

```

*****
*PC GAMESS version 7.1.C (Firefly), build number 5014*
* Compiled on Tuesday, 14-10-2008, 18:38:22 *
*Code development and Intel/AMD specific optimization*
* Copyright (c) 1994, 2008 by Alex A. Granovsky, *
* Laboratory of Chemical Cybernetics, *
* Moscow State University, Moscow, Russia. *
* Some parts of this program include code due to *
* work of Jim Kress, Peter Burger, and Robert Ponec. *
*****
* PC GAMESS homepage: *
* http://classic.chem.msu.su/gran/gameess/index.html *
* e-mail: *
* gran@classic.chem.msu.su *
* This program may not be redistributed without *
* the specific, written permission of its developers.*
*****

```

```

*****
* PARTIALLY BASED ON GAMESS (US) VERSION 6 JUN 1999 *
* FROM IOWA STATE UNIVERSITY *
* M.W.SCHMIDT, K.K.BALDRIDGE, J.A.BOATZ, S.T.ELBERT, *
* M.S.GORDON, J.H.JENSEN, S.KOSEKI, N.MATSUNAGA, *
* K.A.NGUYEN, S.J.SU, T.L.WINDUS, *
* TOGETHER WITH M.DUPOUIS, J.A.MONTGOMERY *
* J.COMPUT.CHEM. 14, 1347-1363(1993) *
*****

```

```

Pentium 4 / Linux PC GAMESS version running under Linux.
Running on Intel CPU: Brand ID 0, Family 15, Model 4, Stepping 3
CPU Brand String : Intel(R) Xeon(TM) CPU 3.20GHz
CPU Features : CMOV, MMX, SSE, SSE2, SSE3, HTT, CID, MWAIT, EM64T
Data cache size : L1 16 KB, L2 2048 KB, L3 0 KB
Operating System successfully passed SSE support test.

```

PARALLEL VERSION (OpenMPI) RUNNING WITH 48 NODES

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

EXECUTION OF PC GAMESS BEGUN 4:35:06 LT 1-SEP-2009

ECHO OF THE FIRST FEW INPUT CARDS -

```

INPUT CARD>! Minimize (Energy/Geometry) B3LYP/SBKJC
INPUT CARD>! $CONTRL EXETYP=check $END
INPUT CARD> $CONTRL RUNTYP=OPTIMIZE NZVAR=0 ICHARG=2 MULT=4
NPRINT=-5
INPUT CARD> SCFTYP=UHF MAXIT=1000 ECP=SBKJC DFTTYP=B3LYP D5=.t.
$END
INPUT CARD> $ZMAT DLC=.true. auto=.true. $END
INPUT CARD> $SCF NCONV=5 DAMP=.T. DIRSCF=.T. SHIFT=.T. SOSCF=.t.
$END
INPUT CARD> $BASIS GBASIS=SBKJC $END
INPUT CARD> $STATPT NSTEP=500 OPTTOL=1d-4 METHOD=GDIIS
HESS=GUESS $END
INPUT CARD> $GUESS GUESS=HUCKEL $END
INPUT CARD> $SYSTEM MWORDS=50 $END
INPUT CARD> $P2P p2p=.t. dlb=.t. $END
INPUT CARD> $DATA
INPUT CARD>Co.inp
INPUT CARD>C1
INPUT CARD>Co 27.0 0.011799 -1.493400 0.831300
INPUT CARD>C 6.0 4.762299 0.657000 0.443300
INPUT CARD>C 6.0 4.993800 -0.687799 0.189999
INPUT CARD>C 6.0 3.885400 -1.514099 0.072099
INPUT CARD>C 6.0 2.581199 -1.030099 0.221199
INPUT CARD>C 6.0 2.297199 0.340900 0.485799
INPUT CARD>C 6.0 3.457800 1.150800 0.579600
INPUT CARD>C 6.0 3.380100 2.470800 0.811600
INPUT CARD>C 6.0 2.188299 3.047700 0.963399
INPUT CARD>C 6.0 1.085600 2.295600 0.884499
INPUT CARD>C 6.0 1.084600 0.963299 0.646100
INPUT CARD>N 7.0 -0.036800 0.352400 0.606500
INPUT CARD>C 6.0 -1.230999 0.778499 0.550000
INPUT CARD>C 6.0 -2.398000 0.084999 0.540700
INPUT CARD>C 6.0 -2.592099 -1.320799 0.533800
INPUT CARD>C 6.0 -3.905499 -1.813100 0.536200
INPUT CARD>C 6.0 -5.033700 -0.998300 0.543400
INPUT CARD>C 6.0 -4.851600 0.379099 0.526400
INPUT CARD>C 6.0 -3.555100 0.891200 0.521300
INPUT CARD>O 8.0 -1.634300 -2.296299 0.502700
INPUT CARD>N 7.0 1.615300 -2.074799 0.017700
INPUT CARD>H 1.0 5.644799 1.315200 0.525699
INPUT CARD>H 1.0 6.017500 -1.082400 0.073900
INPUT CARD>H 1.0 4.054699 -2.582399 -0.147200
INPUT CARD>H 1.0 4.278600 3.108599 0.890300
INPUT CARD>H 1.0 2.123499 4.131900 1.167900
INPUT CARD>H 1.0 0.173899 2.884400 1.064999
INPUT CARD>H 1.0 -1.348500 1.866100 0.459799

```

```

INPUT CARD>H 1.0 -4.061099 -2.905399 0.525799
INPUT CARD>H 1.0 -6.047499 -1.432999 0.546600
INPUT CARD>H 1.0 -5.724599 1.054300 0.519199
INPUT CARD>H 1.0 -3.488699 1.993200 0.513999
INPUT CARD>H 1.0 -1.802699 -2.827499 1.261800
INPUT CARD>H 1.0 1.467899 -2.224700 -1.001900
INPUT CARD>H 1.0 1.942899 -2.960800 0.454399
INPUT CARD> $END
50000000 WORDS OF MEMORY AVAILABLE

```

Loading P2P interface library... loaded successfully (version 1.A).
 Initializing P2P interface... topology done.

BASIS OPTIONS

```

GBASIS=SBKJC   IGAUSS= 0   POLAR=NONE
NDFUNC= 0   NFFUNC= 0   DIFFSP= F
NPFUNC= 0   DIFFS= F

```

RUN TITLE

Co.inp

THE POINT GROUP OF THE MOLECULE IS C1
 THE ORDER OF THE PRINCIPAL AXIS IS 0

ATOM	ATOMIC		COORDINATES (BOHR)		
	CHARGE	X	Y	Z	
CO	27.0	0.0222968769	-2.8221167901	1.5709292136	
C	6.0	8.9994401816	1.2415499739	0.8377155304	
C	6.0	9.4369136375	-1.2997516446	0.3590460479	
C	6.0	7.3423413527	-2.8612322283	0.1362473540	
C	6.0	4.8777588298	-1.9466048502	0.4180054988	
C	6.0	4.3410766493	0.6442075892	0.9180269951	
C	6.0	6.5342945203	2.1746966667	1.0952851825	
C	6.0	6.3874628111	4.6691349705	1.5337016116	
C	6.0	4.1352854892	5.7593178928	1.8205601268	
C	6.0	2.0514865323	4.3380549774	1.6714607464	
C	6.0	2.0495968063	1.8203711542	1.2209519607	
N	7.0	-0.0695419163	0.6659394381	1.1461188116	
C	6.0	-2.3262508012	1.4711497917	1.0393492932	
C	6.0	-4.5315629186	0.1606248192	1.0217748416	
C	6.0	-4.8983568430	-2.4959481949	1.0087357322	
C	6.0	-7.3803229553	-3.4262621883	1.0132710746	

C	6.0	-9.5123137044	-1.8865134535	1.0268771017
C	6.0	-9.1681946020	0.7163932322	0.9947517599
C	6.0	-6.7181648590	1.6841238003	0.9851141574
O	8.0	-3.0883791817	-4.3393758959	0.9499652540
N	7.0	3.0524743880	-3.9208015896	0.0334481500
H	1.0	10.6671233658	2.4853676191	0.9934270620
H	1.0	11.3714261311	-2.0454394091	0.1396507505
H	1.0	7.6622700727	-4.8800265010	-0.2781676654
H	1.0	8.0853816111	5.8744003157	1.6824230469
H	1.0	4.0128312452	7.8081588087	2.2070109811
H	1.0	0.3286214595	5.4507256390	2.0125562872
H	1.0	-2.5482954944	3.5264176657	0.8688941194
H	1.0	-7.6743643190	-5.4904079950	0.9936160346
H	1.0	-11.4281160210	-2.7079754507	1.0329242249
H	1.0	-10.8179234996	1.9923381089	0.9811438431
H	1.0	-6.5926851636	3.7666018387	0.9713172680
H	1.0	-3.4066071483	-5.3431983406	2.3844562513
H	1.0	2.7739268877	-4.2040734049	-1.8933164671
H	1.0	3.6715467318	-5.5951007044	0.8586895991

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.2289592	5.0872973	3.9473535
2 C	5.2289592	0.0000000	1.3878899 *	2.3707410 *
3 C	5.0872973	1.3878899 *	0.0000000	1.3875239 *
4 C	3.9473535	2.3707410 *	1.3875239 *	0.0000000
5 C	2.6811728 *	2.7663747 *	2.4369625 *	1.3990808 *
6 C	2.9507763 *	2.4856475 *	2.9012715 *	2.4768027 *
7 C	4.3508700	1.4014756 *	2.4272477 *	2.7462858 *
8 C	5.2019921	2.3099761 *	3.6009947	4.0843127
9 C	5.0374787	3.5512569	4.7352863	4.9481893
10 C	3.9385784	4.0494175	4.9655843	4.7971534
11 C	2.6871120 *	3.6960001	4.2680203	3.7830489
12 N	1.8600738 *	4.8115244	5.1538746	4.3764204
13 C	2.6048420 *	5.9954789	6.4052910	5.6268938
14 C	2.8953278 *	7.1837702	7.4403572	6.5006013
15 C	2.6265152 *	7.6162359	7.6200231	6.4968089
16 C	3.9413850	9.0133649	8.9768413	7.8104352
17 C	5.0779002	9.9353729	10.0385287	8.9464249
18 C	5.2203320	9.6182737	9.9087506	8.9512992
19 C	4.3017654	8.3210612	8.6998097	7.8325146
20 O	1.8607167 *	7.0457066	6.8276470	5.5914526
21 N	1.8897580 *	4.1889693	3.6561890	2.3389523 *

22 H	6.3017708	1.1040032 *	2.1327211 *	3.3624650
23 H	6.0672086	2.1765795 *	1.1032455 *	2.1753661 *
24 H	4.2998164	3.3679510	2.1412900 *	1.1036390 *
25 H	6.2759435	2.5385254 *	3.9261394	4.7109867
26 H	6.0180210	4.4230352	5.6942442	6.0151791
27 H	4.3870291	5.1382132	6.0628109	5.8401955
28 H	3.6434416	6.2292904	6.8425113	6.2425769
29 H	4.3215241	9.5157682	9.3285426	8.0801241
30 H	6.0662834	11.0104723	11.0721620	9.9445569
31 H	6.2844605	10.4946957	10.8640397	9.9573416
32 H	4.9508126	8.3587916	8.9019953	8.1776377
33 H	2.2929355 *	7.4773574	7.2055168	5.9577578
34 H	2.4526820 *	4.6093242	4.0267438	2.7391128 *
35 H	2.4544784 *	4.5866781	3.8137171	2.4520210 *

C C C C

1 CO	2.6811728 *	2.9507763 *	4.3508700	5.2019921
2 C	2.7663747 *	2.4856475 *	1.4014756 *	2.3099761 *
3 C	2.4369625 *	2.9012715 *	2.4272477 *	3.6009947
4 C	1.3990808 *	2.4768027 *	2.7462858 *	4.0843127
5 C	0.0000000	1.4248886 *	2.3776461 *	3.6391084
6 C	1.4248886 *	0.0000000	1.4183551 *	2.4114923 *
7 C	2.3776461 *	1.4183551 *	0.0000000	1.3424833 *
8 C	3.6391084	2.4114923 *	1.3424833 *	0.0000000
9 C	4.1633731	2.7507685 *	2.3145548 *	1.3327589 *
10 C	3.7063536	2.3340493 *	2.6515775 *	2.3023335 *
11 C	2.5286330 *	1.3723969 *	2.3815241 *	2.7512306 *
12 N	2.9855785 *	2.3371462 *	3.5847448	4.0255298
13 C	4.2322559	3.5558116	4.7036497	4.9187957
14 C	5.1125284	4.7024880	5.9521289	6.2571457
15 C	5.1908803	5.1641827	6.5354554	7.0795873
16 C	6.5413735	6.5662561	7.9375537	8.4562165
17 C	7.6217788	7.4524395	8.7593101	9.1048677
18 C	7.5713597	7.1490163	8.3453269	8.4980843
19 C	6.4370502	5.8782220	7.0179454	7.1187365
20 O	4.4105484	4.7341091	6.1496250	6.9256667
21 N	1.4372790 *	2.5533712 *	3.7569970	4.9403711
22 H	3.8702445	3.4867289	2.1938316 *	2.5585176 *
23 H	3.4398542	4.0045079	3.4343819	4.4861242
24 H	2.1717632 *	3.4691744	3.8498443	5.1874080
25 H	4.5230175	3.4277877	2.1455125 *	1.1046644 *
26 H	5.2680135	3.8557897	3.3186463	2.1131136 *
27 H	4.6723007	3.3635201	3.7449949	3.2426842
28 H	4.8874771	3.9519656	4.8607125	4.7800715
29 H	6.9086651	7.1391884	8.5433885	9.1845871

30 H	8.6442260	8.5313773	9.8502698	10.2073255
31 H	8.5685357	8.0535271	9.1831047	9.2188673
32 H	6.7874686	6.0172673	6.9976989	6.8918116
33 H	4.8509854	5.2392837	6.6306191	7.4253658
34 H	2.0402156 *	3.0794951	4.2254998	5.3845162
35 H	2.0468062 *	3.3208037	4.3835893	5.6298684

C C C N

1 CO	5.0374787	3.9385784	2.6871120 *	1.8600738 *
2 C	3.5512569	4.0494175	3.6960001	4.8115244
3 C	4.7352863	4.9655843	4.2680203	5.1538746
4 C	4.9481893	4.7971534	3.7830489	4.3764204
5 C	4.1633731	3.7063536	2.5286330 *	2.9855785 *
6 C	2.7507685 *	2.3340493 *	1.3723969 *	2.3371462 *
7 C	2.3145548 *	2.6515775 *	2.3815241 *	3.5847448
8 C	1.3327589 *	2.3023335 *	2.7512306 *	4.0255298
9 C	0.0000000	1.3370956 *	2.3798230 *	3.5132726
10 C	1.3370956 *	0.0000000	1.3534626 *	2.2612146 *
11 C	2.3798230 *	1.3534626 *	0.0000000	1.2776164 *
12 N	3.5132726	2.2612146 *	1.2776164 *	0.0000000
13 C	4.1245328	2.7892859 *	2.3249484 *	1.2691981 *
14 C	5.4763501	4.1400995	3.5931912	2.3772039 *
15 C	6.4900342	5.1697970	4.3298765	3.0552305
16 C	7.8066798	6.4740866	5.7115285	4.4340911
17 C	8.2887746	6.9578702	6.4258862	5.1766188
18 C	7.5413909	6.2491243	5.9660781	4.8155402
19 C	6.1508191	4.8621342	4.6419381	3.5603370
20 O	6.5865645	5.3506227	4.2471119	3.0948969
21 N	5.2404838	4.4869043	3.1474702	2.9945642 *
22 H	3.8910834	4.6772018	4.5753410	5.7631658
23 H	5.7019045	6.0325444	5.3708286	6.2447468
24 H	6.0344754	5.8030015	4.6928443	5.0913135
25 H	2.0924652 *	3.2948824	3.8553316	5.1283382
26 H	1.1052191 *	2.1282735 *	3.3751472	4.3893829
27 H	2.0235604 *	1.1002111 *	2.1669060 *	2.5817900 *
28 H	3.7628099	2.5079241 *	2.6018711 *	2.0083241 *
29 H	8.6420979	7.3258151	6.4389063	5.1782960
30 H	9.3850282	8.0559126	7.5245585	6.2705454
31 H	8.1722036	6.9320329	6.8109894	5.7316091
32 H	5.7915660	4.5992312	4.6896919	3.8231385
33 H	7.1088024	5.8932818	4.8047613	3.6958862
34 H	5.6727047	4.9130200	3.6091772	3.3900611
35 H	6.0350124	5.3431909	4.0214400	3.8625946

C C C C

1	CO	2.6048420 *	2.8953278 *	2.6265152 *	3.9413850
2	C	5.9954789	7.1837702	7.6162359	9.0133649
3	C	6.4052910	7.4403572	7.6200231	8.9768413
4	C	5.6268938	6.5006013	6.4968089	7.8104352
5	C	4.2322559	5.1125284	5.1908803	6.5413735
6	C	3.5558116	4.7024880	5.1641827	6.5662561
7	C	4.7036497	5.9521289	6.5354554	7.9375537
8	C	4.9187957	6.2571457	7.0795873	8.4562165
9	C	4.1245328	5.4763501	6.4900342	7.8066798
10	C	2.7892859 *	4.1400995	5.1697970	6.4740866
11	C	2.3249484 *	3.5931912	4.3298765	5.7115285
12	N	1.2691981 *	2.3772039 *	3.0552305	4.4340911
13	C	0.0000000	1.3575419 *	2.5019808 *	3.7241813
14	C	1.3575419 *	0.0000000	1.4191512 *	2.4239128 *
15	C	2.5019808 *	1.4191512 *	0.0000000	1.4026352 *
16	C	3.7241813	2.4239128 *	1.4026352 *	0.0000000
17	C	4.1973317	2.8496418 *	2.4628263 *	1.3916854 *
18	C	3.6426404	2.4712046 *	2.8275524 *	2.3876640 *
19	C	2.3270090 *	1.4103960 *	2.4125644 *	2.7269470 *
20	O	3.1014951	2.5010521 *	1.3674598 *	2.3222723 *
21	N	4.0652270	4.5874648	4.3054711	5.5512656
22	H	6.8967555	8.1363527	8.6484129	10.0496051
23	H	7.4986902	8.5088990	8.6251688	9.9606000
24	H	6.3024064	7.0160917	6.7996558	8.0264319
25	H	5.9917319	7.3376675	8.1824913	9.5565676
26	H	4.7832787	6.1003886	7.2367723	8.4906352
27	H	2.5833663 *	3.8374731	5.0612860	6.2440069
28	H	1.0976423 *	2.0688925 *	3.4217451	4.4811375
29	H	4.6455523	3.4217832	2.1607828 *	1.1033751 *
30	H	5.2999441	3.9526188	3.4572448	2.1754882 *
31	H	4.5021612	3.4650062	3.9311404	3.3957910
32	H	2.5639820 *	2.1980829 *	3.4332016	3.8291167
33	H	3.7197744	3.0589235	1.8502111 *	2.4448453 *
34	H	4.3256963	4.7601995	4.4338466	5.6043351
35	H	4.9056218	5.3035595	4.8230814	5.9605089

C C C O

1	CO	5.0779002	5.2203320	4.3017654	1.8607167 *
2	C	9.9353729	9.6182737	8.3210612	7.0457066
3	C	10.0385287	9.9087506	8.6998097	6.8276470
4	C	8.9464249	8.9512992	7.8325146	5.5914526
5	C	7.6217788	7.5713597	6.4370502	4.4105484
6	C	7.4524395	7.1490163	5.8782220	4.7341091
7	C	8.7593101	8.3453269	7.0179454	6.1496250

8 C	9.1048677	8.4980843	7.1187365	6.9256667
9 C	8.2887746	7.5413909	6.1508191	6.5865645
10 C	6.9578702	6.2491243	4.8621342	5.3506227
11 C	6.4258862	5.9660781	4.6419381	4.2471119
12 N	5.1766188	4.8155402	3.5603370	3.0948969
13 C	4.1973317	3.6426404	2.3270090 *	3.1014951
14 C	2.8496418 *	2.4712046 *	1.4103960 *	2.5010521 *
15 C	2.4628263 *	2.8275524 *	2.4125644 *	1.3674598 *
16 C	1.3916854 *	2.3876640 *	2.7269470 *	2.3222723 *
17 C	0.0000000	1.3894882 *	2.3993659 *	3.6390079
18 C	1.3894882 *	0.0000000	1.3939820 *	4.1844158
19 C	2.3993659 *	1.3939820 *	0.0000000	3.7215546
20 O	3.6390079	4.1844158	3.7215546	0.0000000
21 N	6.7560648	6.9355019	5.9819561	3.2930514
22 H	10.9262499	10.5380585	9.2096654	8.1258068
23 H	11.0614883	10.9762503	9.7841675	7.7593468
24 H	9.2512320	9.4099080	8.3917712	5.7331434
25 H	10.1836089	9.5364116	8.1498390	8.0203206
26 H	8.8280490	7.9465114	6.5701381	7.4756462
27 H	6.5166335	5.6411224	4.2630844	5.5159229
28 H	4.6682412	3.8062209	2.4131506 *	4.1724199
29 H	2.1408618 *	3.3782864	3.8301722	2.5021770 *
30 H	1.1030693 *	2.1712397 *	3.4080191	4.4970590
31 H	2.1658933 *	1.1036646 *	2.1756222 *	5.2874693
32 H	3.3670409	2.1125754 *	1.1040228 *	4.6731922
33 H	3.7817238	4.4854076	4.1770769	0.9416817 *
34 H	6.7943211	7.0036803	6.1040552	3.4485629
35 H	7.2479143	7.5713490	6.7134472	3.6387151

N H H H

1 CO	1.8897580 *	6.3017708	6.0672086	4.2998164
2 C	4.1889693	1.1040032 *	2.1765795 *	3.3679510
3 C	3.6561890	2.1327211 *	1.1032455 *	2.1412900 *
4 C	2.3389523 *	3.3624650	2.1753661 *	1.1036390 *
5 C	1.4372790 *	3.8702445	3.4398542	2.1717632 *
6 C	2.5533712 *	3.4867289	4.0045079	3.4691744
7 C	3.7569970	2.1938316 *	3.4343819	3.8498443
8 C	4.9403711	2.5585176 *	4.4861242	5.1874080
9 C	5.2404838	3.8910834	5.7019045	6.0344754
10 C	4.4869043	4.6772018	6.0325444	5.8030015
11 C	3.1474702	4.5753410	5.3708286	4.6928443
12 N	2.9945642 *	5.7631658	6.2447468	5.0913135
13 C	4.0652270	6.8967555	7.4986902	6.3024064
14 C	4.5874648	8.1363527	8.5088990	7.0160917
15 C	4.3054711	8.6484129	8.6251688	6.7996558

16 C	5.5512656	10.0496051	9.9606000	8.0264319
17 C	6.7560648	10.9262499	11.0614883	9.2512320
18 C	6.9355019	10.5380585	10.9762503	9.4099080
19 C	5.9819561	9.2096654	9.7841675	8.3917712
20 O	3.2930514	8.1258068	7.7593468	5.7331434
21 N	0.0000000	5.2902758	4.5130233	2.4971018 *
22 H	5.2902758	0.0000000	2.4680993 *	4.2629202
23 H	4.5130233	2.4680993 *	0.0000000	2.4802157 *
24 H	2.4971018 *	4.2629202	2.4802157 *	0.0000000
25 H	5.8925557	2.2837937 *	4.6102879	5.7891274
26 H	6.3327986	4.5547530	6.5991669	7.1092076
27 H	5.2695471	5.7169905	7.1320020	6.8129235
28 H	4.9507825	7.0152737	7.9435840	7.0251086
29 H	5.7593026	10.5838515	10.2521069	8.1500573
30 H	7.7077968	12.0109478	12.0793446	10.1910197
31 H	7.9948033	11.3723930	11.9432268	10.4548714
32 H	6.5456653	9.1586356	10.0010410	8.8473806
33 H	3.7144393	8.5538895	8.1001228	6.0294665
34 H	1.0410483 *	5.6842717	4.8125943	2.7477254 *
35 H	1.0406848 *	5.6562641	4.5028368	2.2281849 *

H H H H

1 CO	6.2759435	6.0180210	4.3870291	3.6434416
2 C	2.5385254 *	4.4230352	5.1382132	6.2292904
3 C	3.9261394	5.6942442	6.0628109	6.8425113
4 C	4.7109867	6.0151791	5.8401955	6.2425769
5 C	4.5230175	5.2680135	4.6723007	4.8874771
6 C	3.4277877	3.8557897	3.3635201	3.9519656
7 C	2.1455125 *	3.3186463	3.7449949	4.8607125
8 C	1.1046644 *	2.1131136 *	3.2426842	4.7800715
9 C	2.0924652 *	1.1052191 *	2.0235604 *	3.7628099
10 C	3.2948824	2.1282735 *	1.1002111 *	2.5079241 *
11 C	3.8553316	3.3751472	2.1669060 *	2.6018711 *
12 N	5.1283382	4.3893829	2.5817900 *	2.0083241 *
13 C	5.9917319	4.7832787	2.5833663 *	1.0976423 *
14 C	7.3376675	6.1003886	3.8374731	2.0688925 *
15 C	8.1824913	7.2367723	5.0612860	3.4217451
16 C	9.5565676	8.4906352	6.2440069	4.4811375
17 C	10.1836089	8.8280490	6.5166335	4.6682412
18 C	9.5364116	7.9465114	5.6411224	3.8062209
19 C	8.1498390	6.5701381	4.2630844	2.4131506 *
20 O	8.0203206	7.4756462	5.5159229	4.1724199
21 N	5.8925557	6.3327986	5.2695471	4.9507825
22 H	2.2837937 *	4.5547530	5.7169905	7.0152737
23 H	4.6102879	6.5991669	7.1320020	7.9435840

24 H	5.7891274	7.1092076	6.8129235	7.0251086
25 H	0.0000000	2.4018049 *	4.1145298	5.7787013
26 H	2.4018049 *	0.0000000	2.3168481 *	4.2059522
27 H	4.1145298	2.3168481 *	0.0000000	1.9289636 *
28 H	5.7787013	4.2059522	1.9289636 *	0.0000000
29 H	10.2884213	9.3906934	7.1935886	5.4890575
30 H	11.2859454	9.9055198	7.5904193	5.7421407
31 H	10.2187010	8.4548848	6.1999550	4.4511560
32 H	7.8559946	6.0413898	3.8095226	2.1446547 *
33 H	8.5063194	7.9910627	6.0474342	4.7832389
34 H	6.3185868	6.7486448	5.6612199	5.1771915
35 H	6.5179071	7.1307849	6.1374715	5.8422855

H H H H

1 CO	4.3215241	6.0662834	6.2844605	4.9508126
2 C	9.5157682	11.0104723	10.4946957	8.3587916
3 C	9.3285426	11.0721620	10.8640397	8.9019953
4 C	8.0801241	9.9445569	9.9573416	8.1776377
5 C	6.9086651	8.6442260	8.5685357	6.7874686
6 C	7.1391884	8.5313773	8.0535271	6.0172673
7 C	8.5433885	9.8502698	9.1831047	6.9976989
8 C	9.1845871	10.2073255	9.2188673	6.8918116
9 C	8.6420979	9.3850282	8.1722036	5.7915660
10 C	7.3258151	8.0559126	6.9320329	4.5992312
11 C	6.4389063	7.5245585	6.8109894	4.6896919
12 N	5.1782960	6.2705454	5.7316091	3.8231385
13 C	4.6455523	5.2999441	4.5021612	2.5639820 *
14 C	3.4217832	3.9526188	3.4650062	2.1980829 *
15 C	2.1607828 *	3.4572448	3.9311404	3.4332016
16 C	1.1033751 *	2.1754882 *	3.3957910	3.8291167
17 C	2.1408618 *	1.1030693 *	2.1658933 *	3.3670409
18 C	3.3782864	2.1712397 *	1.1036646 *	2.1125754 *
19 C	3.8301722	3.4080191	2.1756222 *	1.1040228 *
20 O	2.5021770 *	4.4970590	5.2874693	4.6731922
21 N	5.7593026	7.7077968	7.9948033	6.5456653
22 H	10.5838515	12.0109478	11.3723930	9.1586356
23 H	10.2521069	12.0793446	11.9432268	10.0010410
24 H	8.1500573	10.1910197	10.4548714	8.8473806
25 H	10.2884213	11.2859454	10.2187010	7.8559946
26 H	9.3906934	9.9055198	8.4548848	6.0413898
27 H	7.1935886	7.5904193	6.1999550	3.8095226
28 H	5.4890575	5.7421407	4.4511560	2.1446547 *
29 H	0.0000000	2.4726867 *	4.2949379	4.9319421
30 H	2.4726867 *	0.0000000	2.5083205 *	4.2763723
31 H	4.2949379	2.5083205 *	0.0000000	2.4250380 *

32 H	4.9319421	4.2763723	2.4250380 *	0.0000000
33 H	2.3765808 *	4.5248722	5.5678649	5.1614863
34 H	5.7764205	7.7140035	8.0496963	6.6825515
35 H	6.0046781	8.1356707	8.6553886	7.3517294

H H H

1 CO	2.2929355 *	2.4526820 *	2.4544784 *
2 C	7.4773574	4.6093242	4.5866781
3 C	7.2055168	4.0267438	3.8137171
4 C	5.9577578	2.7391128 *	2.4520210 *
5 C	4.8509854	2.0402156 *	2.0468062 *
6 C	5.2392837	3.0794951	3.3208037
7 C	6.6306191	4.2254998	4.3835893
8 C	7.4253658	5.3845162	5.6298684
9 C	7.1088024	5.6727047	6.0350124
10 C	5.8932818	4.9130200	5.3431909
11 C	4.8047613	3.6091772	4.0214400
12 N	3.6958862	3.3900611	3.8625946
13 C	3.7197744	4.3256963	4.9056218
14 C	3.0589235	4.7601995	5.3035595
15 C	1.8502111 *	4.4338466	4.8230814
16 C	2.4448453 *	5.6043351	5.9605089
17 C	3.7817238	6.7943211	7.2479143
18 C	4.4854076	7.0036803	7.5713490
19 C	4.1770769	6.1040552	6.7134472
20 O	0.9416817 *	3.4485629	3.6387151
21 N	3.7144393	1.0410483 *	1.0406848 *
22 H	8.5538895	5.6842717	5.6562641
23 H	8.1001228	4.8125943	4.5028368
24 H	6.0294665	2.7477254 *	2.2281849 *
25 H	8.5063194	6.3185868	6.5179071
26 H	7.9910627	6.7486448	7.1307849
27 H	6.0474342	5.6612199	6.1374715
28 H	4.7832389	5.1771915	5.8422855
29 H	2.3765808 *	5.7764205	6.0046781
30 H	4.5248722	7.7140035	8.1356707
31 H	5.5678649	8.0496963	8.6553886
32 H	5.1614863	6.6825515	7.3517294
33 H	0.0000000	4.0229983	3.8339496
34 H	4.0229983	0.0000000	1.6994926 *
35 H	3.8339496	1.6994926 *	0.0000000

* ... LESS THAN 3.000

ATOMIC BASIS SET

 THE CONTRACTED PRIMITIVE FUNCTIONS HAVE BEEN UNNORMALIZED
 THE CONTRACTED BASIS FUNCTIONS ARE NOW NORMALIZED TO UNITY

SHELL TYPE PRIM EXPONENT CONTRACTION COEFFICIENTS

CO

1	L	1	75.680000	-0.096392 (-0.005271)	-2.572448 (-0.008085)
1	L	2	6.496000	-2.046006 (-0.705525)	-5.779778 (-0.390988)
1	L	3	4.791000	0.802896 (0.347880)	6.871185 (0.680078)
1	L	4	1.594000	1.188595 (1.175595)	1.862653 (0.729594)
2	D	5	51.690000	41.735693 (0.025447)	
2	D	6	14.700000	27.160663 (0.149529)	
2	D	7	4.851000	11.093293 (0.425056)	
2	D	8	1.643000	2.376098 (0.605465)	
3	D	9	0.507500	0.502253 (1.000000)	
4	L	10	2.337000	-0.120253 (-0.089267)	-0.065632 (-0.015935)
4	L	11	0.126900	0.154956 (1.022589)	0.108171 (1.001945)
5	L	12	0.042320	0.066500 (1.000000)	0.027360 (1.000000)
6	L	13	0.557200	0.459641 (1.000000)	0.686205 (1.000000)
7	D	14	0.143300	0.054934 (1.000000)	

C

8	L	15	4.286000	-0.427825 (-0.147220)	1.135964 (0.102570)
8	L	16	1.046000	0.081985 (0.081250)	0.626666 (0.329870)
8	L	17	0.344700	0.313181 (0.713600)	0.228684 (0.482120)
9	L	18	0.112800	0.138721 (0.315210)	0.093181 (0.315930)

C

10	L	19	4.286000	-0.427825 (-0.147220)	1.135964 (0.102570)
10	L	20	1.046000	0.081985 (0.081250)	0.626666 (0.329870)
10	L	21	0.344700	0.313181 (0.713600)	0.228684 (0.482120)
11	L	22	0.112800	0.138721 (0.315210)	0.093181 (0.315930)

C

12	L	23	4.286000	-0.427825 (-0.147220)	1.135964 (0.102570)
12	L	24	1.046000	0.081985 (0.081250)	0.626666 (0.329870)
12	L	25	0.344700	0.313181 (0.713600)	0.228684 (0.482120)
13	L	26	0.112800	0.138721 (0.315210)	0.093181 (0.315930)

C

14	L	27	4.286000	-0.427825 (-0.147220)	1.135964 (0.102570)
14	L	28	1.046000	0.081985 (0.081250)	0.626666 (0.329870)
14	L	29	0.344700	0.313181 (0.713600)	0.228684 (0.482120)
15	L	30	0.112800	0.138721 (0.315210)	0.093181 (0.315930)

C

16	L	31	4.286000	-0.427825 (-0.147220)	1.135964 (0.102570)
16	L	32	1.046000	0.081985 (0.081250)	0.626666 (0.329870)
16	L	33	0.344700	0.313181 (0.713600)	0.228684 (0.482120)
17	L	34	0.112800	0.138721 (0.315210)	0.093181 (0.315930)

C

18	L	35	4.286000	-0.427825 (-0.147220)	1.135964 (0.102570)
18	L	36	1.046000	0.081985 (0.081250)	0.626666 (0.329870)
18	L	37	0.344700	0.313181 (0.713600)	0.228684 (0.482120)
19	L	38	0.112800	0.138721 (0.315210)	0.093181 (0.315930)

C

20	L	39	4.286000	-0.427825 (-0.147220)	1.135964 (0.102570)
20	L	40	1.046000	0.081985 (0.081250)	0.626666 (0.329870)
20	L	41	0.344700	0.313181 (0.713600)	0.228684 (0.482120)
21	L	42	0.112800	0.138721 (0.315210)	0.093181 (0.315930)

C

22	L	43	4.286000	-0.427825 (-0.147220)	1.135964 (0.102570)
22	L	44	1.046000	0.081985 (0.081250)	0.626666 (0.329870)
22	L	45	0.344700	0.313181 (0.713600)	0.228684 (0.482120)

23 L 46 0.112800 0.138721 (0.315210) 0.093181 (0.315930)

C

24 L 47 4.286000 -0.427825 (-0.147220) 1.135964 (0.102570)

24 L 48 1.046000 0.081985 (0.081250) 0.626666 (0.329870)

24 L 49 0.344700 0.313181 (0.713600) 0.228684 (0.482120)

25 L 50 0.112800 0.138721 (0.315210) 0.093181 (0.315930)

C

26 L 51 4.286000 -0.427825 (-0.147220) 1.135964 (0.102570)

26 L 52 1.046000 0.081985 (0.081250) 0.626666 (0.329870)

26 L 53 0.344700 0.313181 (0.713600) 0.228684 (0.482120)

27 L 54 0.112800 0.138721 (0.315210) 0.093181 (0.315930)

N

28 L 55 6.403000 -0.559246 (-0.139550) 1.878681 (0.103360)

28 L 56 1.580000 0.077056 (0.054920) 1.049654 (0.332050)

28 L 57 0.509400 0.430294 (0.716780) 0.374063 (0.487080)

29 L 58 0.162300 0.182242 (0.332100) 0.146838 (0.313120)

C

30 L 59 4.286000 -0.427825 (-0.147220) 1.135964 (0.102570)

30 L 60 1.046000 0.081985 (0.081250) 0.626666 (0.329870)

30 L 61 0.344700 0.313181 (0.713600) 0.228684 (0.482120)

31 L 62 0.112800 0.138721 (0.315210) 0.093181 (0.315930)

C

32 L 63 4.286000 -0.427825 (-0.147220) 1.135964 (0.102570)

32 L 64 1.046000 0.081985 (0.081250) 0.626666 (0.329870)

32 L 65 0.344700 0.313181 (0.713600) 0.228684 (0.482120)

33 L 66 0.112800 0.138721 (0.315210) 0.093181 (0.315930)

C

34 L 67 4.286000 -0.427825 (-0.147220) 1.135964 (0.102570)

34 L 68 1.046000 0.081985 (0.081250) 0.626666 (0.329870)

34 L 69 0.344700 0.313181 (0.713600) 0.228684 (0.482120)

35 L 70 0.112800 0.138721 (0.315210) 0.093181 (0.315930)

C

36 L 71 4.286000 -0.427825 (-0.147220) 1.135964 (0.102570)

36 L 72 1.046000 0.081985 (0.081250) 0.626666 (0.329870)

36 L 73 0.344700 0.313181 (0.713600) 0.228684 (0.482120)

37 L 74 0.112800 0.138721 (0.315210) 0.093181 (0.315930)

C

38 L 75 4.286000 -0.427825 (-0.147220) 1.135964 (0.102570)

38 L 76 1.046000 0.081985 (0.081250) 0.626666 (0.329870)

38 L 77 0.344700 0.313181 (0.713600) 0.228684 (0.482120)

39 L 78 0.112800 0.138721 (0.315210) 0.093181 (0.315930)

C

40 L 79 4.286000 -0.427825 (-0.147220) 1.135964 (0.102570)

40 L 80 1.046000 0.081985 (0.081250) 0.626666 (0.329870)

40 L 81 0.344700 0.313181 (0.713600) 0.228684 (0.482120)

41 L 82 0.112800 0.138721 (0.315210) 0.093181 (0.315930)

C

42 L 83 4.286000 -0.427825 (-0.147220) 1.135964 (0.102570)

42 L 84 1.046000 0.081985 (0.081250) 0.626666 (0.329870)

42 L 85 0.344700 0.313181 (0.713600) 0.228684 (0.482120)

43 L 86 0.112800 0.138721 (0.315210) 0.093181 (0.315930)

O

44 L 87 8.519000 -0.678492 (-0.145510) 2.823932 (0.110070)

44 L 88 2.073000 0.133861 (0.082860) 1.533317 (0.349690)

44 L 89 0.647100 0.501446 (0.743250) 0.492035 (0.480930)

45 L 90 0.200000 0.213149 (0.284720) 0.190646 (0.307270)

N

46	L	91	6.403000	-0.559246 (-0.139550)	1.878681 (0.103360)
46	L	92	1.580000	0.077056 (0.054920)	1.049654 (0.332050)
46	L	93	0.509400	0.430294 (0.716780)	0.374063 (0.487080)

47	L	94	0.162300	0.182242 (0.332100)	0.146838 (0.313120)
----	---	----	----------	----------------------	----------------------

H

48	S	95	13.007734	0.163507 (0.033495)	
48	S	96	1.962079	0.277339 (0.234727)	
48	S	97	0.444529	0.315740 (0.813757)	

49	S	98	0.121949	0.147077 (1.000000)	
----	---	----	----------	----------------------	--

H

50	S	99	13.007734	0.163507 (0.033495)	
50	S	100	1.962079	0.277339 (0.234727)	
50	S	101	0.444529	0.315740 (0.813757)	

51	S	102	0.121949	0.147077 (1.000000)	
----	---	-----	----------	----------------------	--

H

52	S	103	13.007734	0.163507 (0.033495)	
52	S	104	1.962079	0.277339 (0.234727)	
52	S	105	0.444529	0.315740 (0.813757)	

53	S	106	0.121949	0.147077 (1.000000)	
----	---	-----	----------	----------------------	--

H

54	S	107	13.007734	0.163507 (0.033495)	
54	S	108	1.962079	0.277339 (0.234727)	
54	S	109	0.444529	0.315740 (0.813757)	

55	S	110	0.121949	0.147077 (1.000000)	
----	---	-----	----------	----------------------	--

H

56	S	111	13.007734	0.163507 (0.033495)	
56	S	112	1.962079	0.277339 (0.234727)	
56	S	113	0.444529	0.315740 (0.813757)	

57	S	114	0.121949	0.147077 (1.000000)	
----	---	-----	----------	----------------------	--

H

58	S	115	13.007734	0.163507 (0.033495)
58	S	116	1.962079	0.277339 (0.234727)
58	S	117	0.444529	0.315740 (0.813757)
59	S	118	0.121949	0.147077 (1.000000)

H

60	S	119	13.007734	0.163507 (0.033495)
60	S	120	1.962079	0.277339 (0.234727)
60	S	121	0.444529	0.315740 (0.813757)
61	S	122	0.121949	0.147077 (1.000000)

H

62	S	123	13.007734	0.163507 (0.033495)
62	S	124	1.962079	0.277339 (0.234727)
62	S	125	0.444529	0.315740 (0.813757)
63	S	126	0.121949	0.147077 (1.000000)

H

64	S	127	13.007734	0.163507 (0.033495)
64	S	128	1.962079	0.277339 (0.234727)
64	S	129	0.444529	0.315740 (0.813757)
65	S	130	0.121949	0.147077 (1.000000)

H

66	S	131	13.007734	0.163507 (0.033495)
66	S	132	1.962079	0.277339 (0.234727)
66	S	133	0.444529	0.315740 (0.813757)
67	S	134	0.121949	0.147077 (1.000000)

H

68	S	135	13.007734	0.163507 (0.033495)
68	S	136	1.962079	0.277339 (0.234727)
68	S	137	0.444529	0.315740 (0.813757)

69 S 138 0.121949 0.147077 (1.000000)

H

70 S 139 13.007734 0.163507 (0.033495)

70 S 140 1.962079 0.277339 (0.234727)

70 S 141 0.444529 0.315740 (0.813757)

71 S 142 0.121949 0.147077 (1.000000)

H

72 S 143 13.007734 0.163507 (0.033495)

72 S 144 1.962079 0.277339 (0.234727)

72 S 145 0.444529 0.315740 (0.813757)

73 S 146 0.121949 0.147077 (1.000000)

H

74 S 147 13.007734 0.163507 (0.033495)

74 S 148 1.962079 0.277339 (0.234727)

74 S 149 0.444529 0.315740 (0.813757)

75 S 150 0.121949 0.147077 (1.000000)

TOTAL NUMBER OF SHELLS = 75
TOTAL NUMBER OF BASIS FUNCTIONS = 222
NUMBER OF ELECTRONS = 163
CHARGE OF MOLECULE = 2
STATE MULTIPLICITY = 4
NUMBER OF OCCUPIED ORBITALS (ALPHA) = 83
NUMBER OF OCCUPIED ORBITALS (BETA) = 80
TOTAL NUMBER OF ATOMS = 35
THE NUCLEAR REPULSION ENERGY IS 2011.4580931326
TOTAL NUMBER OF CONTAMINANTS DROPPED= 3

\$CONTRL OPTIONS

SCFTYP=UHF RUNTYP=OPTIMIZE EXETYP=RUN
MPLEVL= 0 LOCAL=NONE UNITS=ANGS
MULT = 4 ICHARG= 2 MAXIT = 1000
NPRINT= -5 IREST = 0 COORD=UNIQUE
ECP =SBKJC NORMF = 0 NORMP = 0
ITOL = 20 ICUT = 9 NZVAR = 0

NOSYM = 0 INTTYP=POPLE GEOM =INPUT
PLTORB= F MOLPLT= F RPAC = F
AIMPAC= F FRIEND= CITYP =NONE
DFTTYP=B3LYP

\$SYSTEM OPTIONS

KDIAG = 0 MEMORY= 50000000 TIMLIM= 36000.0 SEC.
COREFL= F PTIME = F XDR = F
BALTYP=NXTVAL

ECP POTENTIALS

PARAMETERS FOR "SBKJC-27" ON ATOM 1 WITH ZCORE 10 AND LMAX 2
ARE

FOR L= 2	COEFF	N	ZETA
1	-3.94746	1	19.44559

FOR L= 0	COEFF	N	ZETA
1	3.07705	0	2.25935
2	215.48382	2	6.66665
3	-174.11816	2	5.76818

FOR L= 1	COEFF	N	ZETA
1	3.95321	0	50.28146
2	90.90043	2	12.52610

PARAMETERS FOR "SBKJC- 6" ON ATOM 2 WITH ZCORE 2 AND LMAX 1
ARE

FOR L= 1	COEFF	N	ZETA
1	-0.89371	1	8.56468

FOR L= 0	COEFF	N	ZETA
1	1.92926	0	2.81497
2	14.88199	2	8.11296

PARAMETERS FOR "SBKJC- 6" ON ATOM 3 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 4 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 5 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 6 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 7 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 8 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 9 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 10 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 11 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 7" ON ATOM 12 WITH ZCORE 2 AND LMAX 1 ARE

FOR L= 1 COEFF N ZETA

1 -0.91212 1 11.99686

FOR L= 0 COEFF N ZETA

1 1.93565 0 3.83895

2 21.73355 2 11.73247

PARAMETERS FOR "SBKJC- 6" ON ATOM 13 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 14 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 15 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 16 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 17 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 18 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 6" ON ATOM 19 ARE THE SAME AS ATOM 2

PARAMETERS FOR "SBKJC- 8" ON ATOM 20 WITH ZCORE 2 AND LMAX 1 ARE

FOR L= 1 COEFF N ZETA

1 -0.92550 1 16.11718

FOR L= 0 COEFF N ZETA

1 1.96069 0 5.05348

2 29.13442 2 15.95333

PARAMETERS FOR "SBKJC- 7" ON ATOM 21 ARE THE SAME AS ATOM 12

THE ECP RUN REMOVES 50 CORE ELECTRONS, AND THE SAME NUMBER OF PROTONS.

THE ADJUSTED NUCLEAR REPULSION ENERGY= 972.3856028573

ECP ANGULAR INTS..... 0.01 SECONDS

PROPERTIES INPUT

```

-----
MOMENTS      FIELD      POTENTIAL      DENSITY
IEMOM =  1  IEFLD =  0  IEPOT =  0  IEDEN =  0
WHERE =ORIGIN  WHERE =NUCLEI  WHERE =NUCLEI  WHERE =NUCLEI
OUTPUT= BOTH  OUTPUT= BOTH  OUTPUT= BOTH  OUTPUT= BOTH
IEMINT=  0  IEFINT=  0           IEDINT=  0
                MORB =  0

```

```

-----
DFT CODE OPTIONS PROGRAM WRITTEN BY ALEX A. GRANOVSKY
-----

```

```

NRAD = 63  LMAX = 29 ( 302 POINTS PER SHELL)
ANGPRN = T  RADPRN = T
KAP = 5.000
CUTOFF = 1.0E-10  CUTAO = 1.0E-10
CUTWGT = 1.0E-20  CUTORB = 1.0E-15
CUTGG1 = 1.0E-13  CUTGG2 = 1.0E-13
CUTGG3 = 1.0E-13  CUTGG4 = 1.0E-30
B3LYP = NWCHEM  O3LYP = DEFAULT

```

```

EXTRAPOLATION IN EFFECT
DAMPING IN EFFECT
LEVEL SHIFTING IN EFFECT
SOSCF IN EFFECT

```

```

-----
INTEGRAL INPUT OPTIONS
-----

```

```

NOPK = 1  NORDER= 0  SCHWRZ= T

```

```

ATTENTION! AO INTEGRALS WILL BE PACKED.
THRESHOLD FOR PACKING PKTHR = 0.10000000D-01

```

```

-----
INTEGRAL TRANSFORMATION OPTIONS
-----

```

```

NWORD = 0  CUTTRF = 1.0E-09
MPTRAN = 0  DIRTRF = F
AOINTS =DUP  IREST = 0

```

```

-----
THE POINT GROUP IS C1 , NAXIS= 0, ORDER= 1

```

DIMENSIONS OF THE SYMMETRY SUBSPACES ARE
A = 222

..... DONE SETTING UP THE RUN

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 0.42 , TOTAL = 1.1 SECONDS (0.0 MIN)
WALL CLOCK TIME: STEP = 0.44 , TOTAL = 0.4 SECONDS (0.0 MIN)
CPU UTILIZATION: STEP = 95.57% , TOTAL = 100.00%

STATIONARY POINT LOCATION RUN

OBTAINING INITIAL HESSIAN, HESS=GUESS
DIAGONAL GUESS HESSIAN IN CARTESIAN COORDS IS H(I,I)= 0.3333

PARAMETERS CONTROLLING GEOMETRY SEARCH ARE
METHOD =GDIIS UPHESS =BFGS
NNEG = 0 NFRZ = 0
NSTEP = 500 IFOLOW = 1
HESS =GUESS RESTAR = F
IHREP = 0 HSEND = F
NPRT = 0 NPUN = 0
OPTTOL = 1.000E-04 RMIN = 1.500E-03
RMAX = 1.000E-01 RLIM = 7.000E-02
DXMAX = 3.000E-01 PURIFY = F
MOVIE = F TRUPD = T
TRMAX = 5.000E-01 TRMIN = 5.000E-02
ITBMAT = 10 STPT = F
STSTEP = 1.000E-02 PROJCT= T
MAXDII = 20 NSKIP = 2
INSERCH= 0

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.0117990000	-1.4934000000	0.8313000000
C	6.0	4.7622990000	0.6570000000	0.4433000000
C	6.0	4.9938000000	-0.6877990000	0.1899990000
C	6.0	3.8854000000	-1.5140990000	0.0720990000
C	6.0	2.5811990000	-1.0300990000	0.2211990000

C	6.0	2.2971990000	0.3409000000	0.4857990000
C	6.0	3.4578000000	1.1508000000	0.5796000000
C	6.0	3.3801000000	2.4708000000	0.8116000000
C	6.0	2.1882990000	3.0477000000	0.9633990000
C	6.0	1.0856000000	2.2956000000	0.8844990000
C	6.0	1.0846000000	0.9632990000	0.6461000000
N	7.0	-0.0368000000	0.3524000000	0.6065000000
C	6.0	-1.2309990000	0.7784990000	0.5500000000
C	6.0	-2.3980000000	0.0849990000	0.5407000000
C	6.0	-2.5920990000	-1.3207990000	0.5338000000
C	6.0	-3.9054990000	-1.8131000000	0.5362000000
C	6.0	-5.0337000000	-0.9983000000	0.5434000000
C	6.0	-4.8516000000	0.3790990000	0.5264000000
C	6.0	-3.5551000000	0.8912000000	0.5213000000
O	8.0	-1.6343000000	-2.2962990000	0.5027000000
N	7.0	1.6153000000	-2.0747990000	0.0177000000
H	1.0	5.6447990000	1.3152000000	0.5256990000
H	1.0	6.0175000000	-1.0824000000	0.0739000000
H	1.0	4.0546990000	-2.5823990000	-0.1472000000
H	1.0	4.2786000000	3.1085990000	0.8903000000
H	1.0	2.1234990000	4.1319000000	1.1679000000
H	1.0	0.1738990000	2.8844000000	1.0649990000
H	1.0	-1.3485000000	1.8661000000	0.4597990000
H	1.0	-4.0610990000	-2.9053990000	0.5257990000
H	1.0	-6.0474990000	-1.4329990000	0.5466000000
H	1.0	-5.7245990000	1.0543000000	0.5191990000
H	1.0	-3.4886990000	1.9932000000	0.5139990000
H	1.0	-1.8026990000	-2.8274990000	1.2618000000
H	1.0	1.4678990000	-2.2247000000	-1.0019000000
H	1.0	1.9428990000	-2.9608000000	0.4543990000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80 , TOTAL = 1.9 SECONDS (0.0 MIN)
WALL CLOCK TIME: STEP = 0.80 , TOTAL = 1.2 SECONDS (0.0 MIN)
CPU UTILIZATION: STEP = 99.65% , TOTAL = 100.00%

GUESS OPTIONS

GUESS =HUCKEL NORB = 0 NORDER= 0
MIX = F PRTMO = F SYMDEN= F
TOLZ = 0.0E+00 TOLE = 0.0E+00

INITIAL GUESS ORBITALS GENERATED BY HUCKEL ROUTINE.
HUCKEL GUESS REQUIRES 380872 WORDS.

SYMMETRIES FOR INITIAL GUESS ORBITALS FOLLOW. ALPHA SET(S).

58 ORBITALS ARE OCCUPIED (4 CORE ORBITALS).

5=A	6=A	7=A	8=A	9=A	10=A	11=A
12=A	13=A	14=A	15=A	16=A	17=A	18=A
19=A	20=A	21=A	22=A	23=A	24=A	25=A
26=A	27=A	28=A	29=A	30=A	31=A	32=A
33=A	34=A	35=A	36=A	37=A	38=A	39=A
40=A	41=A	42=A	43=A	44=A	45=A	46=A
47=A	48=A	49=A	50=A	51=A	52=A	53=A
54=A	55=A	56=A	57=A	58=A	59=A	60=A
61=A	62=A	63=A	64=A	65=A	66=A	67=A
68=A						

SYMMETRIES FOR INITIAL GUESS ORBITALS FOLLOW. BETA SET(S).

55 ORBITALS ARE OCCUPIED (4 CORE ORBITALS).

5=A	6=A	7=A	8=A	9=A	10=A	11=A
12=A	13=A	14=A	15=A	16=A	17=A	18=A
19=A	20=A	21=A	22=A	23=A	24=A	25=A
26=A	27=A	28=A	29=A	30=A	31=A	32=A
33=A	34=A	35=A	36=A	37=A	38=A	39=A
40=A	41=A	42=A	43=A	44=A	45=A	46=A
47=A	48=A	49=A	50=A	51=A	52=A	53=A
54=A	55=A	56=A	57=A	58=A	59=A	60=A
61=A	62=A	63=A	64=A	65=A		

..... END OF INITIAL ORBITAL SELECTION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.57, TOTAL = 3.4 SECONDS (0.1 MIN)
WALL CLOCK TIME: STEP = 1.57, TOTAL = 2.8 SECONDS (0.0 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.00, TOTAL = 3.4 SECONDS (0.1 MIN)
WALL CLOCK TIME: STEP = 0.00, TOTAL = 2.8 SECONDS (0.0 MIN)
CPU UTILIZATION: STEP = 0.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
1	0	-282.236629208	-282.236629208	10.250075485	0.000000000
10357079					211118869

-----START SECOND ORDER SCF-----

SOSCF IS SCALING ROTATION ANGLE MATRIX, SQCDF= 0.206229
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 8.624623
 2 1 -279.358145517 2.878483691 0.406356638 0.327673590 213368284
 10099581
 SOSCF IS SCALING ROTATION ANGLE MATRIX, SQCDF= 0.241348
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 8.494460
 3 2 -280.066559997 -0.708414480 1.140296498 0.633472176 193020319
 12020820
 SOSCF IS SCALING ROTATION ANGLE MATRIX, SQCDF= 0.240822
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 8.395891
 4 3 -280.977199195 -0.910639198 0.739292447 0.592332832 197763848
 11546325
 SOSCF IS SCALING ROTATION ANGLE MATRIX, SQCDF= 0.473650
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 6.783902
 5 4 -281.594656107 -0.617456912 0.756838862 0.506110047 196483389
 11681794
 SOSCF IS SCALING ROTATION ANGLE MATRIX, SQCDF= 2.027676
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 6.872148
 6 5 -282.440972518 -0.846316411 0.672531781 0.340979937 197472382
 11637203
 SOSCF IS SCALING ROTATION ANGLE MATRIX, SQCDF= 0.196163
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 8.446032
 7 6 -283.112394442 -0.671421924 0.346915405 0.257558592 196765879
 11704098
 SOSCF IS SCALING ROTATION ANGLE MATRIX, SQCDF= 0.174401
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 8.386608
 8 7 -283.376990545 -0.264596103 0.298740605 0.246737448 194155769
 11979191
 SOSCF IS SCALING ROTATION ANGLE MATRIX, SQCDF= 0.219050
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 7.591829
 9 8 -283.606712137 -0.229721591 0.312619009 0.230304764 193962013
 12012829
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 5.955304
 10 9 -283.843953858 -0.237241722 0.289467217 0.177814533 194760989
 11928013
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 3.820263
 11 10 -283.996552659 -0.152598801 0.481344966 0.132905294 194479458
 11947076
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 2.050178
 12 11 -284.213835882 -0.217283223 0.308944963 0.087197720 197845042
 11637844
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 1.398749
 13 12 -284.296570930 -0.082735048 0.307864286 0.071766934 196061568
 11780754
 SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX= 1.145760

14 13	-284.367274340	-0.070703410	0.124499754	0.035887479	196678497
11746957	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.390465
15 14	-284.389698886	-0.022424546	0.166448539	0.038466128	193866736
12043028	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.318872
16 15	-284.397895147	-0.008196261	0.089412641	0.033000829	197294228
11727301	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.497344
17 16	-284.403658040	-0.005762893	0.097909344	0.039093994	193937884
12029857	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.298226
18 17	-284.413276600	-0.009618560	0.118836931	0.024955636	192172109
12113353	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.247944
19 18	-284.398478431	0.014798169	0.136064020	0.034026079	195680179
11846445	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.373477
20 19	-284.403602894	-0.005124463	0.096871623	0.044661847	195489524
11893606	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.298226
21 20	-284.404713272	-0.001110377	0.089208985	0.026721719	195007761
11886097	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.247944
22 21	-284.388204911	0.016508361	0.123671716	0.034301144	194200227
12017587	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.448618
23 22	-284.405499694	-0.017294783	0.096373361	0.025412353	196255055
11796217	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.350968
24 23	-284.405313773	0.000185921	0.135138733	0.029158777	193459338
12083716	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.350968
25 24	-284.394353025	0.010960748	0.108883743	0.044308979	195320219
11865340	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.28997388
26 25	-284.407254342	-0.012901317	0.146793393	0.028997388	192587428
12178021	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.18523772
27 26	-284.388730569	0.018523772	0.155860726	0.030566564	196103279
11773777	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.020051014
28 27	-284.408781583	-0.020051014	0.096191474	0.025479741	193965678
12015543	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.011949310
29 28	-284.396832274	0.011949310	0.061068353	0.026653891	195050656
11884742	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				-0.014902810
30 29	-284.411735084	-0.014902810	0.052186835	0.026636182	191978114
12152053	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				0.004942091
31 30	-284.406792993	0.004942091	0.032095119	0.022759157	188041441
12474578	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				-0.003862078
32 31	-284.410655071	-0.003862078	0.035626351	0.023877004	185951159
12656075	SOSCF IS SCALING ROTATION ANGLE MATRIX, DXMAX=				

33 32	-284.407127067	0.003528004	0.031518772	0.026466514	185237532
12726077					
34 33	-284.410139289	-0.003012222	0.010845317	0.022961984	183988056
12830169					
35 34	-284.409508072	0.000631217	0.021770077	0.024572966	173107432
13723126					
36 35	-284.411104380	-0.001596307	0.024081160	0.021647895	179011425
13271727					
37 36	-284.412287065	-0.001182685	0.071261057	0.019815804	179490457
13278576					
38 37	-284.416285860	-0.003998795	0.211281288	0.020400102	186246895
12710871					
39 38	-284.423213348	-0.006927487	0.153625184	0.022231053	194434189
12030212					
40 39	-284.429157436	-0.005944089	0.109436415	0.020628994	193969161
12010330					
41 40	-284.439163406	-0.010005969	0.163761867	0.017375602	190784036
12291306					
42 41	-284.444123506	-0.004960101	0.114030830	0.017715594	189672546
12290275					
43 42	-284.448603019	-0.004479513	0.157448768	0.018796121	190363903
12339917					
44 43	-284.452983949	-0.004380929	0.102017697	0.019028539	192349853
12163673					
45 44	-284.459653542	-0.006669593	0.173761336	0.016549461	188940812
12445094					
46 45	-284.462539559	-0.002886017	0.073676682	0.021786811	192463695
12130275					
47 46	-284.460965691	0.001573867	0.067569843	0.024365762	189821964
12378868					
48 47	-284.466240925	-0.005275233	0.059223289	0.016818943	189204889
12430698					
49 48	-284.468485974	-0.002245050	0.046778925	0.017140505	187127919
12546599					
50 49	-284.469873644	-0.001387670	0.051775961	0.015911820	184396667
12800065					
51 50	-284.470966540	-0.001092895	0.027150238	0.015519481	182861177
12889281					
52 51	-284.472561316	-0.001594776	0.038166367	0.013075362	180291250
13133854					
53 52	-284.474253208	-0.001691892	0.036594633	0.012177736	183114772
12908473					
54 53	-284.475350900	-0.001097692	0.063693741	0.007341690	183627108
12938086					
55 54	-284.476559736	-0.001208836	0.077941814	0.006925098	182626919
12911799					

56 55	-284.477662386	-0.001102650	0.026137850	0.006380787	181106691
13024083					
57 56	-284.478713964	-0.001051578	0.027106168	0.004984335	180555146
13117725					
58 57	-284.479495885	-0.000781922	0.027753174	0.002593384	180672434
13189450					
59 58	-284.480033551	-0.000537665	0.028479755	0.002943533	178187681
13338866					
60 59	-284.480476643	-0.000443093	0.029521081	0.002766895	177051888
13411512					
61 60	-284.480901433	-0.000424790	0.028889950	0.003073155	176240571
13496911					
62 61	-284.481336437	-0.000435004	0.041802144	0.003181222	175235466
13575784					
63 62	-284.481934691	-0.000598254	0.084812396	0.002709499	176204715
13518287					
64 63	-284.482557647	-0.000622957	0.027666780	0.003295424	179681604
13245434					
65 64	-284.482887973	-0.000330326	0.019613809	0.002346392	176480995
13436634					
66 65	-284.483093883	-0.000205909	0.016045620	0.001398347	174012179
13641123					
67 66	-284.483213219	-0.000119336	0.012749191	0.001181518	172238243
13779272					
68 67	-284.483297969	-0.000084750	0.009098369	0.000781179	169732518
13984815					
69 68	-284.483349947	-0.000051979	0.007142209	0.000576806	167265507
14225666					
70 69	-284.483380533	-0.000030585	0.006835153	0.000603755	164662460
14407987					
71 70	-284.483403551	-0.000023018	0.008604936	0.000710805	162983025
14574164					
72 71	-284.483428823	-0.000025272	0.015967816	0.000603865	161913329
14672360					
73 72	-284.483462993	-0.000034170	0.015808761	0.000508044	164476736
14514224					
74 73	-284.483487199	-0.000024206	0.010972416	0.000374594	164717177
14504042					
75 74	-284.483503069	-0.000015870	0.005575360	0.000366172	164234006
14530713					
76 75	-284.483510022	-0.000006953	0.003377511	0.000271259	159832964
14788918					
77 76	-284.483513110	-0.000003088	0.001126093	0.000106498	155849761
15108870					
78 77	-284.483514372	-0.000001262	0.001221789	0.000112569	151147209
15465180					

79 78	-284.483515026	-0.000000654	0.001048505	0.000115953	168788582
14106054					
80 79	-284.483515499	-0.000000473	0.000774459	0.000115445	166014593
14332184					
81 80	-284.483515887	-0.000000388	0.000550273	0.000101121	165719089
14405404					
82 81	-284.483516161	-0.000000275	0.000302679	0.000077210	164147179
14473104					
83 82	-284.483516350	-0.000000189	0.000311249	0.000061612	161719412
14649606					
84 83	-284.483516470	-0.000000120	0.000249674	0.000048321	181934089
12994151					
85 84	-284.483516548	-0.000000078	0.000386154	0.000028940	178361072
13248319					

-----DISABLING FDIFF OPTION-----

86 85	-284.483516614	-0.000000067	0.000401306	0.000017485	212145930
10190916					
87 86	-284.483516641	-0.000000027	0.000225629	0.000012046	212145818
10190936					
88 87	-284.483516653	-0.000000013	0.000140569	0.000011534	212145993
10190925					
89 88	-284.483516659	-0.000000005	0.000121887	0.000008361	212145939
10190928					
90 89	-284.483516662	-0.000000003	0.000058015	0.000005568	212145905
10190927					
91 90	-284.483516663	-0.000000001	0.000057499	0.000005294	212145871
10190933					
92 91	-284.483516663	-0.000000001	0.000026178	0.000003067	212145888
10190934					
93 92	-284.483516664	0.000000000	0.000017063	0.000001437	212145888
10190934					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 340.2 SECONDS (3.7 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 103.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.6
TIME TO SOLVE SCF EQUATIONS= 16.1 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.4835166637 AFTER 93 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -47.2196031438
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998963846

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 358.13 , TOTAL = 361.6 SECONDS (6.0 MIN)
WALL CLOCK TIME: STEP = 330.17 , TOTAL = 333.0 SECONDS (5.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.56 , TOTAL = 365.1 SECONDS (6.1 MIN)
WALL CLOCK TIME: STEP = 3.51 , TOTAL = 336.5 SECONDS (5.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.17 , TOTAL = 368.3 SECONDS (6.1 MIN)
WALL CLOCK TIME: STEP = 3.01 , TOTAL = 339.5 SECONDS (5.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 0 ENERGY= -284.4835167

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0279177	0.0112787	-0.0102851
2 C	6.0	-0.0389078	0.0164381	0.0049049
3 C	6.0	-0.0295722	-0.0081123	-0.0001391
4 C	6.0	0.0061837	0.0176921	0.0006954
5 C	6.0	-0.0334165	0.0047652	0.0014051
6 C	6.0	-0.0411294	0.0465189	0.0095666
7 C	6.0	-0.0293792	0.0455640	0.0081675
8 C	6.0	-0.0579561	-0.0693825	-0.0095534

9 C	6.0	-0.0030497	-0.0895916	-0.0152934
10 C	6.0	0.0710180	-0.0447228	-0.0115436
11 C	6.0	-0.0564470	-0.0613879	-0.0014139
12 N	7.0	0.0670206	0.1160644	-0.0003759
13 C	6.0	-0.0137558	-0.0908743	0.0080246
14 C	6.0	0.0466706	0.0401555	0.0054662
15 C	6.0	0.0896016	-0.0323552	0.0063906
16 C	6.0	-0.0069246	0.0304708	0.0005652
17 C	6.0	0.0222503	0.0078806	-0.0000462
18 C	6.0	0.0156254	-0.0198332	0.0000186
19 C	6.0	0.0214661	-0.0262572	-0.0004724
20 O	8.0	-0.0450303	0.0050904	0.0158257
21 N	7.0	0.0241395	0.0269491	0.0096923
22 H	1.0	0.0043397	-0.0053279	-0.0012319
23 H	1.0	-0.0001257	0.0003879	-0.0000729
24 H	1.0	0.0020929	0.0033422	0.0006276
25 H	1.0	-0.0029435	0.0054387	0.0011521
26 H	1.0	0.0022488	0.0012487	0.0003299
27 H	1.0	0.0083223	0.0077184	0.0009034
28 H	1.0	0.0036453	-0.0064224	0.0001271
29 H	1.0	-0.0015684	0.0038055	0.0011653
30 H	1.0	0.0000143	0.0021370	-0.0001437
31 H	1.0	-0.0011963	-0.0018715	0.0001750
32 H	1.0	-0.0086029	-0.0004536	0.0001886
33 H	1.0	0.0146050	0.0552062	-0.0333461
34 H	1.0	0.0011845	0.0070662	0.0004927
35 H	1.0	-0.0025055	0.0013738	0.0080334

MAXIMUM GRADIENT = 0.1160644 RMS GRADIENT = 0.0299538
 FORCE CONSTANT MATRIX NOT UPDATED --- TAKING FIRST STEP
 MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
 NR STEP HAS LENGTH = 0.920635
 TRIM/QA LAMBDA FOR NON-TS MODES = -0.68972306
 TRIM/QA STEP HAS LENGTH = 0.300000
 RADIUS OF STEP TAKEN= 0.30000 CURRENT TRUST RADIUS= 0.30000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 368.3 SECONDS (6.1 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 339.5 SECONDS (5.7 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

INSERCH= 1

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM CHARGE X Y Z

CO	27.0	0.0262357793	-1.4992323909	0.8366186102
C	6.0	4.7824230065	0.6484978955	0.4407630816
C	6.0	5.0090954824	-0.6836031426	0.1900709456
C	6.0	3.8822017696	-1.5232497073	0.0717393438
C	6.0	2.5984828051	-1.0325636578	0.2204722591
C	6.0	2.3184721018	0.3168394836	0.4808509838
C	6.0	3.4729956247	1.1272333723	0.5753756013
C	6.0	3.4100762150	2.5066861011	0.8165412541
C	6.0	2.1898764220	3.0940386639	0.9713091018
C	6.0	1.0488680639	2.3187315706	0.8904696283
C	6.0	1.1137956594	0.9950501121	0.6468312877
N	7.0	-0.0714640088	0.2923696618	0.6066944212
C	6.0	-1.2238841076	0.8255010610	0.5458495272
C	6.0	-2.4221389389	0.0642297102	0.5378727849
C	6.0	-2.6384426977	-1.3040642131	0.5304946495
C	6.0	-3.9019173627	-1.8288601895	0.5359076833
C	6.0	-5.0452081994	-1.0023760685	0.5434239158
C	6.0	-4.8596817001	0.3893571243	0.5263903713
C	6.0	-3.5662026433	0.9047807665	0.5215443405
O	8.0	-1.6110097201	-2.2989318413	0.4945147836
N	7.0	1.6028147760	-2.0887374865	0.0126869957
H	1.0	5.6425544112	1.3179558883	0.5263362126
H	1.0	6.0175651418	-1.0826006095	0.0739377495
H	1.0	4.0536165633	-2.5841277080	-0.1475246270
H	1.0	4.2801225747	3.1057858934	0.8897041159
H	1.0	2.1223358735	4.1312541211	1.1677293765
H	1.0	0.1695944047	2.8804076738	1.0645317318
H	1.0	-1.3503854334	1.8694219478	0.4597332693
H	1.0	-4.0602876517	-2.9073674125	0.5251962439
H	1.0	-6.0475062642	-1.4341043938	0.5466743085
H	1.0	-5.7239801213	1.0552679930	0.5191085075
H	1.0	-3.4842490873	1.9934345698	0.5139014296
H	1.0	-1.8102532853	-2.8560542089	1.2790481483
H	1.0	1.4672864553	-2.2283549778	-1.0021548152
H	1.0	1.9441950915	-2.9615106019	0.4502437783

 INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.2336186	5.0903994	3.9311691
2 C	5.2336186	0.0000000	1.3743071 *	2.3797194 *
3 C	5.0903994	1.3743071 *	0.0000000	1.4102830 *
4 C	3.9311691	2.3797194 *	1.4102830 *	0.0000000

5 C	2.6858650 *	2.7647949 *	2.4359292 *	1.3823273 *
6 C	2.9460202 *	2.4864952 *	2.8852890 *	2.4491940 *
7 C	4.3412813	1.4006814 *	2.4056582 *	2.7287652 *
8 C	5.2438690	2.3403864 *	3.6231579	4.1252897
9 C	5.0791359	3.6032550	4.7779605	4.9992542
10 C	3.9529135	4.1147720	5.0187621	4.8434409
11 C	2.7276823 *	3.6907166	4.2661303	3.7863752
12 N	1.8089357 *	4.8697618	5.1902006	4.3833918
13 C	2.6555097 *	6.0098335	6.4229283	5.6403478
14 C	2.9203085 *	7.2288666	7.4768620	6.5178281
15 C	2.6892962 *	7.6739689	7.6802149	6.5404360
16 C	3.9534123	9.0312858	8.9909603	7.8039324
17 C	5.1041526	9.9658547	10.0655599	8.9550234
18 C	5.2473995	9.6459665	9.9326289	8.9602064
19 C	4.3340702	8.3529490	8.7274610	7.8470622
20 O	1.8539490 *	7.0403276	6.8211264	5.5637932
21 N	1.8740280 *	4.2172995	3.6889857	2.3492273 *
22 H	6.2909347	1.0933082 *	2.1261663 *	3.3731215
23 H	6.0540310	2.1579710 *	1.0907323 *	2.1803562 *
24 H	4.2854792	3.3655771	2.1538116 *	1.0967779 *
25 H	6.2693352	2.5479635 *	3.9217799	4.7175606
26 H	6.0171130	4.4423118	5.6984250	6.0226021
27 H	4.3879087	5.1622375	6.0735184	5.8447659
28 H	3.6585462	6.2531876	6.8581085	6.2482581
29 H	4.3335323	9.5312559	9.3440434	8.0749330
30 H	6.0810075	11.0288629	11.0877798	9.9414592
31 H	6.3001006	10.5145664	10.8779985	9.9562856
32 H	4.9624966	8.3756833	8.9111334	8.1747889
33 H	2.3258120 *	7.5131876	7.2394014	5.9697577
34 H	2.4473117 *	4.6204356	4.0437695	2.7353680 *
35 H	2.4425624 *	4.5921443	3.8275536	2.4428938 *

C C C C

1 CO	2.6858650 *	2.9460202 *	4.3412813	5.2438690
2 C	2.7647949 *	2.4864952 *	1.4006814 *	2.3403864 *
3 C	2.4359292 *	2.8852890 *	2.4056582 *	3.6231579
4 C	1.3823273 *	2.4491940 *	2.7287652 *	4.1252897
5 C	0.0000000	1.4025305 *	2.3570007 *	3.6797107
6 C	1.4025305 *	0.0000000	1.4137177 *	2.4697603 *
7 C	2.3570007 *	1.4137177 *	0.0000000	1.4017880 *
8 C	3.6797107	2.4697603 *	1.4017880 *	0.0000000
9 C	4.2142095	2.8231049 *	2.3814872 *	1.3630200 *
10 C	3.7525168	2.4056712 *	2.7194387 *	2.3698304 *
11 C	2.5489793 *	1.3923952 *	2.3639803 *	2.7544054 *
12 N	3.0055335	2.3933721 *	3.6415893	4.1313866

13 C	4.2624833	3.5792805	4.7066542	4.9369267
14 C	5.1488194	4.7476790	5.9903251	6.3291376
15 C	5.2531148	5.2154384	6.5774540	7.1545944
16 C	6.5565837	6.5802966	7.9454005	8.5053493
17 C	7.6505700	7.4811786	8.7804358	9.1585995
18 C	7.5986619	7.1786645	8.3654272	8.5414381
19 C	6.4689485	5.9141126	7.0429181	7.1639089
20 O	4.4043859	4.7205163	6.1312525	6.9576554
21 N	1.4662990 *	2.5530655 *	3.7625342	5.0030284
22 H	3.8580911	3.4718621	2.1784777 *	2.5458314 *
23 H	3.4225868	3.9758396	3.4072922	4.4981594
24 H	2.1587466 *	3.4381962	3.8254289	5.2211064
25 H	4.5168264	3.4341601	2.1598441 *	1.0588928 *
26 H	5.2715298	3.8807255	3.3465363	2.1025769 *
27 H	4.6822302	3.3956208	3.7716513	3.2713742
28 H	4.9063557	3.9839018	4.8815184	4.8161616
29 H	6.9243750	7.1474508	8.5458106	9.2305576
30 H	8.6614531	8.5474985	9.8590685	10.2493182
31 H	8.5855468	8.0763716	9.1974294	9.2534354
32 H	6.8001760	6.0401686	7.0112294	6.9200245
33 H	4.8869883	5.2678977	6.6539052	7.4983156
34 H	2.0504485 *	3.0662417	4.2156191	5.4316389
35 H	2.0498106 *	3.2997878	4.3670031	5.6731082

C C C N

1 CO	5.0791359	3.9529135	2.7276823 *	1.8089357 *
2 C	3.6032550	4.1147720	3.6907166	4.8697618
3 C	4.7779605	5.0187621	4.2661303	5.1902006
4 C	4.9992542	4.8434409	3.7863752	4.3833918
5 C	4.2142095	3.7525168	2.5489793 *	3.0055335
6 C	2.8231049 *	2.4056712 *	1.3923952 *	2.3933721 *
7 C	2.3814872 *	2.7194387 *	2.3639803 *	3.6415893
8 C	1.3630200 *	2.3698304 *	2.7544054 *	4.1313866
9 C	0.0000000	1.3818597 *	2.3809638 *	3.6188332
10 C	1.3818597 *	0.0000000	1.3474820 *	2.3327698 *
11 C	2.3809638 *	1.3474820 *	0.0000000	1.3784815 *
12 N	3.6188332	2.3327698 *	1.3784815 *	0.0000000
13 C	4.1208057	2.7411499 *	2.3459946 *	1.2712212 *
14 C	5.5351870	4.1539129	3.6580230	2.3627223 *
15 C	6.5460134	5.1817460	4.4021306	3.0238696
16 C	7.8443903	6.4682693	5.7570957	4.3791551
17 C	8.3252717	6.9489540	6.4756261	5.1398931
18 C	7.5636978	6.2262348	6.0053145	4.7898731
19 C	6.1747538	4.8408925	4.6825452	3.5490134
20 O	6.6149980	5.3436453	4.2776257	3.0162276

21 N	5.3032788	4.5280396	3.1860673	2.9708123 *
22 H	3.9081269	4.7155169	4.5418546	5.8058842
23 H	5.7359212	6.0764904	5.3564722	6.2650338
24 H	6.0800403	5.8432846	4.6993683	5.0852112
25 H	2.0918715 *	3.3257271	3.8131114	5.1895772
26 H	1.0578084 *	2.1247221 *	3.3353056	4.4569667
27 H	2.0336834 *	1.0577806 *	2.1495494 *	2.6392546 *
28 H	3.7808531	2.4786751 *	2.6213966 *	2.0357631 *
29 H	8.6764303	7.3177187	6.4818821	5.1142618
30 H	9.4095094	8.0349550	7.5627421	6.2207231
31 H	8.1847539	6.8996900	6.8392337	5.7044389
32 H	5.7979523	4.5603479	4.7070646	3.8143590
33 H	7.1763045	5.9248608	4.8765526	3.6589644
34 H	5.7222871	4.9429847	3.6379185	3.3630643
35 H	6.0828896	5.3736735	4.0475403	3.8308087

C C C C

1 CO	2.6555097 *	2.9203085 *	2.6892962 *	3.9534123
2 C	6.0098335	7.2288666	7.6739689	9.0312858
3 C	6.4229283	7.4768620	7.6802149	8.9909603
4 C	5.6403478	6.5178281	6.5404360	7.8039324
5 C	4.2624833	5.1488194	5.2531148	6.5565837
6 C	3.5792805	4.7476790	5.2154384	6.5802966
7 C	4.7066542	5.9903251	6.5774540	7.9454005
8 C	4.9369267	6.3291376	7.1545944	8.5053493
9 C	4.1208057	5.5351870	6.5460134	7.8443903
10 C	2.7411499 *	4.1539129	5.1817460	6.4682693
11 C	2.3459946 *	3.6580230	4.4021306	5.7570957
12 N	1.2712212 *	2.3627223 *	3.0238696	4.3791551
13 C	0.0000000	1.4196522 *	2.5566110 *	3.7706226
14 C	1.4196522 *	0.0000000	1.3853050 *	2.4028186 *
15 C	2.5566110 *	1.3853050 *	0.0000000	1.3681405 *
16 C	3.7706226	2.4028186 *	1.3681405 *	0.0000000
17 C	4.2359956	2.8316375 *	2.4256346 *	1.4107609 *
18 C	3.6619154	2.4591573 *	2.7931336 *	2.4161728 *
19 C	2.3437859 *	1.4197445 *	2.3957911 *	2.7542156 *
20 O	3.1487430	2.4988684 *	1.4306204 *	2.3390038 *
21 N	4.0947863	4.5947079	4.3442032	5.5356456
22 H	6.8841027	8.1615710	8.6861913	10.0498500
23 H	7.5034752	8.5298922	8.6708686	9.9582354
24 H	6.3212617	7.0298632	6.8470380	8.0204756
25 H	5.9675811	7.3685249	8.2123294	9.5614686
26 H	4.7446734	6.1310405	7.2535347	8.4978696
27 H	2.5364256 *	3.8633288	5.0675510	6.2477080
28 H	1.0550779 *	2.1008285 *	3.4256551	4.4937077

29 H	4.6882746	3.3932405	2.1429541 *	1.0901255 *
30 H	5.3266451	3.9228014	3.4115813	2.1816278 *
31 H	4.5060373	3.4474141	3.8842141	3.4115085
32 H	2.5444723 *	2.2023814 *	3.4042858	3.8451097
33 H	3.7993760	3.0743785	1.9117801 *	2.4459035 *
34 H	4.3548540	4.7702473	4.4788771	5.5994269
35 H	4.9383523	5.3129706	4.8738217	5.9554400

C C C O

1 CO	5.1041526	5.2473995	4.3340702	1.8539490 *
2 C	9.9658547	9.6459665	8.3529490	7.0403276
3 C	10.0655599	9.9326289	8.7274610	6.8211264
4 C	8.9550234	8.9602064	7.8470622	5.5637932
5 C	7.6505700	7.5986619	6.4689485	4.4043859
6 C	7.4811786	7.1786645	5.9141126	4.7205163
7 C	8.7804358	8.3654272	7.0429181	6.1312525
8 C	9.1585995	8.5414381	7.1639089	6.9576554
9 C	8.3252717	7.5636978	6.1747538	6.6149980
10 C	6.9489540	6.2262348	4.8408925	5.3436453
11 C	6.4756261	6.0053145	4.6825452	4.2776257
12 N	5.1398931	4.7898731	3.5490134	3.0162276
13 C	4.2359956	3.6619154	2.3437859 *	3.1487430
14 C	2.8316375 *	2.4591573 *	1.4197445 *	2.4988684 *
15 C	2.4256346 *	2.7931336 *	2.3957911 *	1.4306204 *
16 C	1.4107609 *	2.4161728 *	2.7542156 *	2.3390038 *
17 C	0.0000000	1.4041480 *	2.4135417 *	3.6711263
18 C	1.4041480 *	0.0000000	1.3923983 *	4.2168452
19 C	2.4135417 *	1.3923983 *	0.0000000	3.7533031
20 O	3.6711263	4.2168452	3.7533031	0.0000000
21 N	6.7570757	6.9403678	5.9949002	3.2565331
22 H	10.9367501	10.5432091	9.2180227	8.1053737
23 H	11.0730216	10.9857122	9.7978896	7.7363752
24 H	9.2610993	9.4203322	8.4072457	5.7080244
25 H	10.1960139	9.5418554	8.1574987	8.0045355
26 H	8.8384164	7.9474322	6.5716935	7.4658140
27 H	6.5224021	5.6381333	4.2607648	5.5064533
28 H	4.6803785	3.8092250	2.4174778 *	4.1766384
29 H	2.1446195 *	3.3922596	3.8440353	2.5239052 *
30 H	1.0913301 *	2.1763158 *	3.4099682	4.5203041
31 H	2.1668460 *	1.0911013 *	2.1630201 *	5.3073333
32 H	3.3782164	2.1130630 *	1.0917609 *	4.6833547
33 H	3.8002893	4.5164369	4.2191290	0.9826372 *
34 H	6.8047354	7.0156534	6.1216183	3.4235812
35 H	7.2593835	7.5846458	6.7318479	3.6166907

	N	H	H	H
1 CO	1.8740280 *	6.2909347	6.0540310	4.2854792
2 C	4.2172995	1.0933082 *	2.1579710 *	3.3655771
3 C	3.6889857	2.1261663 *	1.0907323 *	2.1538116 *
4 C	2.3492273 *	3.3731215	2.1803562 *	1.0967779 *
5 C	1.4662990 *	3.8580911	3.4225868	2.1587466 *
6 C	2.5530655 *	3.4718621	3.9758396	3.4381962
7 C	3.7625342	2.1784777 *	3.4072922	3.8254289
8 C	5.0030284	2.5458314 *	4.4981594	5.2211064
9 C	5.3032788	3.9081269	5.7359212	6.0800403
10 C	4.5280396	4.7155169	6.0764904	5.8432846
11 C	3.1860673	4.5418546	5.3564722	4.6993683
12 N	2.9708123 *	5.8058842	6.2650338	5.0852112
13 C	4.0947863	6.8841027	7.5034752	6.3212617
14 C	4.5947079	8.1615710	8.5298922	7.0298632
15 C	4.3442032	8.6861913	8.6708686	6.8470380
16 C	5.5356456	10.0498500	9.9582354	8.0204756
17 C	6.7570757	10.9367501	11.0730216	9.2610993
18 C	6.9403678	10.5432091	10.9857122	9.4203322
19 C	5.9949002	9.2180227	9.7978896	8.4072457
20 O	3.2565331	8.1053737	7.7363752	5.7080244
21 N	0.0000000	5.3093212	4.5283644	2.5054957 *
22 H	5.3093212	0.0000000	2.4714305 *	4.2667398
23 H	4.5283644	2.4714305 *	0.0000000	2.4820804 *
24 H	2.5054957 *	4.2667398	2.4820804 *	0.0000000
25 H	5.9093324	2.2769701 *	4.6072511	5.7881141
26 H	6.3476232	4.5516998	6.5995055	7.1102807
27 H	5.2775848	5.7170098	7.1334054	6.8129183
28 H	4.9586559	7.0149667	7.9466956	7.0289476
29 H	5.7448716	10.5829345	10.2516596	8.1481580
30 H	7.6968240	12.0096531	12.0794446	10.1900514
31 H	7.9889396	11.3695719	11.9428868	10.4542335
32 H	6.5416789	9.1517740	9.9970013	8.8436972
33 H	3.7204138	8.5751547	8.1161672	6.0410283
34 H	1.0333271 *	5.6873076	4.8141214	2.7470112 *
35 H	1.0342772 *	5.6566320	4.5015833	2.2247256 *

	H	H	H	H
1 CO	6.2693352	6.0171130	4.3879087	3.6585462
2 C	2.5479635 *	4.4423118	5.1622375	6.2531876
3 C	3.9217799	5.6984250	6.0735184	6.8581085
4 C	4.7175606	6.0226021	5.8447659	6.2482581
5 C	4.5168264	5.2715298	4.6822302	4.9063557
6 C	3.4341601	3.8807255	3.3956208	3.9839018

7 C	2.1598441 *	3.3465363	3.7716513	4.8815184
8 C	1.0588928 *	2.1025769 *	3.2713742	4.8161616
9 C	2.0918715 *	1.0578084 *	2.0336834 *	3.7808531
10 C	3.3257271	2.1247221 *	1.0577806 *	2.4786751 *
11 C	3.8131114	3.3353056	2.1495494 *	2.6213966 *
12 N	5.1895772	4.4569667	2.6392546 *	2.0357631 *
13 C	5.9675811	4.7446734	2.5364256 *	1.0550779 *
14 C	7.3685249	6.1310405	3.8633288	2.1008285 *
15 C	8.2123294	7.2535347	5.0675510	3.4256551
16 C	9.5614686	8.4978696	6.2477080	4.4937077
17 C	10.1960139	8.8384164	6.5224021	4.6803785
18 C	9.5418554	7.9474322	5.6381333	3.8092250
19 C	8.1574987	6.5716935	4.2607648	2.4174778 *
20 O	8.0045355	7.4658140	5.5064533	4.1766384
21 N	5.9093324	6.3476232	5.2775848	4.9586559
22 H	2.2769701 *	4.5516998	5.7170098	7.0149667
23 H	4.6072511	6.5995055	7.1334054	7.9466956
24 H	5.7881141	7.1102807	6.8129183	7.0289476
25 H	0.0000000	2.4051874 *	4.1204128	5.7806653
26 H	2.4051874 *	0.0000000	2.3213069 *	4.2043949
27 H	4.1204128	2.3213069 *	0.0000000	1.9230736 *
28 H	5.7806653	4.2043949	1.9230736 *	0.0000000
29 H	10.2885043	9.3904140	7.1889586	5.4923194
30 H	11.2866377	9.9048092	7.5852180	5.7431515
31 H	10.2188079	8.4526371	6.1937745	4.4491238
32 H	7.8526442	6.0358561	3.8000641	2.1381505 *
33 H	8.5315769	8.0187360	6.0722985	4.8179747
34 H	6.3201453	6.7514528	5.6616829	5.1834513
35 H	6.5162696	7.1311872	6.1363317	5.8474148

H H H H

1 CO	4.3335323	6.0810075	6.3001006	4.9624966
2 C	9.5312559	11.0288629	10.5145664	8.3756833
3 C	9.3440434	11.0877798	10.8779985	8.9111334
4 C	8.0749330	9.9414592	9.9562856	8.1747889
5 C	6.9243750	8.6614531	8.5855468	6.8001760
6 C	7.1474508	8.5474985	8.0763716	6.0401686
7 C	8.5458106	9.8590685	9.1974294	7.0112294
8 C	9.2305576	10.2493182	9.2534354	6.9200245
9 C	8.6764303	9.4095094	8.1847539	5.7979523
10 C	7.3177187	8.0349550	6.8996900	4.5603479
11 C	6.4818821	7.5627421	6.8392337	4.7070646
12 N	5.1142618	6.2207231	5.7044389	3.8143590
13 C	4.6882746	5.3266451	4.5060373	2.5444723 *
14 C	3.3932405	3.9228014	3.4474141	2.2023814 *

15 C	2.1429541 *	3.4115813	3.8842141	3.4042858
16 C	1.0901255 *	2.1816278 *	3.4115085	3.8451097
17 C	2.1446195 *	1.0913301 *	2.1668460 *	3.3782164
18 C	3.3922596	2.1763158 *	1.0911013 *	2.1130630 *
19 C	3.8440353	3.4099682	2.1630201 *	1.0917609 *
20 O	2.5239052 *	4.5203041	5.3073333	4.6833547
21 N	5.7448716	7.6968240	7.9889396	6.5416789
22 H	10.5829345	12.0096531	11.3695719	9.1517740
23 H	10.2516596	12.0794446	11.9428868	9.9970013
24 H	8.1481580	10.1900514	10.4542335	8.8436972
25 H	10.2885043	11.2866377	10.2188079	7.8526442
26 H	9.3904140	9.9048092	8.4526371	6.0358561
27 H	7.1889586	7.5852180	6.1937745	3.8000641
28 H	5.4923194	5.7431515	4.4491238	2.1381505 *
29 H	0.0000000	2.4738640 *	4.2977191	4.9345525
30 H	2.4738640 *	0.0000000	2.5104589 *	4.2801150
31 H	4.2977191	2.5104589 *	0.0000000	2.4282872 *
32 H	4.9345525	4.2801150	2.4282872 *	0.0000000
33 H	2.3735165 *	4.5290866	5.5850879	5.1870274
34 H	5.7747671	7.7137420	8.0505116	6.6812901
35 H	6.0051946	8.1369257	8.6567987	7.3500708

H H H

1 CO	2.3258120 *	2.4473117 *	2.4425624 *
2 C	7.5131876	4.6204356	4.5921443
3 C	7.2394014	4.0437695	3.8275536
4 C	5.9697577	2.7353680 *	2.4428938 *
5 C	4.8869883	2.0504485 *	2.0498106 *
6 C	5.2678977	3.0662417	3.2997878
7 C	6.6539052	4.2156191	4.3670031
8 C	7.4983156	5.4316389	5.6731082
9 C	7.1763045	5.7222871	6.0828896
10 C	5.9248608	4.9429847	5.3736735
11 C	4.8765526	3.6379185	4.0475403
12 N	3.6589644	3.3630643	3.8308087
13 C	3.7993760	4.3548540	4.9383523
14 C	3.0743785	4.7702473	5.3129706
15 C	1.9117801 *	4.4788771	4.8738217
16 C	2.4459035 *	5.5994269	5.9554400
17 C	3.8002893	6.8047354	7.2593835
18 C	4.5164369	7.0156534	7.5846458
19 C	4.2191290	6.1216183	6.7318479
20 O	0.9826372 *	3.4235812	3.6166907
21 N	3.7204138	1.0333271 *	1.0342772 *
22 H	8.5751547	5.6873076	5.6566320

23 H	8.1161672	4.8141214	4.5015833
24 H	6.0410283	2.7470112 *	2.2247256 *
25 H	8.5315769	6.3201453	6.5162696
26 H	8.0187360	6.7514528	7.1311872
27 H	6.0722985	5.6616829	6.1363317
28 H	4.8179747	5.1834513	5.8474148
29 H	2.3735165 *	5.7747671	6.0051946
30 H	4.5290866	7.7137420	8.1369257
31 H	5.5850879	8.0505116	8.6567987
32 H	5.1870274	6.6812901	7.3500708
33 H	0.0000000	4.0422964	3.8462866
34 H	4.0422964	0.0000000	1.6954117 *
35 H	3.8462866	1.6954117 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.52 , TOTAL = 368.8 SECONDS (6.1 MIN)
WALL CLOCK TIME: STEP = 0.53 , TOTAL = 340.0 SECONDS (5.7 MIN)
CPU UTILIZATION: STEP = 98.35% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.13 , TOTAL = 370.0 SECONDS (6.2 MIN)
WALL CLOCK TIME: STEP = 1.13 , TOTAL = 341.2 SECONDS (5.7 MIN)
CPU UTILIZATION: STEP = 99.98% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.483310605	-284.483310605	4.049079681	0.049418406	211416096
10250471						
2	1	-284.522211037	-0.038900432	2.389644924	0.016268617	206074174
10703041						
3	2	-284.529399346	-0.007188309	1.326007229	0.009799599	204583595
10851736						
4	3	-284.531162787	-0.001763440	1.028619889	0.006724820	198232434
11439166						
5	4	-284.531856392	-0.000693605	0.261779098	0.003537133	195156019
11663305						

6 5	-284.532061534	-0.000205142	0.458942546	0.002552565	190757058
12090307					
7 6	-284.532118969	-0.000057436	0.116790344	0.001957427	188738819
12233165					
8 7	-284.532177103	-0.000058134	0.213182494	0.001088009	183492052
12695255					
9 8	-284.532195642	-0.000018539	0.065749756	0.000803612	183568347
12676751					
10 9	-284.532202149	-0.000006508	0.068308130	0.000381981	176434401
13253149					
11 10	-284.532204225	-0.000002075	0.028929956	0.000363566	192944696
11880911					
12 11	-284.532206092	-0.000001868	0.025927140	0.000161456	188637812
12232922					
13 12	-284.532206874	-0.000000782	0.007675353	0.000148711	186348016
12457170					
14 13	-284.532207819	-0.000000945	0.020100421	0.000108415	180936824
12905254					
15 14	-284.532208739	-0.000000920	0.010219870	0.000093168	201995590
11150618					
16 15	-284.532208988	-0.000000249	0.009117434	0.000076911	198942349
11386364					
17 16	-284.532209258	-0.000000270	0.008970586	0.000062531	196586392
11599413					
18 17	-284.532209605	-0.000000347	0.005718070	0.000080998	198513685
11462692					
19 18	-284.532209776	-0.000000170	0.004732211	0.000067695	195400093
11736374					
20 19	-284.532209919	-0.000000143	0.007052394	0.000041571	192754775
11943354					
-----DISABLING FDIFF OPTION-----					
21 20	-284.532209997	-0.000000078	0.002523885	0.000024317	210969786
10296136					
22 21	-284.532210028	-0.000000031	0.001923552	0.000021673	210971249
10296027					
23 22	-284.532210048	-0.000000020	0.002429329	0.000016605	210970712
10296077					
24 23	-284.532210069	-0.000000021	0.002539910	0.000010547	210969610
10296161					
25 24	-284.532210088	-0.000000019	0.000880418	0.000016009	210968968
10296240					
26 25	-284.532210104	-0.000000016	0.001722226	0.000018142	210969098
10296241					
27 26	-284.532210117	-0.000000013	0.002432566	0.000012784	210969319
10296201					

28 27	-284.532210124	-0.000000007	0.000520769	0.000009919	210969816
10296143					
29 28	-284.532210126	-0.000000002	0.001060390	0.000008830	210969926
10296136					
30 29	-284.532210127	-0.000000001	0.000240006	0.000003988	210969674
10296158					
31 30	-284.532210127	0.000000000	0.000117461	0.000002478	210969785
10296156					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 113.9 SECONDS (3.7 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 34.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 3.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.5322101268 AFTER 31 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -47.1483986361
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000058978

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 118.46 , TOTAL = 488.4 SECONDS (8.1 MIN)
WALL CLOCK TIME: STEP = 108.64 , TOTAL = 449.8 SECONDS (7.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.94 , TOTAL = 492.4 SECONDS (8.2 MIN)
WALL CLOCK TIME: STEP = 3.91 , TOTAL = 453.7 SECONDS (7.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.13 , TOTAL = 495.5 SECONDS (8.3 MIN)
WALL CLOCK TIME: STEP = 2.96 , TOTAL = 456.7 SECONDS (7.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 1 ENERGY= -284.5322101

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0213994	0.0259338	-0.0147167
2 C	6.0	-0.0276115	0.0079944	0.0028101
3 C	6.0	-0.0108014	0.0133682	0.0029337
4 C	6.0	-0.0208399	0.0065814	-0.0001363
5 C	6.0	-0.0094950	0.0290248	0.0060580
6 C	6.0	-0.0207942	0.0040751	0.0022699
7 C	6.0	-0.0282869	-0.0187285	-0.0030009
8 C	6.0	0.0111168	-0.0043730	-0.0012549
9 C	6.0	-0.0067027	-0.0121112	-0.0011513
10 C	6.0	-0.0048840	-0.0415559	-0.0066490
11 C	6.0	0.0184464	0.0123538	0.0034598
12 N	7.0	-0.0196518	0.0138916	-0.0010328
13 C	6.0	0.0303891	0.0075087	0.0046187
14 C	6.0	0.0115893	-0.0359069	0.0057810
15 C	6.0	0.0186862	0.0118007	0.0053825
16 C	6.0	0.0357797	0.0177109	0.0007037
17 C	6.0	0.0013981	0.0003965	0.0002707
18 C	6.0	0.0142085	-0.0012863	-0.0002508
19 C	6.0	0.0153998	-0.0069578	-0.0005626
20 O	8.0	-0.0031304	0.0057430	-0.0168456
21 N	7.0	0.0061025	0.0115496	0.0047424
22 H	1.0	-0.0025802	-0.0080339	-0.0013785
23 H	1.0	-0.0083227	0.0040189	0.0009850
24 H	1.0	0.0011479	0.0073904	0.0014747
25 H	1.0	-0.0313678	-0.0144131	-0.0012779
26 H	1.0	0.0043058	-0.0351297	-0.0065337
27 H	1.0	0.0343490	-0.0083234	-0.0041680
28 H	1.0	0.0027056	-0.0364958	0.0028927
29 H	1.0	-0.0011971	0.0121318	0.0012515
30 H	1.0	0.0078732	0.0050378	-0.0002005
31 H	1.0	0.0066571	-0.0066819	0.0001726

32 H	1.0	-0.0082628	-0.0086346	0.0001658
33 H	1.0	0.0062807	0.0276326	0.0006426
34 H	1.0	0.0020194	0.0081459	0.0056587
35 H	1.0	-0.0031275	0.0063421	0.0068855

MAXIMUM GRADIENT = 0.0415559 RMS GRADIENT = 0.0141885
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0486934631
 PREDICTED ENERGY CHANGE WAS -0.0770778748 RATIO= 0.632
 MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
 NR STEP HAS LENGTH = 0.539864
 TRIM/QA LAMBDA FOR NON-TS MODES = -0.19952073
 TRIM/QA STEP HAS LENGTH = 0.300000
 RADIUS OF STEP TAKEN= 0.30000 CURRENT TRUST RADIUS= 0.30000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 495.5 SECONDS (8.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 456.7 SECONDS (7.6 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

INSERCH= 2

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.0515766175	-1.5265862356	0.8527193555
C	6.0	4.8155601267	0.6381334757	0.4372501091
C	6.0	5.0241944379	-0.6956361977	0.1871862763
C	6.0	3.9019217308	-1.5324013591	0.0717710871
C	6.0	2.6128599992	-1.0620195840	0.2142635546
C	6.0	2.3451879651	0.3058801111	0.4771792809
C	6.0	3.5053836368	1.1390009573	0.5771322460
C	6.0	3.4076913703	2.5213423149	0.8192058685
C	6.0	2.1969689029	3.1193663395	0.9747252724
C	6.0	1.0431365151	2.3665441152	0.8987728129
C	6.0	1.1039269788	0.9919502036	0.6436151522
N	7.0	-0.0619749056	0.2613384039	0.6077733648
C	6.0	-1.2519342501	0.8315878922	0.5400810859
C	6.0	-2.4405623119	0.0938157194	0.5313340384
C	6.0	-2.6702838995	-1.3109370274	0.5242130369
C	6.0	-3.9363229958	-1.8509363831	0.5351270036
C	6.0	-5.0499039115	-1.0039420088	0.5431630572
C	6.0	-4.8760789598	0.3935821845	0.5266362519
C	6.0	-3.5846490741	0.9155789297	0.5221720238
O	8.0	-1.6012077779	-2.3053775898	0.5088433823

N	7.0	1.5931788036	-2.1041871155	0.0065481012
H	1.0	5.6444645538	1.3267059561	0.5278850045
H	1.0	6.0258277831	-1.0866394455	0.0729732256
H	1.0	4.0521684180	-2.5919456885	-0.1490783033
H	1.0	4.3116306097	3.1192523565	0.8907983407
H	1.0	2.1177365888	4.1658638949	1.1741517511
H	1.0	0.1343335050	2.8875029592	1.0685256209
H	1.0	-1.3536075672	1.9065262983	0.4568491973
H	1.0	-4.0588682325	-2.9199507693	0.5237836797
H	1.0	-6.0553065153	-1.4394128713	0.5468946667
H	1.0	-5.7303956896	1.0621644174	0.5189116456
H	1.0	-3.4747842722	2.0020541259	0.5137092095
H	1.0	-1.8186475046	-2.8916404483	1.2833746964
H	1.0	1.4651102868	-2.2374756274	-1.0078326579
H	1.0	1.9476660376	-2.9679973041	0.4422285617

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.2492061	5.0853063	3.9287494
2 C	5.2492061	0.0000000	1.3729537 *	2.3831768 *
3 C	5.0853063	1.3729537 *	0.0000000	1.4046326 *
4 C	3.9287494	2.3831768 *	1.4046326 *	0.0000000
5 C	2.6802277 *	2.7914389 *	2.4391605 *	1.3795808 *
6 C	2.9596649 *	2.4929351 *	2.8747533 *	2.4427555 *
7 C	4.3715085	1.4096091 *	2.4134493 *	2.7475485 *
8 C	5.2583605	2.3821125 *	3.6553361	4.1515973
9 C	5.1188347	3.6472477	4.8132802	5.0359838
10 C	4.0176829	4.1751151	5.0726843	4.9049323
11 C	2.7375521 *	3.7341657	4.2924087	3.8115786
12 N	1.8081944 *	4.8950384	5.1924765	4.3837515
13 C	2.7125391 *	6.0714485	6.4689056	5.6894631
14 C	2.9899410 *	7.2771180	7.5142708	6.5637553
15 C	2.7500810 *	7.7359097	7.7263950	6.5914822
16 C	4.0136531	9.0994784	9.0413856	7.8583868
17 C	5.1375175	10.0017504	10.0850994	8.9797919
18 C	5.2986004	9.6951361	9.9657933	8.9983116
19 C	4.3926723	8.4052188	8.7647257	7.8895000
20 O	1.8591565 *	7.0600491	6.8257370	5.5743124
21 N	1.8509905 *	4.2531833	3.7132889	2.3793879 *
22 H	6.2870652	1.0814015 *	2.1425869 *	3.3791996
23 H	6.0409630	2.1382907 *	1.0812944 *	2.1701802 *
24 H	4.2594981	3.3704539	2.1572895 *	1.0926952 *
25 H	6.3034377	2.5720812 *	3.9441339	4.7409439

26 H	6.0643486	4.5017950	5.7494157	6.0719673
27 H	4.4201362	5.2318309	6.1258783	5.8926899
28 H	3.7306189	6.2982406	6.8934988	6.2924635
29 H	4.3526337	9.5615339	9.3575050	8.0934409
30 H	6.1151574	11.0681508	11.1102626	9.9689911
31 H	6.3438365	10.5547930	10.9023444	9.9856520
32 H	5.0001452	8.4021388	8.9228241	8.1916712
33 H	2.3551168 *	7.5622709	7.2697008	6.0033679
34 H	2.4423544 *	4.6457406	4.0586228	2.7569411 *
35 H	2.4168830 *	4.6074961	3.8332360	2.4530165 *

C C C C

1 CO	2.6802277 *	2.9596649 *	4.3715085	5.2583605
2 C	2.7914389 *	2.4929351 *	1.4096091 *	2.3821125 *
3 C	2.4391605 *	2.8747533 *	2.4134493 *	3.6553361
4 C	1.3795808 *	2.4427555 *	2.7475485 *	4.1515973
5 C	0.0000000	1.4184226 *	2.4026576 *	3.7199724
6 C	1.4184226 *	0.0000000	1.4318292 *	2.4807597 *
7 C	2.4026576 *	1.4318292 *	0.0000000	1.4067733 *
8 C	3.7199724	2.4807597 *	1.4067733 *	0.0000000
9 C	4.2702758	2.8609833 *	2.4066317 *	1.3592895 *
10 C	3.8324449	2.4737452 *	2.7700137 *	2.3709519 *
11 C	2.5845722 *	1.4279783 *	2.4068731 *	2.7707766 *
12 N	3.0101276	2.4111142 *	3.6738641	4.1461917
13 C	4.3160793	3.6358786	4.7673839	4.9644024
14 C	5.1936082	4.7907525	6.0372827	6.3385982
15 C	5.2980787	5.2698451	6.6440850	7.1913260
16 C	6.6043274	6.6417313	8.0200054	8.5517290
17 C	7.6700390	7.5104841	8.8196544	9.1670468
18 C	7.6354803	7.2219688	8.4146963	8.5576756
19 C	6.5126663	5.9612687	7.0937650	7.1804965
20 O	4.4035308	4.7321991	6.1600067	6.9629463
21 N	1.4727554 *	2.5681580 *	3.8079341	5.0347186
22 H	3.8723371	3.4539662	2.1478654 *	2.5524847 *
23 H	3.4159798	3.9559579	3.4000427	4.5198489
24 H	2.1317364 *	3.4210196	3.8400935	5.2439145
25 H	4.5636122	3.4573170	2.1609758 *	1.0861529 *
26 H	5.3382861	3.9289922	3.3828828	2.1200050 *
27 H	4.7404204	3.4499775	3.8291913	3.3031963
28 H	4.9602397	4.0303312	4.9207071	4.8144853
29 H	6.9325081	7.1707805	8.5846282	9.2436171
30 H	8.6827519	8.5801641	9.9023193	10.2620692
31 H	8.6148061	8.1110270	9.2362824	9.2587263
32 H	6.8218493	6.0622123	7.0336070	6.9087958
33 H	4.9121044	5.3114607	6.7149204	7.5385976

34 H	2.0475706 *	3.0738340	4.2515201	5.4550930
35 H	2.0315517 *	3.2981083	4.3945555	5.6926826

	C	C	C	N
--	---	---	---	---

1 CO	5.1188347	4.0176829	2.7375521 *	1.8081944 *
2 C	3.6472477	4.1751151	3.7341657	4.8950384
3 C	4.8132802	5.0726843	4.2924087	5.1924765
4 C	5.0359838	4.9049323	3.8115786	4.3837515
5 C	4.2702758	3.8324449	2.5845722 *	3.0101276
6 C	2.8609833 *	2.4737452 *	1.4279783 *	2.4111142 *
7 C	2.4066317 *	2.7700137 *	2.4068731 *	3.6738641
8 C	1.3592895 *	2.3709519 *	2.7707766 *	4.1461917
9 C	0.0000000	1.3797968 *	2.4145960 *	3.6613938
10 C	1.3797968 *	0.0000000	1.3993961 *	2.3953795 *
11 C	2.4145960 *	1.3993961 *	0.0000000	1.3763740 *
12 N	3.6613938	2.3953795 *	1.3763740 *	0.0000000
13 C	4.1614635	2.7842594 *	2.3635815 *	1.3212759 *
14 C	5.5549301	4.1756991	3.6582314	2.3857043 *
15 C	6.5970220	5.2396234	4.4229192	3.0466881
16 C	7.9066064	6.5356252	5.7877365	4.4133384
17 C	8.3489570	6.9722146	6.4701863	5.1463137
18 C	7.5933319	6.2504541	6.0110065	4.8166035
19 C	6.2039173	4.8645172	4.6907703	3.5839352
20 O	6.6386022	5.3825137	4.2671171	2.9945043 *
21 N	5.3467224	4.5919548	3.1986385	2.9490196 *
22 H	3.9113327	4.7319173	4.5543316	5.8055871
23 H	5.7588021	6.1183032	5.3731997	6.2581465
24 H	6.1093195	5.8939703	4.7079507	5.0636183
25 H	2.1163265 *	3.3540553	3.8569258	5.2322271
26 H	1.0682723 *	2.1138000 *	3.3738712	4.5074656
27 H	2.0777449 *	1.0611960 *	2.1711243 *	2.6734940 *
28 H	3.7875810	2.4801805 *	2.6288414 *	2.0970780 *
29 H	8.7070200	7.3565004	6.4785634	5.1090910
30 H	9.4374550	8.0620730	7.5614486	6.2302717
31 H	8.2026188	6.9084325	6.8358209	5.7254007
32 H	5.7991126	4.5489268	4.6906057	3.8322587
33 H	7.2355126	5.9988525	4.9023474	3.6720037
34 H	5.7586378	5.0010203	3.6451234	3.3445842
35 H	6.1156930	5.4299115	4.0538422	3.8071867

	C	C	C	C
--	---	---	---	---

1 CO	2.7125391 *	2.9899410 *	2.7500810 *	4.0136531
2 C	6.0714485	7.2771180	7.7359097	9.0994784
3 C	6.4689056	7.5142708	7.7263950	9.0413856

4 C	5.6894631	6.5637553	6.5914822	7.8583868
5 C	4.3160793	5.1936082	5.2980787	6.6043274
6 C	3.6358786	4.7907525	5.2698451	6.6417313
7 C	4.7673839	6.0372827	6.6440850	8.0200054
8 C	4.9644024	6.3385982	7.1913260	8.5517290
9 C	4.1614635	5.5549301	6.5970220	7.9066064
10 C	2.7842594 *	4.1756991	5.2396234	6.5356252
11 C	2.3635815 *	3.6582314	4.4229192	5.7877365
12 N	1.3212759 *	2.3857043 *	3.0466881	4.4133384
13 C	0.0000000	1.3990071 *	2.5695098 *	3.7949841
14 C	1.3990071 *	0.0000000	1.4234300 *	2.4534415 *
15 C	2.5695098 *	1.4234300 *	0.0000000	1.3764350 *
16 C	3.7949841	2.4534415 *	1.3764350 *	0.0000000
17 C	4.2182642	2.8308789 *	2.3994159 *	1.3991163 *
18 C	3.6505417	2.4538996 *	2.7876376 *	2.4333263 *
19 C	2.3342951 *	1.4086565 *	2.4069568 *	2.7888079 *
20 O	3.1565044	2.5418793 *	1.4601616 *	2.3790693 *
21 N	4.1228753	4.6236008	4.3674176	5.5604786
22 H	6.9141599	8.1784894	8.7230852	10.0940058
23 H	7.5407961	8.5605683	8.7106995	10.0021090
24 H	6.3505140	7.0591662	6.8764576	8.0519083
25 H	6.0257502	7.4077386	8.2769616	9.6362865
26 H	4.7826900	6.1459645	7.3036230	8.5593151
27 H	2.5353064 *	3.8371020	5.0782924	6.2695746
28 H	1.0829393 *	2.1149322 *	3.4771029	4.5601614
29 H	4.6854227	3.4207835	2.1253451 *	1.0760752 *
30 H	5.3131795	3.9265007	3.3875358	2.1586063 *
31 H	4.4844432	3.4294106	3.8724569	3.4212740
32 H	2.5123194 *	2.1705528 *	3.4092875	3.8805944
33 H	3.8387600	3.1409062	1.9494190 *	2.4753765 *
34 H	4.3814973	4.8018988	4.5063425	5.6307742
35 H	4.9682859	5.3515593	4.9069371	5.9898065

C C C O

1 CO	5.1375175	5.2986004	4.3926723	1.8591565 *
2 C	10.0017504	9.6951361	8.4052188	7.0600491
3 C	10.0850994	9.9657933	8.7647257	6.8257370
4 C	8.9797919	8.9983116	7.8895000	5.5743124
5 C	7.6700390	7.6354803	6.5126663	4.4035308
6 C	7.5104841	7.2219688	5.9612687	4.7321991
7 C	8.8196544	8.4146963	7.0937650	6.1600067
8 C	9.1670468	8.5576756	7.1804965	6.9629463
9 C	8.3489570	7.5933319	6.2039173	6.6386022
10 C	6.9722146	6.2504541	4.8645172	5.3825137
11 C	6.4701863	6.0110065	4.6907703	4.2671171

12 N	5.1463137	4.8166035	3.5839352	2.9945043 *
13 C	4.2182642	3.6505417	2.3342951 *	3.1565044
14 C	2.8308789 *	2.4538996 *	1.4086565 *	2.5418793 *
15 C	2.3994159 *	2.7876376 *	2.4069568 *	1.4601616 *
16 C	1.3991163 *	2.4333263 *	2.7888079 *	2.3790693 *
17 C	0.0000000	1.4083899 *	2.4149478 *	3.6862471
18 C	1.4083899 *	0.0000000	1.3929435 *	4.2437580
19 C	2.4149478 *	1.3929435 *	0.0000000	3.7826945
20 O	3.6862471	4.2437580	3.7826945	0.0000000
21 N	6.7549273	6.9541814	6.0162078	3.2398895
22 H	10.9453949	10.5618444	9.2382680	8.1050701
23 H	11.0860160	11.0112868	9.8271015	7.7360828
24 H	9.2654560	9.4384092	8.4305568	5.6987406
25 H	10.2352289	9.5904066	8.2062960	8.0333155
26 H	8.8600288	7.9726308	6.5959557	7.4933403
27 H	6.5035119	5.6229457	4.2447400	5.5037584
28 H	4.7054099	3.8342763	2.4420872 *	4.2194957
29 H	2.1572243 *	3.4128203	3.8647347	2.5333808 *
30 H	1.0956656 *	2.1796465 *	3.4133189	4.5376578
31 H	2.1754202 *	1.0848590 *	2.1507502 *	5.3282862
32 H	3.3938005	2.1333016 *	1.0920486 *	4.6972631
33 H	3.8147525	4.5511787	4.2653383	0.9954310 *
34 H	6.8097432	7.0347524	6.1467664	3.4215820
35 H	7.2686784	7.6072884	6.7598126	3.6108182

N H H H

1 CO	1.8509905 *	6.2870652	6.0409630	4.2594981
2 C	4.2531833	1.0814015 *	2.1382907 *	3.3704539
3 C	3.7132889	2.1425869 *	1.0812944 *	2.1572895 *
4 C	2.3793879 *	3.3791996	2.1701802 *	1.0926952 *
5 C	1.4727554 *	3.8723371	3.4159798	2.1317364 *
6 C	2.5681580 *	3.4539662	3.9559579	3.4210196
7 C	3.8079341	2.1478654 *	3.4000427	3.8400935
8 C	5.0347186	2.5524847 *	4.5198489	5.2439145
9 C	5.3467224	3.9113327	5.7588021	6.1093195
10 C	4.5919548	4.7319173	6.1183032	5.8939703
11 C	3.1986385	4.5543316	5.3731997	4.7079507
12 N	2.9490196 *	5.8055871	6.2581465	5.0636183
13 C	4.1228753	6.9141599	7.5407961	6.3505140
14 C	4.6236008	8.1784894	8.5605683	7.0591662
15 C	4.3674176	8.7230852	8.7106995	6.8764576
16 C	5.5604786	10.0940058	10.0021090	8.0519083
17 C	6.7549273	10.9453949	11.0860160	9.2654560
18 C	6.9541814	10.5618444	11.0112868	9.4384092
19 C	6.0162078	9.2382680	9.8271015	8.4305568

20	O	3.2398895	8.1050701	7.7360828	5.6987406
21	N	0.0000000	5.3343918	4.5484275	2.5117241 *
22	H	5.3343918	0.0000000	2.4852804 *	4.2836336
23	H	4.5484275	2.4852804 *	0.0000000	2.4921045 *
24	H	2.5117241 *	4.2836336	2.4921045 *	0.0000000
25	H	5.9545108	2.2630455 *	4.6148495	5.8108904
26	H	6.3993749	4.5734329	6.6388675	7.1526886
27	H	5.3078240	5.7523842	7.1759764	6.8451696
28	H	4.9972135	7.0224106	7.9726074	7.0587401
29	H	5.7339898	10.5919204	10.2598906	8.1455047
30	H	7.6963126	12.0223300	12.0955718	10.1967524
31	H	7.9951887	11.3779395	11.9593064	10.4640954
32	H	6.5423757	9.1442329	9.9997953	8.8430277
33	H	3.7270535	8.6060010	8.1399566	6.0504726
34	H	1.0310847 *	5.7034044	4.8262521	2.7488139 *
35	H	1.0303624 *	5.6672862	4.5063577	2.2181048 *

H H H H

1	CO	6.3034377	6.0643486	4.4201362	3.7306189
2	C	2.5720812 *	4.5017950	5.2318309	6.2982406
3	C	3.9441339	5.7494157	6.1258783	6.8934988
4	C	4.7409439	6.0719673	5.8926899	6.2924635
5	C	4.5636122	5.3382861	4.7404204	4.9602397
6	C	3.4573170	3.9289922	3.4499775	4.0303312
7	C	2.1609758 *	3.3828828	3.8291913	4.9207071
8	C	1.0861529 *	2.1200050 *	3.3031963	4.8144853
9	C	2.1163265 *	1.0682723 *	2.0777449 *	3.7875810
10	C	3.3540553	2.1138000 *	1.0611960 *	2.4801805 *
11	C	3.8569258	3.3738712	2.1711243 *	2.6288414 *
12	N	5.2322271	4.5074656	2.6734940 *	2.0970780 *
13	C	6.0257502	4.7826900	2.5353064 *	1.0829393 *
14	C	7.4077386	6.1459645	3.8371020	2.1149322 *
15	C	8.2769616	7.3036230	5.0782924	3.4771029
16	C	9.6362865	8.5593151	6.2695746	4.5601614
17	C	10.2352289	8.8600288	6.5035119	4.7054099
18	C	9.5904066	7.9726308	5.6229457	3.8342763
19	C	8.2062960	6.5959557	4.2447400	2.4420872 *
20	O	8.0333155	7.4933403	5.5037584	4.2194957
21	N	5.9545108	6.3993749	5.3078240	4.9972135
22	H	2.2630455 *	4.5734329	5.7523842	7.0224106
23	H	4.6148495	6.6388675	7.1759764	7.9726074
24	H	5.8108904	7.1526886	6.8451696	7.0587401
25	H	0.0000000	2.4472139 *	4.1874940	5.8098141
26	H	2.4472139 *	0.0000000	2.3620439 *	4.2034937
27	H	4.1874940	2.3620439 *	0.0000000	1.8842590 *

28 H	5.8098141	4.2034937	1.8842590 *	0.0000000
29 H	10.3282102	9.4224304	7.1837458	5.5333350
30 H	11.3301846	9.9303179	7.5700689	5.7714288
31 H	10.2573000	8.4649554	6.1667645	4.4579225
32 H	7.8751879	6.0327893	3.7573358	2.1240879 *
33 H	8.5944900	8.0817954	6.1039982	4.8909928
34 H	6.3562577	6.7963030	5.6874982	5.2214189
35 H	6.5455444	7.1733264	6.1617616	5.8872406

H H H H

1 CO	4.3526337	6.1151574	6.3438365	5.0001452
2 C	9.5615339	11.0681508	10.5547930	8.4021388
3 C	9.3575050	11.1102626	10.9023444	8.9228241
4 C	8.0934409	9.9689911	9.9856520	8.1916712
5 C	6.9325081	8.6827519	8.6148061	6.8218493
6 C	7.1707805	8.5801641	8.1110270	6.0622123
7 C	8.5846282	9.9023193	9.2362824	7.0336070
8 C	9.2436171	10.2620692	9.2587263	6.9087958
9 C	8.7070200	9.4374550	8.2026188	5.7991126
10 C	7.3565004	8.0620730	6.9084325	4.5489268
11 C	6.4785634	7.5614486	6.8358209	4.6906057
12 N	5.1090910	6.2302717	5.7254007	3.8322587
13 C	4.6854227	5.3131795	4.4844432	2.5123194 *
14 C	3.4207835	3.9265007	3.4294106	2.1705528 *
15 C	2.1253451 *	3.3875358	3.8724569	3.4092875
16 C	1.0760752 *	2.1586063 *	3.4212740	3.8805944
17 C	2.1572243 *	1.0956656 *	2.1754202 *	3.3938005
18 C	3.4128203	2.1796465 *	1.0848590 *	2.1333016 *
19 C	3.8647347	3.4133189	2.1507502 *	1.0920486 *
20 O	2.5333808 *	4.5376578	5.3282862	4.6972631
21 N	5.7339898	7.6963126	7.9951887	6.5423757
22 H	10.5919204	12.0223300	11.3779395	9.1442329
23 H	10.2598906	12.0955718	11.9593064	9.9997953
24 H	8.1455047	10.1967524	10.4640954	8.8430277
25 H	10.3282102	11.3301846	10.2573000	7.8751879
26 H	9.4224304	9.9303179	8.4649554	6.0327893
27 H	7.1837458	7.5700689	6.1667645	3.7573358
28 H	5.5333350	5.7714288	4.4579225	2.1240879 *
29 H	0.0000000	2.4856171 *	4.3187115	4.9565500
30 H	2.4856171 *	0.0000000	2.5227443 *	4.3016150
31 H	4.3187115	2.5227443 *	0.0000000	2.4436044 *
32 H	4.9565500	4.3016150	2.4436044 *	0.0000000
33 H	2.3656646 *	4.5387936	5.6141563	5.2233534
34 H	5.7728641	7.7207998	8.0618781	6.6851522
35 H	6.0072801	8.1483185	8.6718346	7.3559152

	H	H	H
1 CO	2.3551168 *	2.4423544 *	2.4168830 *
2 C	7.5622709	4.6457406	4.6074961
3 C	7.2697008	4.0586228	3.8332360
4 C	6.0033679	2.7569411 *	2.4530165 *
5 C	4.9121044	2.0475706 *	2.0315517 *
6 C	5.3114607	3.0738340	3.2981083
7 C	6.7149204	4.2515201	4.3945555
8 C	7.5385976	5.4550930	5.6926826
9 C	7.2355126	5.7586378	6.1156930
10 C	5.9988525	5.0010203	5.4299115
11 C	4.9023474	3.6451234	4.0538422
12 N	3.6720037	3.3445842	3.8071867
13 C	3.8387600	4.3814973	4.9682859
14 C	3.1409062	4.8018988	5.3515593
15 C	1.9494190 *	4.5063425	4.9069371
16 C	2.4753765 *	5.6307742	5.9898065
17 C	3.8147525	6.8097432	7.2686784
18 C	4.5511787	7.0347524	7.6072884
19 C	4.2653383	6.1467664	6.7598126
20 O	0.9954310 *	3.4215820	3.6108182
21 N	3.7270535	1.0310847 *	1.0303624 *
22 H	8.6060010	5.7034044	5.6672862
23 H	8.1399566	4.8262521	4.5063577
24 H	6.0504726	2.7488139 *	2.2181048 *
25 H	8.5944900	6.3562577	6.5455444
26 H	8.0817954	6.7963030	7.1733264
27 H	6.1039982	5.6874982	6.1617616
28 H	4.8909928	5.2214189	5.8872406
29 H	2.3656646 *	5.7728641	6.0072801
30 H	4.5387936	7.7207998	8.1483185
31 H	5.6141563	8.0618781	8.6718346
32 H	5.2233534	6.6851522	7.3559152
33 H	0.0000000	4.0571699	3.8598543
34 H	4.0571699	0.0000000	1.6938712 *
35 H	3.8598543	1.6938712 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.66 , TOTAL = 496.2 SECONDS (8.3 MIN)
WALL CLOCK TIME: STEP = 0.65 , TOTAL = 457.4 SECONDS (7.6 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.89, TOTAL = 497.1 SECONDS (8.3 MIN)
WALL CLOCK TIME: STEP = 0.90, TOTAL = 458.3 SECONDS (7.6 MIN)
CPU UTILIZATION: STEP = 98.77%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.542681320	-284.542681320	5.624945896	0.026996782	209690727
10402119						
2	1	-284.554603091	-0.011921771	2.858617687	0.008508430	202148030
11066291						
3	2	-284.556355526	-0.001752435	2.723079425	0.007230785	199368374
11351486						
4	3	-284.558432957	-0.002077431	2.719593778	0.006347703	196576525
11563973						
5	4	-284.558764413	-0.000331456	0.386786899	0.001990898	194879246
11719297						
6	5	-284.558910264	-0.000145851	0.920147437	0.001068318	184059392
12661700						
7	6	-284.558933832	-0.000023568	0.271978966	0.001410589	187104316
12400007						
8	7	-284.558953572	-0.000019740	0.345795938	0.000811706	178095590
13185568						
9	8	-284.558958373	-0.000004801	0.239743832	0.000634138	179177532
13066062						
10	9	-284.558965108	-0.000006735	0.099902830	0.000157885	175170456
13430986						
11	10	-284.558966309	-0.000001201	0.063925746	0.000217381	169737322
13842905						
12	11	-284.558967965	-0.000001656	0.070046847	0.000128941	163464551
14423457						
13	12	-284.558970335	-0.000002370	0.023323424	0.000236536	186523535
12461272						
14	13	-284.558972648	-0.000002314	0.021453675	0.000222898	180517385
13068856						
15	14	-284.558974137	-0.000001488	0.016959881	0.000196777	181901523
12872271						
16	15	-284.558974887	-0.000000751	0.014348670	0.000083068	177895619
13226885						

17 16 -284.558975325 -0.000000437 0.016738921 0.000131070 176415614
13311551
18 17 -284.558975603 -0.000000279 0.020870591 0.000075622 196392973
11634578

-----DISABLING FDIFF OPTION-----

19 18 -284.558975708 -0.000000105 0.003433826 0.000043695 209397944
10432314
20 19 -284.558975836 -0.000000127 0.015052848 0.000041259 209398945
10432273
21 20 -284.558976016 -0.000000180 0.019198200 0.000062448 209400131
10432139
22 21 -284.558976210 -0.000000194 0.002922632 0.000055653 209402296
10431913
23 22 -284.558976282 -0.000000073 0.011548413 0.000026835 209403495
10431841
24 23 -284.558976319 -0.000000037 0.010577709 0.000017775 209401039
10432019
25 24 -284.558976332 -0.000000013 0.001524721 0.000016166 209399548
10432184
26 25 -284.558976338 -0.000000006 0.001191214 0.000009605 209399707
10432180
27 26 -284.558976341 -0.000000003 0.000990506 0.000010919 209399921
10432160
28 27 -284.558976343 -0.000000002 0.001248318 0.000005979 209399834
10432159
29 28 -284.558976343 -0.000000001 0.000347616 0.000002044 209399756
10432147
30 29 -284.558976343 0.000000000 0.000203644 0.000000941 209399850
10432142
31 30 -284.558976343 0.000000000 0.000159889 0.000001205 209399857
10432144
32 31 -284.558976343 0.000000000 0.000076520 0.000000368 209399794
10432144

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 116.4 SECONDS (3.6 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 35.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.3, LAST ITERATION= 3.7
TIME TO SOLVE SCF EQUATIONS= 4.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.5589763433 AFTER 32 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -47.0466407580
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999972135

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 121.90 , TOTAL = 619.0 SECONDS (10.3 MIN)
WALL CLOCK TIME: STEP = 111.83 , TOTAL = 570.1 SECONDS (9.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.85 , TOTAL = 622.8 SECONDS (10.4 MIN)
WALL CLOCK TIME: STEP = 3.82 , TOTAL = 573.9 SECONDS (9.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.29 , TOTAL = 626.1 SECONDS (10.4 MIN)
WALL CLOCK TIME: STEP = 3.12 , TOTAL = 577.0 SECONDS (9.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 2 ENERGY= -284.5589763

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0081721	0.0208135	-0.0185888
2 C	6.0	-0.0086884	0.0004074	0.0004351
3 C	6.0	-0.0110672	0.0066189	0.0013546
4 C	6.0	-0.0121125	0.0135010	0.0015438
5 C	6.0	-0.0040520	0.0064798	0.0021632
6 C	6.0	-0.0028090	-0.0097517	-0.0008210

7 C	6.0	-0.0115792	-0.0046031	-0.0006617
8 C	6.0	-0.0217214	-0.0069107	-0.0005096
9 C	6.0	0.0049064	-0.0217926	-0.0035329
10 C	6.0	-0.0016186	0.0167295	0.0041400
11 C	6.0	-0.0101969	-0.0160195	-0.0021908
12 N	7.0	0.0300151	-0.0199132	0.0023654
13 C	6.0	-0.0277824	0.0060233	0.0023947
14 C	6.0	0.0211386	0.0123578	0.0047357
15 C	6.0	0.0015611	-0.0030493	0.0029549
16 C	6.0	0.0052796	0.0030475	0.0014465
17 C	6.0	0.0204882	-0.0039827	0.0005414
18 C	6.0	0.0072316	0.0038921	-0.0005289
19 C	6.0	0.0189031	-0.0128337	0.0007864
20 O	8.0	0.0137497	0.0015857	-0.0237450
21 N	7.0	-0.0112673	0.0091256	0.0070730
22 H	1.0	-0.0129792	-0.0096405	-0.0011375
23 H	1.0	-0.0145405	0.0078048	0.0019778
24 H	1.0	-0.0027926	0.0102131	0.0020304
25 H	1.0	-0.0120971	-0.0048753	-0.0003456
26 H	1.0	0.0004394	-0.0267859	-0.0048121
27 H	1.0	0.0281743	-0.0107388	-0.0046558
28 H	1.0	-0.0007377	-0.0129215	0.0015839
29 H	1.0	0.0041993	0.0215777	0.0010385
30 H	1.0	0.0063269	0.0022373	-0.0001876
31 H	1.0	0.0115090	-0.0075911	-0.0000354
32 H	1.0	-0.0037750	-0.0087351	0.0001171
33 H	1.0	0.0040418	0.0181141	0.0091854
34 H	1.0	0.0030859	0.0085996	0.0072362
35 H	1.0	-0.0030608	0.0110160	0.0066488

MAXIMUM GRADIENT = 0.0300151 RMS GRADIENT = 0.0109095
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0267662166
 PREDICTED ENERGY CHANGE WAS -0.0298954402 RATIO= 0.895
 NR STEP HAS LENGTH = 0.752618
 RADIUS OF STEP TAKEN= 0.42426 CURRENT TRUST RADIUS= 0.42426

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.01 , TOTAL = 626.1 SECONDS (10.4 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 577.0 SECONDS (9.6 MIN)
 CPU UTILIZATION: STEP = 62.20% , TOTAL = 100.00%

INSERCH= 3

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.0823884080	-1.5754984233	0.8895276775
C	6.0	4.8532607692	0.6293698632	0.4338885579
C	6.0	5.0502249785	-0.7141665600	0.1830749110
C	6.0	3.9337696521	-1.5568560758	0.0698402854
C	6.0	2.6292674316	-1.0945046757	0.2064067057
C	6.0	2.3700437413	0.3101592093	0.4753779254
C	6.0	3.5463354843	1.1554395030	0.5795795960
C	6.0	3.4323665363	2.5409541279	0.8218754004
C	6.0	2.1965001601	3.1664015699	0.9817666718
C	6.0	1.0418065995	2.3837943116	0.9001214631
C	6.0	1.1077438665	1.0086911979	0.6437322461
N	7.0	-0.0912050508	0.2633335740	0.6056374327
C	6.0	-1.2398671853	0.8272157214	0.5324158955
C	6.0	-2.4818718287	0.1032019708	0.5199970080
C	6.0	-2.6968658558	-1.3133214030	0.5153792585
C	6.0	-3.9715781746	-1.8724685094	0.5326480345
C	6.0	-5.0795157366	-1.0000016020	0.5422568558
C	6.0	-4.8985456522	0.3917275155	0.5275153700
C	6.0	-3.6235965125	0.9403786424	0.5216775945
O	8.0	-1.6115172418	-2.3126243949	0.5512736052
N	7.0	1.6000647495	-2.1280779939	-0.0073629201
H	1.0	5.6626937109	1.3461325779	0.5305920131
H	1.0	6.0512071003	-1.0999303907	0.0696514162
H	1.0	4.0545782934	-2.6113737146	-0.1529397295
H	1.0	4.3530154351	3.1366882171	0.8921636088
H	1.0	2.1134240023	4.2286398169	1.1855998802
H	1.0	0.0694272875	2.9072123618	1.0777818783
H	1.0	-1.3552552761	1.9535146180	0.4524501302
H	1.0	-4.0630885580	-2.9578106331	0.5213155890
H	1.0	-6.0698196075	-1.4466084797	0.5473144121
H	1.0	-5.7504053043	1.0775114078	0.5187983312
H	1.0	-3.4623170054	2.0203095960	0.5134048840
H	1.0	-1.8304593955	-2.9430908849	1.2745918766
H	1.0	1.4593968761	-2.2558482656	-1.0217456602
H	1.0	1.9543903028	-2.9873887956	0.4272787952

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.2754407	5.0912050	3.9376862
2 C	5.2754407	0.0000000	1.3808666 *	2.3994956 *
3 C	5.0912050	1.3808666 *	0.0000000	1.4033603 *

4 C	3.9376862	2.3994956 *	1.4033603 *	0.0000000
5 C	2.6804108 *	2.8230547 *	2.4507625 *	1.3907355 *
6 C	2.9934247 *	2.5039935 *	2.8841040 *	2.4688956 *
7 C	4.4218796	1.4163435 *	2.4319388 *	2.7868417 *
8 C	5.3077408	2.4132196 *	3.6907103	4.1963091
9 C	5.1926479	3.7141725	4.8826696	5.1145750
10 C	4.0738918	4.2216775	5.1165355	4.9579777
11 C	2.7910223 *	3.7705193	4.3270777	3.8597677
12 N	1.8686978 *	4.9609699	5.2505589	4.4497854
13 C	2.7656688 *	6.0971353	6.4856116	5.7152684
14 C	3.0870728	7.3544842	7.5838045	6.6422052
15 C	2.8165543 *	7.7964801	7.7773279	6.6500482
16 C	4.0804656	9.1731527	9.1025709	7.9251704
17 C	5.2054825	10.0661137	10.1401361	9.0428191
18 C	5.3675632	9.7551509	10.0159711	9.0562817
19 C	4.4943604	8.4830150	8.8367048	7.9720839
20 O	1.8780540 *	7.1036937	6.8607177	5.6172209
21 N	1.8474573 *	4.2873658	3.7334994	2.4038372 *
22 H	6.3090863	1.0854870 *	2.1773191 *	3.4101046
23 H	6.0436048	2.1349996 *	1.0787232 *	2.1661769 *
24 H	4.2353357	3.3889054	2.1687815 *	1.0845428 *
25 H	6.3594784	2.5974808 *	3.9771837	4.7834444
26 H	6.1563613	4.5854683	5.8361966	6.1668907
27 H	4.4866807	5.3374364	6.2227993	5.9897408
28 H	3.8355950	6.3481789	6.9440092	6.3594715
29 H	4.3853559	9.6112847	9.3915296	8.1311896
30 H	6.1630663	11.1191833	11.1500912	10.0155846
31 H	6.4185188	10.6134714	10.9533755	10.0461286
32 H	5.0632243	8.4314809	8.9470581	8.2276948
33 H	2.3827653 *	7.6250491	7.3145971	6.0497446
34 H	2.4519368 *	4.6863276	4.0893058	2.7933261 *
35 H	2.3898744 *	4.6351307	3.8485539	2.4682238 *

C C C C

1 CO	2.6804108 *	2.9934247 *	4.4218796	5.3077408
2 C	2.8230547 *	2.5039935 *	1.4163435 *	2.4132196 *
3 C	2.4507625 *	2.8841040 *	2.4319388 *	3.6907103
4 C	1.3907355 *	2.4688956 *	2.7868417 *	4.1963091
5 C	0.0000000	1.4534865 *	2.4581539 *	3.7736363
6 C	1.4534865 *	0.0000000	1.4522462 *	2.4950022 *
7 C	2.4581539 *	1.4522462 *	0.0000000	1.4111509 *
8 C	3.7736363	2.4950022 *	1.4111509 *	0.0000000
9 C	4.3524467	2.9059710 *	2.4551534 *	1.3943154 *
10 C	3.8858507	2.4989165 *	2.8078938 *	2.3969978 *
11 C	2.6324362 *	1.4524776 *	2.4438453 *	2.7898809 *

12 N	3.0666073	2.4651381 *	3.7454283	4.2011750
13 C	4.3323774	3.6471986	4.7976756	4.9850230
14 C	5.2589528	4.8565324	6.1196436	6.4040598
15 C	5.3395731	5.3207953	6.7139009	7.2468524
16 C	6.6545341	6.7069600	8.1049032	8.6244043
17 C	7.7166744	7.5641874	8.8911545	9.2232692
18 C	7.6798416	7.2692340	8.4795038	8.6087119
19 C	6.5831948	6.0268602	7.1733903	7.2414484
20 O	4.4257207	4.7683941	6.2154415	7.0050848
21 N	1.4741877 *	2.6020967 *	3.8618595	5.0837808
22 H	3.9068506	3.4522215	2.1254966 *	2.5469205 *
23 H	3.4246755	3.9628185	3.4089737	4.5475495
24 H	2.1122340 *	3.4304219	3.8708884	5.2805203
25 H	4.6200176	3.4778087	2.1618945 *	1.0988330 *
26 H	5.4369827	3.9905838	3.4445691	2.1725993 *
27 H	4.8296807	3.5214218	3.9250228	3.3924908
28 H	5.0226866	4.0717313	4.9677639	4.8376526
29 H	6.9540424	7.2157417	8.6501766	9.3009998
30 H	8.7128819	8.6210615	9.9620346	10.3086168
31 H	8.6622259	8.1567400	9.2972661	9.3035917
32 H	6.8486288	6.0780336	7.0621236	6.9211911
33 H	4.9444367	5.3727652	6.7963900	7.6142655
34 H	2.0556445 *	3.1072578	4.3077186	5.5046218
35 H	2.0216958 *	3.3239892	4.4407782	5.7360871

C C C N

1 CO	5.1926479	4.0738918	2.7910223 *	1.8686978 *
2 C	3.7141725	4.2216775	3.7705193	4.9609699
3 C	4.8826696	5.1165355	4.3270777	5.2505589
4 C	5.1145750	4.9579777	3.8597677	4.4497854
5 C	4.3524467	3.8858507	2.6324362 *	3.0666073
6 C	2.9059710 *	2.4989165 *	1.4524776 *	2.4651381 *
7 C	2.4551534 *	2.8078938 *	2.4438453 *	3.7454283
8 C	1.3943154 *	2.3969978 *	2.7898809 *	4.2011750
9 C	0.0000000	1.3973036 *	2.4403630 *	3.7152217
10 C	1.3973036 *	0.0000000	1.4003541 *	2.4221457 *
11 C	2.4403630 *	1.4003541 *	0.0000000	1.4122633 *
12 N	3.7152217	2.4221457 *	1.4122633 *	0.0000000
13 C	4.1811873	2.7864277 *	2.3572446 *	1.2816978 *
14 C	5.6110237	4.2144876	3.7041277	2.3975538 *
15 C	6.6505989	5.2720359	4.4590663	3.0468764
16 C	7.9772871	6.5867167	5.8406278	4.4299293
17 C	8.3959807	7.0034798	6.5059454	5.1461905
18 C	7.6318304	6.2765397	6.0390119	4.8096894
19 C	6.2482306	4.8982298	4.7334074	3.5976699

20	O	6.6862580	5.4053835	4.2934912	2.9916323 *
21	N	5.4190060	4.6359650	3.2412383	2.9924926 *
22	H	3.9409942	4.7503570	4.5688331	5.8553767
23	H	5.8217101	6.1579308	5.4049683	6.3146652
24	H	6.1743583	5.9276838	4.7353341	5.1016567
25	H	2.1585805 *	3.3957350	3.8886858	5.2999396
26	H	1.0848040 *	2.1525140 *	3.4165893	4.5738823
27	H	2.1449562 *	1.1185040 *	2.2070077 *	2.6905052 *
28	H	3.7902820	2.4761777 *	2.6449282 *	2.1161288 *
29	H	8.7692897	7.3983912	6.5181002	5.1145614
30	H	9.4763206	8.0852759	7.5865150	6.2186120
31	H	8.2298911	6.9271874	6.8596323	5.7181268
32	H	5.7926765	4.5352839	4.6825008	3.8026132
33	H	7.3231174	6.0634846	4.9646353	3.7085932
34	H	5.8273644	5.0392696	3.6816701	3.3762434
35	H	6.1834626	5.4686376	4.0905156	3.8449276

C C C C

1	CO	2.7656688 *	3.0870728	2.8165543 *	4.0804656
2	C	6.0971353	7.3544842	7.7964801	9.1731527
3	C	6.4856116	7.5838045	7.7773279	9.1025709
4	C	5.7152684	6.6422052	6.6500482	7.9251704
5	C	4.3323774	5.2589528	5.3395731	6.6545341
6	C	3.6471986	4.8565324	5.3207953	6.7069600
7	C	4.7976756	6.1196436	6.7139009	8.1049032
8	C	4.9850230	6.4040598	7.2468524	8.6244043
9	C	4.1811873	5.6110237	6.6505989	7.9772871
10	C	2.7864277 *	4.2144876	5.2720359	6.5867167
11	C	2.3572446 *	3.7041277	4.4590663	5.8406278
12	N	1.2816978 *	2.3975538 *	3.0468764	4.4299293
13	C	0.0000000	1.4376807 *	2.5894081 *	3.8406432
14	C	1.4376807 *	0.0000000	1.4327534 *	2.4744007 *
15	C	2.5894081 *	1.4327534 *	0.0000000	1.3920615 *
16	C	3.8406432	2.4744007 *	1.3920615 *	0.0000000
17	C	4.2522607	2.8222876 *	2.4033127 *	1.4102540 *
18	C	3.6845084	2.4338480 *	2.7847321 *	2.4466055 *
19	C	2.3864381 *	1.4157694 *	2.4368080 *	2.8343113 *
20	O	3.1618152	2.5680172 *	1.4757630 *	2.4008273 *
21	N	4.1340459	4.6817652	4.4046226	5.6035839
22	H	6.9220391	8.2388674	8.7724092	10.1576863
23	H	7.5556474	8.6292395	8.7620197	10.0631708
24	H	6.3501782	7.1096375	6.9075023	8.0892026
25	H	6.0616349	7.4870709	8.3453807	9.7221274
26	H	4.8208813	6.2112002	7.3689496	8.6415925
27	H	2.5175508 *	3.8318045	5.0775565	6.2826941

28 H	1.1350146 *	2.1673681 *	3.5321518	4.6357010
29 H	4.7219833	3.4452933	2.1379767 *	1.0892521 *
30 H	5.3384397	3.9084560	3.3757373	2.1410719 *
31 H	4.5174979	3.4106585	3.8781692	3.4448221
32 H	2.5225221 *	2.1532807 *	3.4203823	3.9259952
33 H	3.8877804	3.2052538	1.9957987 *	2.5062128 *
34 H	4.3825481	4.8451716	4.5305220	5.6620323
35 H	4.9764990	5.4074735	4.9441326	6.0308583

C C C O

1 CO	5.2054825	5.3675632	4.4943604	1.8780540 *
2 C	10.0661137	9.7551509	8.4830150	7.1036937
3 C	10.1401361	10.0159711	8.8367048	6.8607177
4 C	9.0428191	9.0562817	7.9720839	5.6172209
5 C	7.7166744	7.6798416	6.5831948	4.4257207
6 C	7.5641874	7.2692340	6.0268602	4.7683941
7 C	8.8911545	8.4795038	7.1733903	6.2154415
8 C	9.2232692	8.6087119	7.2414484	7.0050848
9 C	8.3959807	7.6318304	6.2482306	6.6862580
10 C	7.0034798	6.2765397	4.8982298	5.4053835
11 C	6.5059454	6.0390119	4.7334074	4.2934912
12 N	5.1461905	4.8096894	3.5976699	2.9916323 *
13 C	4.2522607	3.6845084	2.3864381 *	3.1618152
14 C	2.8222876 *	2.4338480 *	1.4157694 *	2.5680172 *
15 C	2.4033127 *	2.7847321 *	2.4368080 *	1.4757630 *
16 C	1.4102540 *	2.4466055 *	2.8343113 *	2.4008273 *
17 C	0.0000000	1.4035232 *	2.4259431 *	3.7081091
18 C	1.4035232 *	0.0000000	1.3880012 *	4.2565995
19 C	2.4259431 *	1.3880012 *	0.0000000	3.8250971
20 O	3.7081091	4.2565995	3.8250971	0.0000000
21 N	6.7964280	6.9905259	6.0812784	3.2650254
22 H	10.9954329	10.6042763	9.2951548	8.1425472
23 H	11.1411998	11.0603693	9.8979298	7.7730259
24 H	9.3011554	9.4678437	8.4867203	5.7175000
25 H	10.3056917	9.6570782	8.2817494	8.0862144
26 H	8.9157705	8.0201427	6.6458151	7.5541839
27 H	6.4857322	5.5956423	4.2209136	5.5090363
28 H	4.7540971	3.8729473	2.4852784 *	4.2749712
29 H	2.2060324 *	3.4521635	3.9228858	2.5352248 *
30 H	1.0863632 *	2.1798518 *	3.4179485	4.5416362
31 H	2.1832781 *	1.0936363 *	2.1312272 *	5.3501841
32 H	3.4261413	2.1714584 *	1.0919388 *	4.7118161
33 H	3.8559406	4.5926344	4.3432196	0.9841814 *
34 H	6.8396369	7.0592705	6.1995841	3.4508154
35 H	7.3101821	7.6414138	6.8227711	3.6313053

	N	H	H	H
1 CO	1.8474573 *	6.3090863	6.0436048	4.2353357
2 C	4.2873658	1.0854870 *	2.1349996 *	3.3889054
3 C	3.7334994	2.1773191 *	1.0787232 *	2.1687815 *
4 C	2.4038372 *	3.4101046	2.1661769 *	1.0845428 *
5 C	1.4741877 *	3.9068506	3.4246755	2.1122340 *
6 C	2.6020967 *	3.4522215	3.9628185	3.4304219
7 C	3.8618595	2.1254966 *	3.4089737	3.8708884
8 C	5.0837808	2.5469205 *	4.5475495	5.2805203
9 C	5.4190060	3.9409942	5.8217101	6.1743583
10 C	4.6359650	4.7503570	6.1579308	5.9276838
11 C	3.2412383	4.5688331	5.4049683	4.7353341
12 N	2.9924926 *	5.8553767	6.3146652	5.1016567
13 C	4.1340459	6.9220391	7.5556474	6.3501782
14 C	4.6817652	8.2388674	8.6292395	7.1096375
15 C	4.4046226	8.7724092	8.7620197	6.9075023
16 C	5.6035839	10.1576863	10.0631708	8.0892026
17 C	6.7964280	10.9954329	11.1411998	9.3011554
18 C	6.9905259	10.6042763	11.0603693	9.4678437
19 C	6.0812784	9.2951548	9.8979298	8.4867203
20 O	3.2650254	8.1425472	7.7730259	5.7175000
21 N	0.0000000	5.3725682	4.5689919	2.5058739 *
22 H	5.3725682	0.0000000	2.5192525 *	4.3260960
23 H	4.5689919	2.5192525 *	0.0000000	2.5140673 *
24 H	2.5058739 *	4.3260960	2.5140673 *	0.0000000
25 H	6.0087976	2.2476834 *	4.6378140	5.8499164
26 H	6.4880320	4.6190041	6.7190131	7.2350227
27 H	5.3735034	5.8327537	7.2701589	6.9174342
28 H	5.0601129	7.0446169	8.0203333	7.1042946
29 H	5.7479790	10.6355467	10.2934298	8.1529844
30 H	7.7200514	12.0603296	12.1353878	10.2152076
31 H	8.0362964	11.4162658	12.0092065	10.4974668
32 H	6.5656704	9.1498978	10.0219736	8.8543899
33 H	3.7518196	8.6659285	8.1835071	6.0647796
34 H	1.0320296 *	5.7490628	4.8592196	2.7597443 *
35 H	1.0260970 *	5.7045241	4.5248541	2.2110700 *

	H	H	H	H
1 CO	6.3594784	6.1563613	4.4866807	3.8355950
2 C	2.5974808 *	4.5854683	5.3374364	6.3481789
3 C	3.9771837	5.8361966	6.2227993	6.9440092
4 C	4.7834444	6.1668907	5.9897408	6.3594715
5 C	4.6200176	5.4369827	4.8296807	5.0226866

6 C	3.4778087	3.9905838	3.5214218	4.0717313
7 C	2.1618945 *	3.4445691	3.9250228	4.9677639
8 C	1.0988330 *	2.1725993 *	3.3924908	4.8376526
9 C	2.1585805 *	1.0848040 *	2.1449562 *	3.7902820
10 C	3.3957350	2.1525140 *	1.1185040 *	2.4761777 *
11 C	3.8886858	3.4165893	2.2070077 *	2.6449282 *
12 N	5.2999396	4.5738823	2.6905052 *	2.1161288 *
13 C	6.0616349	4.8208813	2.5175508 *	1.1350146 *
14 C	7.4870709	6.2112002	3.8318045	2.1673681 *
15 C	8.3453807	7.3689496	5.0775565	3.5321518
16 C	9.7221274	8.6415925	6.2826941	4.6357010
17 C	10.3056917	8.9157705	6.4857322	4.7540971
18 C	9.6570782	8.0201427	5.5956423	3.8729473
19 C	8.2817494	6.6458151	4.2209136	2.4852784 *
20 O	8.0862144	7.5541839	5.5090363	4.2749712
21 N	6.0087976	6.4880320	5.3735034	5.0601129
22 H	2.2476834 *	4.6190041	5.8327537	7.0446169
23 H	4.6378140	6.7190131	7.2701589	8.0203333
24 H	5.8499164	7.2350227	6.9174342	7.1042946
25 H	0.0000000	2.5088310 *	4.2937444	5.8461613
26 H	2.5088310 *	0.0000000	2.4363329 *	4.2125336
27 H	4.2937444	2.4363329 *	0.0000000	1.8249108 *
28 H	5.8461613	4.2125336	1.8249108 *	0.0000000
29 H	10.3976560	9.4992448	7.1962377	5.6087627
30 H	11.3912695	9.9790444	7.5450317	5.8135147
31 H	10.3178836	8.4978848	6.1262321	4.4820896
32 H	7.9037447	6.0346878	3.6848793	2.1090012 *
33 H	8.6801686	8.1850997	6.1542141	4.9878333
34 H	6.4121390	6.8810400	5.7443212	5.2739222
35 H	6.5934695	7.2575073	6.2227456	5.9470088

H H H H

1 CO	4.3853559	6.1630663	6.4185188	5.0632243
2 C	9.6112847	11.1191833	10.6134714	8.4314809
3 C	9.3915296	11.1500912	10.9533755	8.9470581
4 C	8.1311896	10.0155846	10.0461286	8.2276948
5 C	6.9540424	8.7128819	8.6622259	6.8486288
6 C	7.2157417	8.6210615	8.1567400	6.0780336
7 C	8.6501766	9.9620346	9.2972661	7.0621236
8 C	9.3009998	10.3086168	9.3035917	6.9211911
9 C	8.7692897	9.4763206	8.2298911	5.7926765
10 C	7.3983912	8.0852759	6.9271874	4.5352839
11 C	6.5181002	7.5865150	6.8596323	4.6825008
12 N	5.1145614	6.2186120	5.7181268	3.8026132
13 C	4.7219833	5.3384397	4.5174979	2.5225221 *

14 C	3.4452933	3.9084560	3.4106585	2.1532807 *
15 C	2.1379767 *	3.3757373	3.8781692	3.4203823
16 C	1.0892521 *	2.1410719 *	3.4448221	3.9259952
17 C	2.2060324 *	1.0863632 *	2.1832781 *	3.4261413
18 C	3.4521635	2.1798518 *	1.0936363 *	2.1714584 *
19 C	3.9228858	3.4179485	2.1312272 *	1.0919388 *
20 O	2.5352248 *	4.5416362	5.3501841	4.7118161
21 N	5.7479790	7.7200514	8.0362964	6.5656704
22 H	10.6355467	12.0603296	11.4162658	9.1498978
23 H	10.2934298	12.1353878	12.0092065	10.0219736
24 H	8.1529844	10.2152076	10.4974668	8.8543899
25 H	10.3976560	11.3912695	10.3178836	7.9037447
26 H	9.4992448	9.9790444	8.4978848	6.0346878
27 H	7.1962377	7.5450317	6.1262321	3.6848793
28 H	5.6087627	5.8135147	4.4820896	2.1090012 *
29 H	0.0000000	2.5122455 *	4.3738848	5.0142467
30 H	2.5122455 *	0.0000000	2.5444095 *	4.3381725
31 H	4.3738848	2.5444095 *	0.0000000	2.4747213 *
32 H	5.0142467	4.3381725	2.4747213 *	0.0000000
33 H	2.3563266 *	4.5541813	5.6659017	5.2799346
34 H	5.7768187	7.7334287	8.0910945	6.6981700
35 H	6.0182863	8.1716802	8.7118118	7.3773423

H H H

1 CO	2.3827653 *	2.4519368 *	2.3898744 *
2 C	7.6250491	4.6863276	4.6351307
3 C	7.3145971	4.0893058	3.8485539
4 C	6.0497446	2.7933261 *	2.4682238 *
5 C	4.9444367	2.0556445 *	2.0216958 *
6 C	5.3727652	3.1072578	3.3239892
7 C	6.7963900	4.3077186	4.4407782
8 C	7.6142655	5.5046218	5.7360871
9 C	7.3231174	5.8273644	6.1834626
10 C	6.0634846	5.0392696	5.4686376
11 C	4.9646353	3.6816701	4.0905156
12 N	3.7085932	3.3762434	3.8449276
13 C	3.8877804	4.3825481	4.9764990
14 C	3.2052538	4.8451716	5.4074735
15 C	1.9957987 *	4.5305220	4.9441326
16 C	2.5062128 *	5.6620323	6.0308583
17 C	3.8559406	6.8396369	7.3101821
18 C	4.5926344	7.0592705	7.6414138
19 C	4.3432196	6.1995841	6.8227711
20 O	0.9841814 *	3.4508154	3.6313053
21 N	3.7518196	1.0320296 *	1.0260970 *

22 H	8.6659285	5.7490628	5.7045241
23 H	8.1835071	4.8592196	4.5248541
24 H	6.0647796	2.7597443 *	2.2110700 *
25 H	8.6801686	6.4121390	6.5934695
26 H	8.1850997	6.8810400	7.2575073
27 H	6.1542141	5.7443212	6.2227456
28 H	4.9878333	5.2739222	5.9470088
29 H	2.3563266 *	5.7768187	6.0182863
30 H	4.5541813	7.7334287	8.1716802
31 H	5.6659017	8.0910945	8.7118118
32 H	5.2799346	6.6981700	7.3773423
33 H	0.0000000	4.0704573	3.8787871
34 H	4.0704573	0.0000000	1.6970097 *
35 H	3.8787871	1.6970097 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.81 , TOTAL = 626.9 SECONDS (10.4 MIN)
WALL CLOCK TIME: STEP = 0.80 , TOTAL = 577.8 SECONDS (9.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.53 , TOTAL = 628.5 SECONDS (10.5 MIN)
WALL CLOCK TIME: STEP = 1.53 , TOTAL = 579.4 SECONDS (9.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.565871761	-284.565871761	3.708830103	0.025238020	207110560
10613635						
2	1	-284.579347951	-0.013476190	1.859823564	0.005465678	198631146
11362645						
3	2	-284.579491495	-0.000143544	1.291463717	0.005669022	194752719
11730200						
4	3	-284.581703810	-0.002212315	1.130232159	0.003472482	190692231
12054566						
5	4	-284.581688335	0.000015475	0.030655173	0.002884255	188737759
12233446						

6 5	-284.581933847	-0.000245512	0.612270501	0.001059171	173399566
13516775					
7 6	-284.581937097	-0.000003250	0.110912769	0.000893935	183333534
12700270					
8 7	-284.581970407	-0.000033310	0.266850975	0.000454716	170616570
13791765					
9 8	-284.581972826	-0.000002419	0.094113716	0.000539391	176444765
13285086					
10 9	-284.581981601	-0.000008774	0.140322342	0.000268242	167418681
14060075					
11 10	-284.581985397	-0.000003796	0.006064997	0.000264607	189659995
12176621					
12 11	-284.581991232	-0.000005834	0.120438276	0.000259856	172260872
13731621					
13 12	-284.581996839	-0.000005607	0.004990585	0.000280632	205430206
10823994					
14 13	-284.582000305	-0.000003466	0.036142163	0.000254198	191654511
12044166					

-----DISABLING FDIFF OPTION-----

15 14	-284.582003495	-0.000003189	0.007180347	0.000145863	206558301
10667789					
16 15	-284.582006882	-0.000003387	0.023683714	0.000101215	206560013
10667643					
17 16	-284.582007724	-0.000000842	0.011659924	0.000098733	206552569
10668313					
18 17	-284.582008398	-0.000000673	0.022582584	0.000072956	206555431
10668098					
19 18	-284.582008926	-0.000000528	0.005409271	0.000045114	206562064
10667590					
20 19	-284.582009201	-0.000000275	0.009923978	0.000035269	206561060
10667668					
21 20	-284.582009280	-0.000000079	0.001246716	0.000027775	206558196
10667911					
22 21	-284.582009328	-0.000000047	0.003103478	0.000020950	206558243
10667888					
23 22	-284.582009366	-0.000000038	0.005729670	0.000017888	206557525
10667927					
24 23	-284.582009415	-0.000000049	0.002482138	0.000018017	206556187
10668041					
25 24	-284.582009452	-0.000000037	0.004074655	0.000021983	206556727
10668006					
26 25	-284.582009464	-0.000000012	0.000662245	0.000009005	206557736
10667928					
27 26	-284.582009469	-0.000000005	0.001097594	0.000008067	206557824
10667918					

28 27	-284.582009471	-0.000000001	0.000291414	0.000003865	206558162
10667892					
29 28	-284.582009471	-0.000000001	0.000829268	0.000002140	206558142
10667894					
30 29	-284.582009471	0.000000000	0.000439293	0.000000909	206558031
10667906					
31 30	-284.582009471	0.000000000	0.000122657	0.000001062	206557973
10667911					
32 31	-284.582009471	0.000000000	0.000112482	0.000000402	206558024
10667904					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 114.3 SECONDS (3.6 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 35.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.2, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 3.9 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.5820094713 AFTER 32 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.9006672498
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000220061

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 119.08 , TOTAL = 747.5 SECONDS (12.5 MIN)
WALL CLOCK TIME: STEP = 109.90 , TOTAL = 689.3 SECONDS (11.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.78 , TOTAL = 751.3 SECONDS (12.5 MIN)
WALL CLOCK TIME: STEP = 3.77 , TOTAL = 693.0 SECONDS (11.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.93 , TOTAL = 754.3 SECONDS (12.6 MIN)

WALL CLOCK TIME: STEP = 2.85 , TOTAL = 695.9 SECONDS (11.6 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 3 ENERGY= -284.5820095

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0041835	-0.0009348	-0.0142769
2 C	6.0	-0.0027101	-0.0027076	-0.0006983
3 C	6.0	-0.0113285	-0.0029806	-0.0007931
4 C	6.0	0.0057604	0.0054021	-0.0000083
5 C	6.0	-0.0099645	-0.0204665	-0.0024249
6 C	6.0	0.0043886	-0.0022397	0.0004460
7 C	6.0	0.0058764	0.0080330	0.0014930
8 C	6.0	-0.0035751	-0.0236754	-0.0042260
9 C	6.0	-0.0123746	-0.0025558	0.0001244
10 C	6.0	0.0215671	-0.0082704	-0.0033305
11 C	6.0	-0.0111793	0.0022427	0.0004262
12 N	7.0	-0.0291210	0.0054072	-0.0034615
13 C	6.0	0.0396578	-0.0298598	0.0068419
14 C	6.0	-0.0032061	0.0074133	0.0025553
15 C	6.0	0.0072314	0.0003742	-0.0022229
16 C	6.0	-0.0048414	-0.0039623	0.0023186
17 C	6.0	0.0067162	0.0091305	0.0011773
18 C	6.0	0.0194742	-0.0101213	-0.0003839
19 C	6.0	-0.0025770	-0.0001459	0.0022719
20 O	8.0	0.0074916	-0.0122642	-0.0134297
21 N	7.0	-0.0144929	0.0047394	0.0076772
22 H	1.0	-0.0146788	-0.0037849	0.0001141
23 H	1.0	-0.0164839	0.0089357	0.0023153
24 H	1.0	-0.0074707	0.0159020	0.0031885
25 H	1.0	-0.0038205	-0.0020353	-0.0002440
26 H	1.0	-0.0009928	-0.0134629	-0.0022137
27 H	1.0	-0.0097742	0.0066439	0.0015350

28 H	1.0	-0.0042324	0.0201436	0.0001033
29 H	1.0	0.0068952	0.0109816	0.0004091
30 H	1.0	0.0140547	0.0021505	-0.0001923
31 H	1.0	0.0089366	-0.0014116	-0.0005212
32 H	1.0	0.0022382	-0.0088685	0.0001022
33 H	1.0	0.0096778	0.0188816	0.0022202
34 H	1.0	0.0033697	0.0080386	0.0064531
35 H	1.0	-0.0046958	0.0153275	0.0066546

MAXIMUM GRADIENT = 0.0396578 RMS GRADIENT = 0.0099888
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0230331280
 PREDICTED ENERGY CHANGE WAS -0.0288434667 RATIO= 0.799
 GDIIS STEP HAS LENGTH = 0.669873
 RADIUS OF STEP TAKEN= 0.50000 CURRENT TRUST RADIUS= 0.50000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 754.3 SECONDS (12.6 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 695.9 SECONDS (11.6 MIN)
 CPU UTILIZATION: STEP = 99.51%, TOTAL = 100.00%

INSERCH= 4

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1034635766	-1.6190266251	0.9434452535
C	6.0	4.8898610833	0.6260423514	0.4320418005
C	6.0	5.0887941969	-0.7276413270	0.1803672517
C	6.0	3.9555794146	-1.5862652103	0.0680897921
C	6.0	2.6567015182	-1.0953583942	0.2026271590
C	6.0	2.3844879906	0.3200910694	0.4736374383
C	6.0	3.5743446997	1.1619777242	0.5802091192
C	6.0	3.4571019317	2.5887394084	0.8297900155
C	6.0	2.2134080869	3.2085830602	0.9872509948
C	6.0	1.0141253279	2.4087934800	0.9053917379
C	6.0	1.1239291031	1.0175736811	0.6431692233
N	7.0	-0.0733089989	0.2644278076	0.6085290631
C	6.0	-1.2855415471	0.8601845159	0.5160513681
C	6.0	-2.5130652096	0.1036365588	0.5061444647
C	6.0	-2.7265623483	-1.3179275305	0.5106958646
C	6.0	-3.9978436050	-1.8850597821	0.5270866612
C	6.0	-5.1153590136	-1.0088142114	0.5397444220
C	6.0	-4.9461529053	0.4031819522	0.5288841728

C	6.0	-3.6549454274	0.9621462506	0.5179647661
O	8.0	-1.6344331909	-2.3016592476	0.6107754169
N	7.0	1.6285039692	-2.1554522780	-0.0306413248
H	1.0	5.7007766632	1.3692808307	0.5328726787
H	1.0	6.0982334932	-1.1249689524	0.0632638270
H	1.0	4.0675571973	-2.6518350196	-0.1610237805
H	1.0	4.3967302194	3.1560999596	0.8938409961
H	1.0	2.1109607705	4.3062297067	1.1994081691
H	1.0	0.0233855647	2.9165915714	1.0842726684
H	1.0	-1.3505598471	1.9682229337	0.4482201903
H	1.0	-4.0769089826	-3.0084406552	0.5185124095
H	1.0	-6.1032679966	-1.4562257821	0.5479755140
H	1.0	-5.7817976993	1.0936918882	0.5194472618
H	1.0	-3.4544069040	2.0498607534	0.5129893639
H	1.0	-1.8543229679	-3.0145090102	1.2612879715
H	1.0	1.4493624233	-2.2839445300	-1.0438282430
H	1.0	1.9671664132	-3.0271219479	0.4043933126

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3114470	5.1215600	3.9504578
2 C	5.3114470	0.0000000	1.3911772 *	2.4289191 *
3 C	5.1215600	1.3911772 *	0.0000000	1.4261897 *
4 C	3.9504578	2.4289191 *	1.4261897 *	0.0000000
5 C	2.7096243 *	2.8289315 *	2.4598346 *	1.3950533 *
6 C	3.0305064	2.5243278 *	2.9149653 *	2.5033960 *
7 C	4.4623919	1.4282029 *	2.4544024 *	2.8214261 *
8 C	5.3819237	2.4623530 *	3.7526725	4.2730938
9 C	5.2687380	3.7604753	4.9409280	5.1836848
10 C	4.1296595	4.2922709	5.1928615	5.0312743
11 C	2.8430928 *	3.7921122	4.3566175	3.8895934
12 N	1.9211502 *	4.9794548	5.2739770	4.4664394
13 C	2.8737586 *	6.1804108	6.5776919	5.8013046
14 C	3.1630718	7.4217058	7.6541113	6.7000764
15 C	2.8787114 *	7.8609867	7.8445747	6.7021581
16 C	4.1309622	9.2361227	9.1666143	7.9722578
17 C	5.2698617	10.1384804	10.2143503	9.1015291
18 C	5.4552557	9.8390150	10.1044737	9.1329661
19 C	4.5792057	8.5518458	8.9119210	8.0384623
20 O	1.8965605 *	7.1533068	6.9184225	5.6616727
21 N	1.8874176 *	4.3112919	3.7492369	2.3977076 *
22 H	6.3583382	1.1046060 *	2.2126602 *	3.4636670
23 H	6.0791511	2.1592132 *	1.0911233 *	2.1917536 *

24 H	4.2427094	3.4310917	2.2049930 *	1.0956601 *
25 H	6.4215600	2.6187073 *	4.0089205	4.8338914
26 H	6.2613277	4.6749243	5.9368168	6.2772602
27 H	4.5385105	5.4179890	6.3052235	6.0638680
28 H	3.9022803	6.3831469	6.9860368	6.3979683
29 H	4.4256699	9.6757382	9.4512699	8.1698429
30 H	6.2214482	11.1891987	11.2217747	10.0711276
31 H	6.4942218	10.6822580	11.0273296	10.1095206
32 H	5.1287883	8.4652596	8.9895184	8.2660296
33 H	2.4251440 *	7.7087795	7.3895216	6.1007022
34 H	2.4905452 *	4.7416502	4.1432111	2.8291769 *
35 H	2.3972271 *	4.6785166	3.8836013	2.4784984 *

C C C C

1 CO	2.7096243 *	3.0305064	4.4623919	5.3819237
2 C	2.8289315 *	2.5243278 *	1.4282029 *	2.4623530 *
3 C	2.4598346 *	2.9149653 *	2.4544024 *	3.7526725
4 C	1.3950533 *	2.5033960 *	2.8214261 *	4.2730938
5 C	0.0000000	1.4666438 *	2.4658069 *	3.8218517
6 C	1.4666438 *	0.0000000	1.4614683 *	2.5345829 *
7 C	2.4658069 *	1.4614683 *	0.0000000	1.4531639 *
8 C	3.8218517	2.5345829 *	1.4531639 *	0.0000000
9 C	4.3972782	2.9387843 *	2.4912697 *	1.3984901 *
10 C	3.9333211	2.5351496 *	2.8661850 *	2.4507613 *
11 C	2.6472534 *	1.4505970 *	2.4554741 *	2.8190574 *
12 N	3.0768055	2.4621251 *	3.7565643	4.2326330
13 C	4.4117642	3.7098001	4.8696704	5.0575687
14 C	5.3156561	4.9024419	6.1791691	6.4748265
15 C	5.3966632	5.3672445	6.7717200	7.3213094
16 C	6.7090888	6.7527553	8.1624319	8.6995817
17 C	7.7798498	7.6169590	8.9568368	9.3012690
18 C	7.7559952	7.3313200	8.5543723	8.6880319
19 C	6.6460252	6.0736279	7.2323193	7.3023461
20 O	4.4761126	4.8004280	6.2553243	7.0631223
21 N	1.4951266 *	2.6370673 *	3.8941978	5.1566915
22 H	3.9306363	3.4788042	2.1370373 *	2.5708589 *
23 H	3.4444798	4.0060592	3.4449052	4.6211220
24 H	2.1319886 *	3.4738828	3.9163570	5.3682388
25 H	4.6454682	3.5026613	2.1797262 *	1.0995007 *
26 H	5.5198333	4.0608942	3.5229562	2.2132525 *
27 H	4.8792821	3.5622317	3.9927510	3.4587074
28 H	5.0501475	4.0825932	4.9922076	4.8625351
29 H	7.0072232	7.2684791	8.7142343	9.3907741
30 H	8.7741983	8.6719565	10.0255781	10.3846924
31 H	8.7235649	8.2029738	9.3565889	9.3642269

32 H	6.8799981	6.0898559	7.0849279	6.9397195
33 H	5.0153010	5.4504559	6.8831201	7.7326462
34 H	2.1033439 *	3.1556558	4.3620439	5.5932559
35 H	2.0610383 *	3.3738386	4.4902661	5.8256990

C C C N

1 CO	5.2687380	4.1296595	2.8430928 *	1.9211502 *
2 C	3.7604753	4.2922709	3.7921122	4.9794548
3 C	4.9409280	5.1928615	4.3566175	5.2739770
4 C	5.1836848	5.0312743	3.8895934	4.4664394
5 C	4.3972782	3.9333211	2.6472534 *	3.0768055
6 C	2.9387843 *	2.5351496 *	1.4505970 *	2.4621251 *
7 C	2.4912697 *	2.8661850 *	2.4554741 *	3.7565643
8 C	1.3984901 *	2.4507613 *	2.8190574 *	4.2326330
9 C	0.0000000	1.4438294 *	2.4710077 *	3.7470729
10 C	1.4438294 *	0.0000000	1.4199683 *	2.4225906 *
11 C	2.4710077 *	1.4199683 *	0.0000000	1.4148525 *
12 N	3.7470729	2.4225906 *	1.4148525 *	0.0000000
13 C	4.2402421	2.7996863 *	2.4179494 *	1.3538781 *
14 C	5.6755358	4.2325193	3.7525704	2.4471916 *
15 C	6.7171207	5.2949956	4.5053745	3.0908208
16 C	8.0459056	6.6106069	5.8882350	4.4753661
17 C	8.4674393	7.0273977	6.5609192	5.2007831
18 C	7.7032259	6.2999327	6.1021663	4.8754696
19 C	6.3011333	4.9033774	4.7808357	3.6500866
20 O	6.7312990	5.4120260	4.3158915	3.0036505
21 N	5.4910011	4.6995700	3.2827900	3.0266361
22 H	3.9687822	4.8149826	4.5916660	5.8793273
23 H	5.8928171	6.2485848	5.4470619	6.3494625
24 H	6.2530716	6.0058845	4.7724452	5.1228482
25 H	2.1859496 *	3.4641906	3.9175704	5.3314558
26 H	1.1226461 *	2.2112797 *	3.4783461	4.6320984
27 H	2.2115313 *	1.1275738 *	2.2387580 *	2.6962297 *
28 H	3.8119437	2.4484371 *	2.6579757 *	2.1354125 *
29 H	8.8565901	7.4441072	6.5782253	5.1719033
30 H	9.5457061	8.1069975	7.6394452	6.2709426
31 H	8.2834124	6.9327495	6.9072544	5.7690951
32 H	5.8044542	4.5000658	4.6950744	3.8247512
33 H	7.4396510	6.1454754	5.0507175	3.7880776
34 H	5.9056674	5.1000667	3.7218127	3.3975012
35 H	6.2677249	5.5415217	4.1385536	3.8780809

C C C C

1 CO	2.8737586 *	3.1630718	2.8787114 *	4.1309622
------	-------------	-----------	-------------	-----------

2 C	6.1804108	7.4217058	7.8609867	9.2361227
3 C	6.5776919	7.6541113	7.8445747	9.1666143
4 C	5.8013046	6.7000764	6.7021581	7.9722578
5 C	4.4117642	5.3156561	5.3966632	6.7090888
6 C	3.7098001	4.9024419	5.3672445	6.7527553
7 C	4.8696704	6.1791691	6.7717200	8.1624319
8 C	5.0575687	6.4748265	7.3213094	8.6995817
9 C	4.2402421	5.6755358	6.7171207	8.0459056
10 C	2.7996863 *	4.2325193	5.2949956	6.6106069
11 C	2.4179494 *	3.7525704	4.5053745	5.8882350
12 N	1.3538781 *	2.4471916 *	3.0908208	4.4753661
13 C	0.0000000	1.4419699 *	2.6116550 *	3.8591541
14 C	1.4419699 *	0.0000000	1.4375139 *	2.4819183 *
15 C	2.6116550 *	1.4375139 *	0.0000000	1.3921436 *
16 C	3.8591541	2.4819183 *	1.3921436 *	0.0000000
17 C	4.2615982	2.8303019 *	2.4088886 *	1.4201434 *
18 C	3.6890502	2.4515628 *	2.8087597 *	2.4769627 *
19 C	2.3715975 *	1.4286599 *	2.4618457 *	2.8677944 *
20 O	3.1824447	2.5628870 *	1.4732583 *	2.4013054 *
21 N	4.2290187	4.7480750	4.4677843	5.6603851
22 H	7.0048629	8.3108223	8.8454295	10.2300538
23 H	7.6593723	8.7097692	8.8382380	10.1352673
24 H	6.4380415	7.1653561	6.9563336	8.1309366
25 H	6.1402089	7.5639351	8.4205118	9.7988096
26 H	4.8865562	6.2868132	7.4503087	8.7236215
27 H	2.5029933 *	3.8315181	5.0815702	6.2878133
28 H	1.1120151 *	2.1980574 *	3.5631546	4.6756945
29 H	4.7705344	3.4829276	2.1636385 *	1.1261925 *
30 H	5.3457707	3.9146490	3.3797422	2.1487547 *
31 H	4.5023168	3.4154061	3.8923576	3.4721048
32 H	2.4737251 *	2.1619342 *	3.4455422	3.9722943
33 H	3.9864947	3.2752122	2.0500192 *	2.5316769 *
34 H	4.4495473	4.8789130	4.5593949	5.6832153
35 H	5.0698844	5.4666697	4.9963722	6.0745950

C C C O

1 CO	5.2698617	5.4552557	4.5792057	1.8965605 *
2 C	10.1384804	9.8390150	8.5518458	7.1533068
3 C	10.2143503	10.1044737	8.9119210	6.9184225
4 C	9.1015291	9.1329661	8.0384623	5.6616727
5 C	7.7798498	7.7559952	6.6460252	4.4761126
6 C	7.6169590	7.3313200	6.0736279	4.8004280
7 C	8.9568368	8.5543723	7.2323193	6.2553243
8 C	9.3012690	8.6880319	7.3023461	7.0631223
9 C	8.4674393	7.7032259	6.3011333	6.7312990

10 C	7.0273977	6.2999327	4.9033774	5.4120260
11 C	6.5609192	6.1021663	4.7808357	4.3158915
12 N	5.2007831	4.8754696	3.6500866	3.0036505
13 C	4.2615982	3.6890502	2.3715975 *	3.1824447
14 C	2.8303019 *	2.4515628 *	1.4286599 *	2.5628870 *
15 C	2.4088886 *	2.8087597 *	2.4618457 *	1.4732583 *
16 C	1.4201434 *	2.4769627 *	2.8677944 *	2.4013054 *
17 C	0.0000000	1.4221399 *	2.4531546 *	3.7139384
18 C	1.4221399 *	0.0000000	1.4070455 *	4.2767230
19 C	2.4531546 *	1.4070455 *	0.0000000	3.8397278
20 O	3.7139384	4.2767230	3.8397278	0.0000000
21 N	6.8643868	7.0771315	6.1591580	3.3285959
22 H	11.0744830	10.6906722	9.3645884	8.2028759
23 H	11.2243121	11.1593243	9.9843529	7.8408229
24 H	9.3550277	9.5423305	8.5532995	5.7646328
25 H	10.3899825	9.7468567	8.3536936	8.1389308
26 H	8.9946954	8.0923567	6.7002189	7.6183109
27 H	6.4893773	5.5966058	4.2036508	5.4956987
28 H	4.8005041	3.9222633	2.5154021 *	4.2823944
29 H	2.2532943 *	3.5206337	3.9929455	2.5443546 *
30 H	1.0845317 *	2.1901317 *	3.4414688	4.5485367
31 H	2.2056936 *	1.0840642 *	2.1309169 *	5.3607259
32 H	3.4806566	2.2219608 *	1.1060575 *	4.7177953
33 H	3.8958687	4.6665232	4.4281551	0.9897843 *
34 H	6.8723524	7.1131350	6.2474204	3.4996889
35 H	7.3657350	7.7185793	6.8945849	3.6797295

N H H H

1 CO	1.8874176 *	6.3583382	6.0791511	4.2427094
2 C	4.3112919	1.1046060 *	2.1592132 *	3.4310917
3 C	3.7492369	2.2126602 *	1.0911233 *	2.2049930 *
4 C	2.3977076 *	3.4636670	2.1917536 *	1.0956601 *
5 C	1.4951266 *	3.9306363	3.4444798	2.1319886 *
6 C	2.6370673 *	3.4788042	4.0060592	3.4738828
7 C	3.8941978	2.1370373 *	3.4449052	3.9163570
8 C	5.1566915	2.5708589 *	4.6211220	5.3682388
9 C	5.4910011	3.9687822	5.8928171	6.2530716
10 C	4.6995700	4.8149826	6.2485848	6.0058845
11 C	3.2827900	4.5916660	5.4470619	4.7724452
12 N	3.0266361	5.8793273	6.3494625	5.1228482
13 C	4.2290187	7.0048629	7.6593723	6.4380415
14 C	4.7480750	8.3108223	8.7097692	7.1653561
15 C	4.4677843	8.8454295	8.8382380	6.9563336
16 C	5.6603851	10.2300538	10.1352673	8.1309366
17 C	6.8643868	11.0744830	11.2243121	9.3550277

18 C	7.0771315	10.6906722	11.1593243	9.5423305
19 C	6.1591580	9.3645884	9.9843529	8.5532995
20 O	3.3285959	8.2028759	7.8408229	5.7646328
21 N	0.0000000	5.4152282	4.5879403	2.4924639 *
22 H	5.4152282	0.0000000	2.5690049 *	4.3952555
23 H	4.5879403	2.5690049 *	0.0000000	2.5505433 *
24 H	2.4924639 *	4.3952555	2.5505433 *	0.0000000
25 H	6.0605554	2.2413295 *	4.6810814	5.9121234
26 H	6.5953863	4.6857994	6.8327949	7.3548426
27 H	5.4355374	5.9102438	7.3675266	6.9938160
28 H	5.1096797	7.0772342	8.0746857	7.1464751
29 H	5.7949026	10.7129729	10.3580037	8.1805419
30 H	7.7848579	12.1375115	12.2156177	10.2653712
31 H	8.1100004	11.4858889	12.0940357	10.5594415
32 H	6.6193787	9.1804668	10.0764446	8.8960767
33 H	3.8127606	8.7651430	8.2612818	6.1010792
34 H	1.0368942 *	5.8229343	4.9174058	2.7874058 *
35 H	1.0313852 *	5.7692902	4.5607314	2.2073011 *

H H H H

1 CO	6.4215600	6.2613277	4.5385105	3.9022803
2 C	2.6187073 *	4.6749243	5.4179890	6.3831469
3 C	4.0089205	5.9368168	6.3052235	6.9860368
4 C	4.8338914	6.2772602	6.0638680	6.3979683
5 C	4.6454682	5.5198333	4.8792821	5.0501475
6 C	3.5026613	4.0608942	3.5622317	4.0825932
7 C	2.1797262 *	3.5229562	3.9927510	4.9922076
8 C	1.0995007 *	2.2132525 *	3.4587074	4.8625351
9 C	2.1859496 *	1.1226461 *	2.2115313 *	3.8119437
10 C	3.4641906	2.2112797 *	1.1275738 *	2.4484371 *
11 C	3.9175704	3.4783461	2.2387580 *	2.6579757 *
12 N	5.3314558	4.6320984	2.6962297 *	2.1354125 *
13 C	6.1402089	4.8865562	2.5029933 *	1.1120151 *
14 C	7.5639351	6.2868132	3.8315181	2.1980574 *
15 C	8.4205118	7.4503087	5.0815702	3.5631546
16 C	9.7988096	8.7236215	6.2878133	4.6756945
17 C	10.3899825	8.9946954	6.4893773	4.8005041
18 C	9.7468567	8.0923567	5.5966058	3.9222633
19 C	8.3536936	6.7002189	4.2036508	2.5154021 *
20 O	8.1389308	7.6183109	5.4956987	4.2823944
21 N	6.0605554	6.5953863	5.4355374	5.1096797
22 H	2.2413295 *	4.6857994	5.9102438	7.0772342
23 H	4.6810814	6.8327949	7.3675266	8.0746857
24 H	5.9121234	7.3548426	6.9938160	7.1464751
25 H	0.0000000	2.5769966 *	4.3840360	5.8856582

26 H	2.5769966 *	0.0000000	2.5104423 *	4.2441353
27 H	4.3840360	2.5104423 *	0.0000000	1.7865307 *
28 H	5.8856582	4.2441353	1.7865307 *	0.0000000
29 H	10.4854658	9.6050900	7.2276211	5.6749538
30 H	11.4735842	10.0550391	7.5461931	5.8587571
31 H	10.3921186	8.5485895	6.1108219	4.5172720
32 H	7.9378314	6.0444759	3.6294114	2.1064264 *
33 H	8.7913081	8.3258945	6.2237511	5.0737042
34 H	6.4834885	6.9928691	5.7972234	5.3053465
35 H	6.6614242	7.3777213	6.2903299	5.9968908

H H H H

1 CO	4.4256699	6.2214482	6.4942218	5.1287883
2 C	9.6757382	11.1891987	10.6822580	8.4652596
3 C	9.4512699	11.2217747	11.0273296	8.9895184
4 C	8.1698429	10.0711276	10.1095206	8.2660296
5 C	7.0072232	8.7741983	8.7235649	6.8799981
6 C	7.2684791	8.6719565	8.2029738	6.0898559
7 C	8.7142343	10.0255781	9.3565889	7.0849279
8 C	9.3907741	10.3846924	9.3642269	6.9397195
9 C	8.8565901	9.5457061	8.2834124	5.8044542
10 C	7.4441072	8.1069975	6.9327495	4.5000658
11 C	6.5782253	7.6394452	6.9072544	4.6950744
12 N	5.1719033	6.2709426	5.7690951	3.8247512
13 C	4.7705344	5.3457707	4.5023168	2.4737251 *
14 C	3.4829276	3.9146490	3.4154061	2.1619342 *
15 C	2.1636385 *	3.3797422	3.8923576	3.4455422
16 C	1.1261925 *	2.1487547 *	3.4721048	3.9722943
17 C	2.2532943 *	1.0845317 *	2.2056936 *	3.4806566
18 C	3.5206337	2.1901317 *	1.0840642 *	2.2219608 *
19 C	3.9929455	3.4414688	2.1309169 *	1.1060575 *
20 O	2.5443546 *	4.5485367	5.3607259	4.7177953
21 N	5.7949026	7.7848579	8.1100004	6.6193787
22 H	10.7129729	12.1375115	11.4858889	9.1804668
23 H	10.3580037	12.2156177	12.0940357	10.0764446
24 H	8.1805419	10.2653712	10.5594415	8.8960767
25 H	10.4854658	11.4735842	10.3921186	7.9378314
26 H	9.6050900	10.0550391	8.5485895	6.0444759
27 H	7.2276211	7.5461931	6.1108219	3.6294114
28 H	5.6749538	5.8587571	4.5172720	2.1064264 *
29 H	0.0000000	2.5527181 *	4.4423122	5.0964647
30 H	2.5527181 *	0.0000000	2.5702601 *	4.3943523
31 H	4.4423122	2.5702601 *	0.0000000	2.5161575 *
32 H	5.0964647	4.3943523	2.5161575 *	0.0000000
33 H	2.3434250 *	4.5815494	5.7317275	5.3635865

34 H	5.7883917	7.7628077	8.1327692	6.7269981
35 H	6.0451815	8.2231528	8.7772882	7.4283917

H H H

1 CO	2.4251440 *	2.4905452 *	2.3972271 *
2 C	7.7087795	4.7416502	4.6785166
3 C	7.3895216	4.1432111	3.8836013
4 C	6.1007022	2.8291769 *	2.4784984 *
5 C	5.0153010	2.1033439 *	2.0610383 *
6 C	5.4504559	3.1556558	3.3738386
7 C	6.8831201	4.3620439	4.4902661
8 C	7.7326462	5.5932559	5.8256990
9 C	7.4396510	5.9056674	6.2677249
10 C	6.1454754	5.1000667	5.5415217
11 C	5.0507175	3.7218127	4.1385536
12 N	3.7880776	3.3975012	3.8780809
13 C	3.9864947	4.4495473	5.0698844
14 C	3.2752122	4.8789130	5.4666697
15 C	2.0500192 *	4.5593949	4.9963722
16 C	2.5316769 *	5.6832153	6.0745950
17 C	3.8958687	6.8723524	7.3657350
18 C	4.6665232	7.1131350	7.7185793
19 C	4.4281551	6.2474204	6.8945849
20 O	0.9897843 *	3.4996889	3.6797295
21 N	3.8127606	1.0368942 *	1.0313852 *
22 H	8.7651430	5.8229343	5.7692902
23 H	8.2612818	4.9174058	4.5607314
24 H	6.1010792	2.7874058 *	2.2073011 *
25 H	8.7913081	6.4834885	6.6614242
26 H	8.3258945	6.9928691	7.3777213
27 H	6.2237511	5.7972234	6.2903299
28 H	5.0737042	5.3053465	5.9968908
29 H	2.3434250 *	5.7883917	6.0451815
30 H	4.5815494	7.7628077	8.2231528
31 H	5.7317275	8.1327692	8.7772882
32 H	5.3635865	6.7269981	7.4283917
33 H	0.0000000	4.0940960	3.9164025
34 H	4.0940960	0.0000000	1.7081508 *
35 H	3.9164025	1.7081508 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.75 , TOTAL = 755.0 SECONDS (12.6 MIN)
WALL CLOCK TIME: STEP = 0.74 , TOTAL = 696.7 SECONDS (11.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.13 , TOTAL = 756.1 SECONDS (12.6 MIN)
WALL CLOCK TIME: STEP = 1.13 , TOTAL = 697.8 SECONDS (11.6 MIN)
CPU UTILIZATION: STEP = 99.97% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.581332946	-284.581332946	1.782215039	0.031157047	203902439
10884694						
2	1	-284.594362950	-0.013030004	0.550368422	0.006652200	193231536
11817804						
3	2	-284.593507130	0.000855820	0.580765126	0.012460257	186426771
12424727						
4	3	-284.596332924	-0.002825794	0.234513499	0.004125643	184800674
12561439						
5	4	-284.596225811	0.000107113	0.042093589	0.003390759	179035798
13047431						
6	5	-284.596582847	-0.000357035	0.098930776	0.000416507	168488911
13925155						
7	6	-284.596575879	0.000006967	0.008816410	0.000554542	171325119
13688601						
8	7	-284.596606427	-0.000030548	0.033370494	0.000238768	179154618
13023179						
9	8	-284.596607260	-0.000000832	0.006120309	0.000243438	181078467
12877015						
10	9	-284.596612639	-0.000005379	0.018321648	0.000167717	171290038
13699363						
11	10	-284.596615064	-0.000002426	0.004114353	0.000163435	193772246
11821650						
12	11	-284.596617788	-0.000002724	0.013448401	0.000153683	185253116
12671440						
-----DISABLING FDIFF OPTION-----						
13	12	-284.596619518	-0.000001730	0.006638367	0.000128719	203226396
10947236						

14 13	-284.596620915	-0.000001398	0.004995826	0.000128942	203222224
10947500					
15 14	-284.596621966	-0.000001050	0.004627436	0.000105456	203225110
10947280					
16 15	-284.596622803	-0.000000837	0.005620973	0.000074183	203227141
10947087					
17 16	-284.596623043	-0.000000240	0.001607346	0.000065295	203224327
10947308					
18 17	-284.596623212	-0.000000168	0.006700868	0.000038893	203225180
10947273					
19 18	-284.596623431	-0.000000220	0.001743236	0.000033106	203228370
10947013					
20 19	-284.596623590	-0.000000158	0.005329196	0.000030055	203228277
10947042					
21 20	-284.596623644	-0.000000054	0.001350631	0.000030569	203224630
10947265					
22 21	-284.596623690	-0.000000046	0.002245752	0.000027639	203225468
10947199					
23 22	-284.596623778	-0.000000088	0.002828775	0.000028798	203226710
10947107					
24 23	-284.596623826	-0.000000048	0.000627388	0.000016897	203225085
10947223					
25 24	-284.596623860	-0.000000033	0.001908641	0.000010098	203225198
10947239					
26 25	-284.596623874	-0.000000014	0.000283595	0.000007408	203225818
10947177					
27 26	-284.596623879	-0.000000005	0.000277018	0.000003732	203225554
10947189					
28 27	-284.596623880	-0.000000001	0.000053530	0.000002118	203225416
10947197					
29 28	-284.596623880	-0.000000001	0.000056317	0.000000895	203225379
10947198					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 102.4 SECONDS (3.5 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 31.8 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 3.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.5966238803 AFTER 29 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.7020684794
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999855797

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 106.65 , TOTAL = 862.8 SECONDS (14.4 MIN)
WALL CLOCK TIME: STEP = 98.14 , TOTAL = 795.9 SECONDS (13.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.72 , TOTAL = 866.5 SECONDS (14.4 MIN)
WALL CLOCK TIME: STEP = 3.69 , TOTAL = 799.6 SECONDS (13.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.95 , TOTAL = 869.5 SECONDS (14.5 MIN)
WALL CLOCK TIME: STEP = 2.79 , TOTAL = 802.4 SECONDS (13.4 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 4 ENERGY= -284.5966239

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0024835	-0.0138511	-0.0029390
2 C	6.0	-0.0021294	-0.0085184	-0.0018221
3 C	6.0	-0.0044087	0.0031038	-0.0003708
4 C	6.0	-0.0069556	-0.0081302	-0.0010128
5 C	6.0	-0.0018366	-0.0099949	0.0009612

6 C	6.0	-0.0097328	0.0003179	0.0012378
7 C	6.0	0.0091583	-0.0111148	-0.0016794
8 C	6.0	-0.0003306	0.0084705	0.0013495
9 C	6.0	0.0158484	-0.0085522	-0.0028149
10 C	6.0	-0.0167988	-0.0101868	-0.0016992
11 C	6.0	0.0057336	-0.0125865	-0.0031028
12 N	7.0	0.0329914	-0.0071348	-0.0000970
13 C	6.0	-0.0329168	0.0256900	-0.0016269
14 C	6.0	-0.0029070	-0.0049690	0.0006282
15 C	6.0	0.0020147	0.0013705	-0.0070908
16 C	6.0	0.0017878	0.0113375	0.0022997
17 C	6.0	-0.0006125	-0.0024529	0.0020721
18 C	6.0	-0.0037816	0.0000783	0.0000314
19 C	6.0	0.0047704	0.0087192	0.0035741
20 O	8.0	-0.0002011	-0.0098757	-0.0126062
21 N	7.0	-0.0019705	-0.0029428	-0.0023933
22 H	1.0	-0.0063368	0.0066748	0.0017337
23 H	1.0	-0.0082612	0.0047630	0.0011253
24 H	1.0	-0.0067077	0.0070578	0.0013038
25 H	1.0	-0.0016287	-0.0045539	-0.0008852
26 H	1.0	-0.0039855	0.0111657	0.0025999
27 H	1.0	-0.0174290	0.0075315	0.0018316
28 H	1.0	0.0021420	0.0087477	0.0025832
29 H	1.0	0.0062817	-0.0136350	-0.0002753
30 H	1.0	0.0154868	0.0028940	-0.0000511
31 H	1.0	0.0161869	-0.0040213	-0.0010927
32 H	1.0	0.0077277	0.0005589	0.0004226
33 H	1.0	0.0120733	0.0094041	0.0063522
34 H	1.0	0.0005451	0.0048294	0.0022663
35 H	1.0	-0.0063005	0.0098057	0.0091869

MAXIMUM GRADIENT = 0.0329914 RMS GRADIENT = 0.0085067
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0146144090
 PREDICTED ENERGY CHANGE WAS -0.0305776620 RATIO= 0.478
 GDIIS STEP HAS LENGTH = 0.323236
 RADIUS OF STEP TAKEN= 0.32324 CURRENT TRUST RADIUS= 0.50000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 869.5 SECONDS (14.5 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 802.4 SECONDS (13.4 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 5

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1094188652	-1.6168992131	0.9731827157
C	6.0	4.9119267538	0.6366025961	0.4337544911
C	6.0	5.1143889515	-0.7377058283	0.1798151034
C	6.0	3.9741097772	-1.5868432137	0.0691448009
C	6.0	2.6746242224	-1.0785636930	0.1997997853
C	6.0	2.4064740817	0.3216224455	0.4704069866
C	6.0	3.5733874961	1.1803140355	0.5827798863
C	6.0	3.4637057187	2.6029564399	0.8324998614
C	6.0	2.2027441185	3.2379683319	0.9932760528
C	6.0	1.0208957551	2.4462057092	0.9128865027
C	6.0	1.1212453672	1.0347186128	0.6464356906
N	7.0	-0.0978589803	0.2670829303	0.6114524346
C	6.0	-1.2773253552	0.8455412691	0.5093355089
C	6.0	-2.5191777494	0.1163855983	0.4986654097
C	6.0	-2.7472198751	-1.3240518980	0.5194039914
C	6.0	-4.0144573321	-1.9081408603	0.5208926734
C	6.0	-5.1279512238	-1.0123469684	0.5353826665
C	6.0	-4.9669632654	0.4117839065	0.5294517559
C	6.0	-3.6733112694	0.9574363710	0.5107764364
O	8.0	-1.6424612191	-2.2797961050	0.6559012691
N	7.0	1.6441674675	-2.1642095314	-0.0385311539
H	1.0	5.7280641724	1.3697479064	0.5312785280
H	1.0	6.1332007980	-1.1440905975	0.0585192844
H	1.0	4.0841936052	-2.6828145732	-0.1670602924
H	1.0	4.4210029427	3.1726867500	0.8960369916
H	1.0	2.1154478499	4.3265046346	1.2021118886
H	1.0	0.0323110325	2.9068421153	1.0836434391
H	1.0	-1.3511093284	1.9590895048	0.4424999284
H	1.0	-4.0928474262	-3.0106543416	0.5176097997
H	1.0	-6.1438839514	-1.4654510614	0.5483660012
H	1.0	-5.8199831878	1.1063592499	0.5214214683
H	1.0	-3.4624072619	2.0635990453	0.5121613754
H	1.0	-1.8850045268	-3.0647250303	1.2476703520
H	1.0	1.4436766881	-2.3047187581	-1.0577203171
H	1.0	1.9829732883	-3.0613307792	0.3796356841

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3322917	5.1431643	3.9691339

2 C	5.3322917	0.0000000	1.4121614 *	2.4405229 *
3 C	5.1431643	1.4121614 *	0.0000000	1.4260150 *
4 C	3.9691339	2.4405229 *	1.4260150 *	0.0000000
5 C	2.7328016 *	2.8287900 *	2.4635412 *	1.4014569 *
6 C	3.0474764	2.5254404 *	2.9222291 *	2.5021459 *
7 C	4.4694401	1.4524180 *	2.4931639 *	2.8428082 *
8 C	5.3924219	2.4744473 *	3.7829588	4.2892475
9 C	5.2869796	3.7973463	4.9945350	5.2221223
10 C	4.1645225	4.3179107	5.2374968	5.0694040
11 C	2.8568573 *	3.8174592	4.3936794	3.9172294
12 N	1.9295600 *	5.0265370	5.3257337	4.5068913
13 C	2.8638832 *	6.1932390	6.5931227	5.8041221
14 C	3.1841738	7.4495740	7.6878136	6.7266826
15 C	2.9072426 *	7.9065814	7.8907551	6.7415180
16 C	4.1588151	9.2824375	9.2098907	8.0077783
17 C	5.2902928	10.1748962	10.2521894	9.1320829
18 C	5.4847158	9.8819112	10.1526959	9.1732862
19 C	4.5989206	8.5915760	8.9558203	8.0716446
20 O	1.8997852 *	7.1773764	6.9469220	5.6894935
21 N	1.9179590 *	4.3296481	3.7583274	2.4028269 *
22 H	6.3784415	1.1014051 *	2.2229451 *	3.4686243
23 H	6.1111460	2.1916158 *	1.1035574 *	2.2040456 *
24 H	4.2702651	3.4734206	2.2282444 *	1.1265276 *
25 H	6.4448307	2.6242016 *	4.0354588	4.8514523
26 H	6.2769905	4.6931913	5.9736895	6.3012635
27 H	4.5257467	5.4209771	6.3187935	6.0630184
28 H	3.8990335	6.4011459	7.0103050	6.4086653
29 H	4.4507462	9.7157333	9.4896576	8.2039111
30 H	6.2695456	11.2544532	11.2877877	10.1300635
31 H	6.5404918	10.7425438	11.0940419	10.1677013
32 H	5.1494223	8.4954068	9.0287982	8.2960098
33 H	2.4797717 *	7.7820666	7.4529754	6.1564826
34 H	2.5254518 *	4.7858779	4.1786543	2.8615139 *
35 H	2.4390340 *	4.7176698	3.9044750	2.4970268 *

C C C C

1 CO	2.7328016 *	3.0474764	4.4694401	5.3924219
2 C	2.8287900 *	2.5254404 *	1.4524180 *	2.4744473 *
3 C	2.4635412 *	2.9222291 *	2.4931639 *	3.7829588
4 C	1.4014569 *	2.5021459 *	2.8428082 *	4.2892475
5 C	0.0000000	1.4510872 *	2.4610928 *	3.8179248
6 C	1.4510872 *	0.0000000	1.4531572 *	2.5403415 *
7 C	2.4610928 *	1.4531572 *	0.0000000	1.4485515 *
8 C	3.8179248	2.5403415 *	1.4485515 *	0.0000000
9 C	4.4141504	2.9698436 *	2.5062146 *	1.4209550 *

10	C	3.9581953	2.5747756 *	2.8682166 *	2.4491536 *
11	C	2.6605322 *	1.4803057 *	2.4572853 *	2.8250859 *
12	N	3.1091616	2.5088947 *	3.7832346	4.2649631
13	C	4.4063474	3.7210731	4.8628060	5.0665885
14	C	5.3378651	4.9300068	6.1853351	6.4876324
15	C	5.4368010	5.4102871	6.7989663	7.3549317
16	C	6.7479709	6.7972607	8.1925437	8.7389943
17	C	7.8100694	7.6518796	8.9734778	9.3260531
18	C	7.7925391	7.3742250	8.5750262	8.7160343
19	C	6.6737012	6.1130744	7.2504829	7.3313201
20	O	4.5042441	4.8161877	6.2596155	7.0672060
21	N	1.5156747 *	2.6494320 *	3.9107231	5.1764163
22	H	3.9277988	3.4835661	2.1636010 *	2.5959308 *
23	H	3.4620811	4.0257246	3.4971918	4.6653629
24	H	2.1668163 *	3.4996784	3.9682422	5.4151178
25	H	4.6484100	3.5168246	2.1877228 *	1.1158170 *
26	H	5.5255834	4.0815646	3.5224530	2.2192410 *
27	H	4.8627624	3.5631545	3.9712701	3.4539672
28	H	5.0490366	4.0989645	4.9876687	4.8733057
29	H	7.0450444	7.3039357	8.7372548	9.4187726
30	H	8.8338704	8.7354640	10.0710785	10.4373584
31	H	8.7769974	8.2639587	9.3938622	9.4086903
32	H	6.9017325	6.1220907	7.0913741	6.9544636
33	H	5.0826257	5.5216190	6.9466884	7.8040811
34	H	2.1447715 *	3.1874473	4.4014046	5.6337133
35	H	2.1076260 *	3.4105666	4.5345601	5.8721209

C C C N

1	CO	5.2869796	4.1645225	2.8568573 *	1.9295600 *
2	C	3.7973463	4.3179107	3.8174592	5.0265370
3	C	4.9945350	5.2374968	4.3936794	5.3257337
4	C	5.2221223	5.0694040	3.9172294	4.5068913
5	C	4.4141504	3.9581953	2.6605322 *	3.1091616
6	C	2.9698436 *	2.5747756 *	1.4803057 *	2.5088947 *
7	C	2.5062146 *	2.8682166 *	2.4572853 *	3.7832346
8	C	1.4209550 *	2.4491536 *	2.8250859 *	4.2649631
9	C	0.0000000	1.4248214 *	2.4787592 *	3.7768670
10	C	1.4248214 *	0.0000000	1.4399173 *	2.4680054 *
11	C	2.4787592 *	1.4399173 *	0.0000000	1.4410773 *
12	N	3.7768670	2.4680054 *	1.4410773 *	0.0000000
13	C	4.2507398	2.8296290 *	2.4099224 *	1.3176429 *
14	C	5.6820300	4.2581406	3.7573730	2.4286241 *
15	C	6.7482388	5.3449384	4.5326547	3.0918111
16	C	8.0845024	6.6684911	5.9204413	4.4810202
17	C	8.4861028	7.0648719	6.5768737	5.1908145

18 C	7.7205670	6.3356412	6.1211124	4.8719441
19 C	6.3215235	4.9410228	4.7970980	3.6428811
20 O	6.7338808	5.4308936	4.3155731	2.9789872 *
21 N	5.5281244	4.7486411	3.3129697	3.0607708
22 H	4.0164127	4.8437403	4.6204205	5.9298970
23 H	5.9602601	6.3052227	5.4965946	6.4127414
24 H	6.3199607	6.0709907	4.8229546	5.1766342
25 H	2.2213485 *	3.4768934	3.9397473	5.3799289
26 H	1.1118203 *	2.1948165 *	3.4832556	4.6611705
27 H	2.1974054 *	1.1039219 *	2.2094739 *	2.6848160 *
28 H	3.8169045	2.4667699 *	2.6473740 *	2.1123607 *
29 H	8.8829059	7.4889208	6.6006365	5.1683944
30 H	9.5909488	8.1711690	7.6839163	6.2896798
31 H	8.3144788	6.9818377	6.9427239	5.7840467
32 H	5.8055624	4.5174079	4.6996272	3.8154310
33 H	7.5165384	6.2391261	5.1190292	3.8340066
34 H	5.9585359	5.1607478	3.7629711	3.4317100
35 H	6.3329316	5.6163073	4.1942077	3.9321673

C C C C

1 CO	2.8638832 *	3.1841738	2.9072426 *	4.1588151
2 C	6.1932390	7.4495740	7.9065814	9.2824375
3 C	6.5931227	7.6878136	7.8907551	9.2098907
4 C	5.8041221	6.7266826	6.7415180	8.0077783
5 C	4.4063474	5.3378651	5.4368010	6.7479709
6 C	3.7210731	4.9300068	5.4102871	6.7972607
7 C	4.8628060	6.1853351	6.7989663	8.1925437
8 C	5.0665885	6.4876324	7.3549317	8.7389943
9 C	4.2507398	5.6820300	6.7482388	8.0845024
10 C	2.8296290 *	4.2581406	5.3449384	6.6684911
11 C	2.4099224 *	3.7573730	4.5326547	5.9204413
12 N	1.3176429 *	2.4286241 *	3.0918111	4.4810202
13 C	0.0000000	1.4401317 *	2.6206537 *	3.8826267
14 C	1.4401317 *	0.0000000	1.4585244 *	2.5169550 *
15 C	2.6206537 *	1.4585244 *	0.0000000	1.3953684 *
16 C	3.8826267	2.5169550 *	1.3953684 *	0.0000000
17 C	4.2754820	2.8427248 *	2.4011033 *	1.4291694 *
18 C	3.7151013	2.4657376 *	2.8178871 *	2.5078660 *
19 C	2.3985977 *	1.4281237 *	2.4622974 *	2.8858302 *
20 O	3.1500063	2.5563728 *	1.4671640 *	2.4047288 *
21 N	4.2301156	4.7773568	4.5057118	5.6919734
22 H	7.0250094	8.3420010	8.8930950	10.2791725
23 H	7.6862064	8.7547806	8.8941932	10.1868802
24 H	6.4538897	7.2030011	6.9989770	8.1646522
25 H	6.1673406	7.5937467	8.4702969	9.8545691

26 H	4.9099852	6.3007693	7.4860147	8.7698690
27 H	2.5087723 *	3.8260870	5.0935864	6.3148305
28 H	1.1179896 *	2.1824519 *	3.5684810	4.6962792
29 H	4.7746704	3.5007391	2.1576247 *	1.1053017 *
30 H	5.3875413	3.9551451	3.3997293	2.1751291 *
31 H	4.5501552	3.4461402	3.9177515	3.5138490
32 H	2.5016506 *	2.1636784 *	3.4623293	4.0099318
33 H	4.0254931	3.3290613	2.0745434 *	2.5299134 *
34 H	4.4478820	4.8977850	4.5839549	5.6956580
35 H	5.0901885	5.5119337	5.0410714	6.1089258

C C C O

1 CO	5.2902928	5.4847158	4.5989206	1.8997852 *
2 C	10.1748962	9.8819112	8.5915760	7.1773764
3 C	10.2521894	10.1526959	8.9558203	6.9469220
4 C	9.1320829	9.1732862	8.0716446	5.6894935
5 C	7.8100694	7.7925391	6.6737012	4.5042441
6 C	7.6518796	7.3742250	6.1130744	4.8161877
7 C	8.9734778	8.5750262	7.2504829	6.2596155
8 C	9.3260531	8.7160343	7.3313201	7.0672060
9 C	8.4861028	7.7205670	6.3215235	6.7338808
10 C	7.0648719	6.3356412	4.9410228	5.4308936
11 C	6.5768737	6.1211124	4.7970980	4.3155731
12 N	5.1908145	4.8719441	3.6428811	2.9789872 *
13 C	4.2754820	3.7151013	2.3985977 *	3.1500063
14 C	2.8427248 *	2.4657376 *	1.4281237 *	2.5563728 *
15 C	2.4011033 *	2.8178871 *	2.4622974 *	1.4671640 *
16 C	1.4291694 *	2.5078660 *	2.8858302 *	2.4047288 *
17 C	0.0000000	1.4332135 *	2.4488016 *	3.7107402
18 C	1.4332135 *	0.0000000	1.4041442 *	4.2793582
19 C	2.4488016 *	1.4041442 *	0.0000000	3.8242760
20 O	3.7107402	4.2793582	3.8242760	0.0000000
21 N	6.8933124	7.1179629	6.1904759	3.3611791
22 H	11.1142909	10.7378448	9.4104347	8.2255302
23 H	11.2720140	11.2185634	10.0393541	7.8808383
24 H	9.3886900	9.5908868	8.5959160	5.7995056
25 H	10.4320230	9.7923888	8.4008144	8.1579919
26 H	9.0230092	8.1202252	6.7333719	7.6199367
27 H	6.5029947	5.6147295	4.2261088	5.4670871
28 H	4.8065161	3.9339694	2.5299392 *	4.2542423
29 H	2.2505528 *	3.5323225	3.9902132	2.5607950 *
30 H	1.1124708 *	2.2157417 *	3.4605673	4.5757544
31 H	2.2289054 *	1.1000647 *	2.1518577 *	5.3792028
32 H	3.4980023	2.2343860 *	1.1260898 *	4.7114696
33 H	3.9033720	4.7011086	4.4630523	1.0124877 *

34 H	6.8843660	7.1410648	6.2678069	3.5300662
35 H	7.4018808	7.7708808	6.9398301	3.7189911

	N	H	H	H
--	---	---	---	---

1 CO	1.9179590 *	6.3784415	6.1111460	4.2702651
2 C	4.3296481	1.1014051 *	2.1916158 *	3.4734206
3 C	3.7583274	2.2229451 *	1.1035574 *	2.2282444 *
4 C	2.4028269 *	3.4686243	2.2040456 *	1.1265276 *
5 C	1.5156747 *	3.9277988	3.4620811	2.1668163 *
6 C	2.6494320 *	3.4835661	4.0257246	3.4996784
7 C	3.9107231	2.1636010 *	3.4971918	3.9682422
8 C	5.1764163	2.5959308 *	4.6653629	5.4151178
9 C	5.5281244	4.0164127	5.9602601	6.3199607
10 C	4.7486411	4.8437403	6.3052227	6.0709907
11 C	3.3129697	4.6204205	5.4965946	4.8229546
12 N	3.0607708	5.9298970	6.4127414	5.1766342
13 C	4.2301156	7.0250094	7.6862064	6.4538897
14 C	4.7773568	8.3420010	8.7547806	7.2030011
15 C	4.5057118	8.8930950	8.8941932	6.9989770
16 C	5.6919734	10.2791725	10.1868802	8.1646522
17 C	6.8933124	11.1142909	11.2720140	9.3886900
18 C	7.1179629	10.7378448	11.2185634	9.5908868
19 C	6.1904759	9.4104347	10.0393541	8.5959160
20 O	3.3611791	8.2255302	7.8808383	5.7995056
21 N	0.0000000	5.4306308	4.6045067	2.4978388 *
22 H	5.4306308	0.0000000	2.5897917 *	4.4286849
23 H	4.6045067	2.5897917 *	0.0000000	2.5723507 *
24 H	2.4978388 *	4.4286849	2.5723507 *	0.0000000
25 H	6.0882423	2.2565563 *	4.7188583	5.9607476
26 H	6.6250035	4.7162935	6.8831355	7.4081812
27 H	5.4380991	5.9253160	7.3947137	7.0161438
28 H	5.1190496	7.1042172	8.1112309	7.1736570
29 H	5.8257275	10.7535304	10.4051375	8.2122014
30 H	7.8413300	12.2058100	12.2910550	10.3250849
31 H	8.1684584	11.5510549	12.1719929	10.6265970
32 H	6.6524231	9.2166458	10.1277223	8.9409714
33 H	3.8626801	8.8394899	8.3303381	6.1464335
34 H	1.0481822 *	5.8636677	4.9582946	2.8122164 *
35 H	1.0461737 *	5.8037195	4.5829373	2.2039233 *

	H	H	H	H
--	---	---	---	---

1 CO	6.4448307	6.2769905	4.5257467	3.8990335
2 C	2.6242016 *	4.6931913	5.4209771	6.4011459
3 C	4.0354588	5.9736895	6.3187935	7.0103050

4 C	4.8514523	6.3012635	6.0630184	6.4086653
5 C	4.6484100	5.5255834	4.8627624	5.0490366
6 C	3.5168246	4.0815646	3.5631545	4.0989645
7 C	2.1877228 *	3.5224530	3.9712701	4.9876687
8 C	1.1158170 *	2.2192410 *	3.4539672	4.8733057
9 C	2.2213485 *	1.1118203 *	2.1974054 *	3.8169045
10 C	3.4768934	2.1948165 *	1.1039219 *	2.4667699 *
11 C	3.9397473	3.4832556	2.2094739 *	2.6473740 *
12 N	5.3799289	4.6611705	2.6848160 *	2.1123607 *
13 C	6.1673406	4.9099852	2.5087723 *	1.1179896 *
14 C	7.5937467	6.3007693	3.8260870	2.1824519 *
15 C	8.4702969	7.4860147	5.0935864	3.5684810
16 C	9.8545691	8.7698690	6.3148305	4.6962792
17 C	10.4320230	9.0230092	6.5029947	4.8065161
18 C	9.7923888	8.1202252	5.6147295	3.9339694
19 C	8.4008144	6.7333719	4.2261088	2.5299392 *
20 O	8.1579919	7.6199367	5.4670871	4.2542423
21 N	6.0882423	6.6250035	5.4380991	5.1190496
22 H	2.2565563 *	4.7162935	5.9253160	7.1042172
23 H	4.7188583	6.8831355	7.3947137	8.1112309
24 H	5.9607476	7.4081812	7.0161438	7.1736570
25 H	0.0000000	2.5962592 *	4.4007370	5.9157243
26 H	2.5962592 *	0.0000000	2.5236750 *	4.2659915
27 H	4.4007370	2.5236750 *	0.0000000	1.7953139 *
28 H	5.9157243	4.2659915	1.7953139 *	0.0000000
29 H	10.5291292	9.6356305	7.2356127	5.6763653
30 H	11.5433978	10.1089414	7.5860961	5.8914662
31 H	10.4540826	8.5909104	6.1487543	4.5501880
32 H	7.9702944	6.0588152	3.6401520	2.1150305 *
33 H	8.8766369	8.4045209	6.2739635	5.1158632
34 H	6.5332695	7.0378435	5.8084213	5.3142780
35 H	6.7136900	7.4346573	6.3182116	6.0269958

H H H H

1 CO	4.4507462	6.2695456	6.5404918	5.1494223
2 C	9.7157333	11.2544532	10.7425438	8.4954068
3 C	9.4896576	11.2877877	11.0940419	9.0287982
4 C	8.2039111	10.1300635	10.1677013	8.2960098
5 C	7.0450444	8.8338704	8.7769974	6.9017325
6 C	7.3039357	8.7354640	8.2639587	6.1220907
7 C	8.7372548	10.0710785	9.3938622	7.0913741
8 C	9.4187726	10.4373584	9.4086903	6.9544636
9 C	8.8829059	9.5909488	8.3144788	5.8055624
10 C	7.4889208	8.1711690	6.9818377	4.5174079
11 C	6.6006365	7.6839163	6.9427239	4.6996272

12 N	5.1683944	6.2896798	5.7840467	3.8154310
13 C	4.7746704	5.3875413	4.5501552	2.5016506 *
14 C	3.5007391	3.9551451	3.4461402	2.1636784 *
15 C	2.1576247 *	3.3997293	3.9177515	3.4623293
16 C	1.1053017 *	2.1751291 *	3.5138490	4.0099318
17 C	2.2505528 *	1.1124708 *	2.2289054 *	3.4980023
18 C	3.5323225	2.2157417 *	1.1000647 *	2.2343860 *
19 C	3.9902132	3.4605673	2.1518577 *	1.1260898 *
20 O	2.5607950 *	4.5757544	5.3792028	4.7114696
21 N	5.8257275	7.8413300	8.1684584	6.6524231
22 H	10.7535304	12.2058100	11.5510549	9.2166458
23 H	10.4051375	12.2910550	12.1719929	10.1277223
24 H	8.2122014	10.3250849	10.6265970	8.9409714
25 H	10.5291292	11.5433978	10.4540826	7.9702944
26 H	9.6356305	10.1089414	8.5909104	6.0588152
27 H	7.2356127	7.5860961	6.1487543	3.6401520
28 H	5.6763653	5.8914662	4.5501880	2.1150305 *
29 H	0.0000000	2.5681413 *	4.4646179	5.1132702
30 H	2.5681413 *	0.0000000	2.5922666 *	4.4323608
31 H	4.4646179	2.5922666 *	0.0000000	2.5445153 *
32 H	5.1132702	4.4323608	2.5445153 *	0.0000000
33 H	2.3260443 *	4.6026903	5.7800898	5.4156145
34 H	5.7994059	7.8009589	8.1786244	6.7539906
35 H	6.0775984	8.2837860	8.8473653	7.4789463

H H H

1 CO	2.4797717 *	2.5254518 *	2.4390340 *
2 C	7.7820666	4.7858779	4.7176698
3 C	7.4529754	4.1786543	3.9044750
4 C	6.1564826	2.8615139 *	2.4970268 *
5 C	5.0826257	2.1447715 *	2.1076260 *
6 C	5.5216190	3.1874473	3.4105666
7 C	6.9466884	4.4014046	4.5345601
8 C	7.8040811	5.6337133	5.8721209
9 C	7.5165384	5.9585359	6.3329316
10 C	6.2391261	5.1607478	5.6163073
11 C	5.1190292	3.7629711	4.1942077
12 N	3.8340066	3.4317100	3.9321673
13 C	4.0254931	4.4478820	5.0901885
14 C	3.3290613	4.8977850	5.5119337
15 C	2.0745434 *	4.5839549	5.0410714
16 C	2.5299134 *	5.6956580	6.1089258
17 C	3.9033720	6.8843660	7.4018808
18 C	4.7011086	7.1410648	7.7708808
19 C	4.4630523	6.2678069	6.9398301

20	O	1.0124877 *	3.5300662	3.7189911
21	N	3.8626801	1.0481822 *	1.0461737 *
22	H	8.8394899	5.8636677	5.8037195
23	H	8.3303381	4.9582946	4.5829373
24	H	6.1464335	2.8122164 *	2.2039233 *
25	H	8.8766369	6.5332695	6.7136900
26	H	8.4045209	7.0378435	7.4346573
27	H	6.2739635	5.8084213	6.3182116
28	H	5.1158632	5.3142780	6.0269958
29	H	2.3260443 *	5.7994059	6.0775984
30	H	4.6026903	7.8009589	8.2837860
31	H	5.7800898	8.1786244	8.8473653
32	H	5.4156145	6.7539906	7.4789463
33	H	0.0000000	4.1197760	3.9641832
34	H	4.1197760	0.0000000	1.7115183 *
35	H	3.9641832	1.7115183 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.82 , TOTAL = 870.3 SECONDS (14.5 MIN)
WALL CLOCK TIME: STEP = 0.82 , TOTAL = 803.2 SECONDS (13.4 MIN)
CPU UTILIZATION: STEP = 99.71% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.89 , TOTAL = 871.2 SECONDS (14.5 MIN)
WALL CLOCK TIME: STEP = 0.88 , TOTAL = 804.1 SECONDS (13.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.593752413	-284.593752413	2.190782564	0.013342808	201945375
11057099						
2	1	-284.602293038	-0.008540625	1.350002513	0.007478234	191339834
11969426						
3	2	-284.603324400	-0.001031362	0.748624126	0.003050980	187501677
12330799						

4 3	-284.603920397	-0.000595997	0.551281926	0.002959294	182094129
12783174					
5 4	-284.603972562	-0.000052165	0.083859362	0.002850034	178697803
13091750					
6 5	-284.604092791	-0.000120229	0.354423289	0.001183665	168702227
13883087					
7 6	-284.604105142	-0.000012351	0.027683906	0.000639027	174072694
13478456					
8 7	-284.604124079	-0.000018938	0.130362073	0.000370794	161121287
14516257					
9 8	-284.604126992	-0.000002912	0.053355501	0.000390303	165425454
14193997					
10 9	-284.604129471	-0.000002479	0.050250045	0.000131926	158350290
14786596					
11 10	-284.604130348	-0.000000877	0.002266660	0.000181448	156908372
14925777					
12 11	-284.604132271	-0.000001922	0.037664170	0.000144201	140806401
16240388					
13 12	-284.604136855	-0.000004584	0.005349274	0.000193166	178380371
13213313					
14 13	-284.604138187	-0.000001332	0.009007635	0.000193386	171361754
13771705					
15 14	-284.604139102	-0.000000915	0.009837897	0.000146486	186928807
12411668					

-----DISABLING FDIFF OPTION-----

16 15	-284.604139844	-0.000000742	0.016219763	0.000073392	201671463
11081645					
17 16	-284.604140145	-0.000000301	0.003730189	0.000042296	201665899
11082103					
18 17	-284.604140341	-0.000000196	0.009875092	0.000039721	201668199
11081998					
19 18	-284.604140401	-0.000000061	0.006132367	0.000036831	201670925
11081731					
20 19	-284.604140469	-0.000000068	0.002873208	0.000028850	201672790
11081543					
21 20	-284.604140556	-0.000000086	0.002990195	0.000030341	201673750
11081427					
22 21	-284.604140592	-0.000000036	0.004486551	0.000021629	201672542
11081537					
23 22	-284.604140617	-0.000000025	0.003246729	0.000016512	201671087
11081694					
24 23	-284.604140627	-0.000000010	0.001605622	0.000013485	201670419
11081770					
25 24	-284.604140633	-0.000000007	0.001124736	0.000014646	201669975
11081814					

26	25	-284.604140640	-0.000000006	0.002291280	0.000011362	201670353
11081787						
27	26	-284.604140643	-0.000000003	0.000563736	0.000003049	201670967
11081738						
28	27	-284.604140643	0.000000000	0.000254855	0.000001766	201671116
11081712						
29	28	-284.604140643	0.000000000	0.000320361	0.000001237	201671064
11081717						
30	29	-284.604140644	0.000000000	0.000064318	0.000000819	201671000
11081726						
31	30	-284.604140644	0.000000000	0.000066722	0.000000351	201671002
11081726						

 DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 108.5 SECONDS (3.5 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 34.0 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
 TIME TO SOLVE SCF EQUATIONS= 3.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6041406436 AFTER 31 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6156767755
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999848185

 SPIN SZ = 1.500
 S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
 PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 112.94 , TOTAL = 984.1 SECONDS (16.4 MIN)
 WALL CLOCK TIME: STEP = 103.57 , TOTAL = 907.7 SECONDS (15.1 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
 END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 3.74 , TOTAL = 987.9 SECONDS (16.5 MIN)

WALL CLOCK TIME: STEP = 3.72 , TOTAL = 911.4 SECONDS (15.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.89 , TOTAL = 990.8 SECONDS (16.5 MIN)

WALL CLOCK TIME: STEP = 2.74 , TOTAL = 914.2 SECONDS (15.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 5 ENERGY= -284.6041406

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0024771	-0.0111881	0.0022926
2 C	6.0	0.0097922	0.0050234	0.0002799
3 C	6.0	-0.0067798	-0.0121656	-0.0028056
4 C	6.0	-0.0067179	0.0073453	0.0030313
5 C	6.0	-0.0029628	0.0131493	0.0054890
6 C	6.0	0.0191048	-0.0162243	-0.0030061
7 C	6.0	-0.0155795	-0.0026894	0.0005948
8 C	6.0	0.0063076	-0.0053187	-0.0011447
9 C	6.0	-0.0114675	-0.0002002	-0.0000836
10 C	6.0	-0.0138204	0.0230817	0.0043928
11 C	6.0	-0.0012244	-0.0078330	-0.0022624
12 N	7.0	-0.0128741	-0.0006151	-0.0030504
13 C	6.0	-0.0009297	0.0020892	-0.0004776
14 C	6.0	0.0080996	0.0166836	-0.0011108
15 C	6.0	-0.0022111	-0.0096391	-0.0063551
16 C	6.0	0.0020301	-0.0139063	0.0007719
17 C	6.0	0.0159269	0.0031176	0.0020514
18 C	6.0	0.0038430	0.0069628	0.0011705
19 C	6.0	-0.0045208	-0.0113502	0.0030063
20 O	8.0	0.0018087	0.0092094	-0.0216270
21 N	7.0	0.0023772	-0.0010004	-0.0048665
22 H	1.0	-0.0069072	0.0040727	0.0012239
23 H	1.0	-0.0003380	0.0006927	-0.0002011
24 H	1.0	-0.0038463	-0.0126617	-0.0029887

25 H	1.0	0.0081747	0.0004920	-0.0003937
26 H	1.0	-0.0029069	0.0045945	0.0012240
27 H	1.0	-0.0050641	-0.0021831	-0.0007933
28 H	1.0	0.0012151	0.0110983	0.0029746
29 H	1.0	0.0074411	-0.0007790	-0.0002308
30 H	1.0	-0.0023600	-0.0046967	0.0004527
31 H	1.0	0.0062417	0.0031231	-0.0014920
32 H	1.0	0.0106890	0.0119992	0.0010420
33 H	1.0	0.0061735	-0.0078580	0.0172551
34 H	1.0	-0.0018759	0.0002883	-0.0052902
35 H	1.0	-0.0043619	-0.0027143	0.0109265

MAXIMUM GRADIENT = 0.0230817 RMS GRADIENT = 0.0076224
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0075167633
 PREDICTED ENERGY CHANGE WAS -0.0087721892 RATIO= 0.857
 GDIIS STEP HAS LENGTH = 0.258005
 RADIUS OF STEP TAKEN= 0.25800 CURRENT TRUST RADIUS= 0.45712

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 990.8 SECONDS (16.5 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 914.2 SECONDS (15.2
 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

INSERCH= 6

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1155401543	-1.5933383493	0.9835282871
C	6.0	4.9115747854	0.6367709335	0.4345884148
C	6.0	5.1375773265	-0.7261639131	0.1836622476
C	6.0	3.9936186739	-1.5926606142	0.0661651157
C	6.0	2.6894383807	-1.0855535760	0.1904679732
C	6.0	2.3962024572	0.3410414147	0.4719055776
C	6.0	3.5918498263	1.1960510548	0.5836594099
C	6.0	3.4536453856	2.6160729357	0.8354184631
C	6.0	2.2105106059	3.2539253943	0.9969741142
C	6.0	1.0464588446	2.4455145305	0.9131349455
C	6.0	1.1173922092	1.0547383078	0.6514102232
N	7.0	-0.0945150321	0.2624288903	0.6180033511
C	6.0	-1.2718704322	0.8310669219	0.5068532994
C	6.0	-2.5295178877	0.1062243973	0.4966284971
C	6.0	-2.7589981589	-1.3152107158	0.5350661566

C	6.0	-4.0278402384	-1.9055815686	0.5161244806
C	6.0	-5.1521810101	-1.0192020959	0.5297100938
C	6.0	-4.9822043135	0.4083422448	0.5279975371
C	6.0	-3.6750615257	0.9661799125	0.5019810519
O	8.0	-1.6444994839	-2.2781861176	0.7086358126
N	7.0	1.6460474763	-2.1659449489	-0.0342060053
H	1.0	5.7509870102	1.3608154823	0.5281047136
H	1.0	6.1518034764	-1.1550391034	0.0563610138
H	1.0	4.0995415348	-2.6819668068	-0.1661437104
H	1.0	4.4225144338	3.1818983004	0.8980115887
H	1.0	2.1227380737	4.3238571880	1.2004469835
H	1.0	0.0533865451	2.9002301852	1.0830125477
H	1.0	-1.3541263392	1.9358035502	0.4347640606
H	1.0	-4.1123467921	-3.0026246689	0.5176390704
H	1.0	-6.1657848676	-1.4645523171	0.5479126281
H	1.0	-5.8512544924	1.1085633339	0.5248245233
H	1.0	-3.4838415901	2.0526598410	0.5101620007
H	1.0	-1.9132670582	-3.0823166647	1.2176597440
H	1.0	1.4436595177	-2.3162671415	-1.0571111777
H	1.0	1.9988195049	-3.0764712172	0.3495339667

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3175813	5.1587435	3.9851033
2 C	5.3175813	0.0000000	1.4041483 *	2.4390048 *
3 C	5.1587435	1.4041483 *	0.0000000	1.4398832 *
4 C	3.9851033	2.4390048 *	1.4398832 *	0.0000000
5 C	2.7407558 *	2.8220359 *	2.4743871 *	1.4048114 *
6 C	3.0339749	2.5329719 *	2.9558666 *	2.5407809 *
7 C	4.4749656	1.4410727 *	2.4988361 *	2.8646346 *
8 C	5.3743861	2.4907548 *	3.7988104	4.3123961
9 C	5.2806295	3.8028309	5.0070257	5.2474066
10 C	4.1453465	4.2941450	5.2277074	5.0704997
11 C	2.8506701 *	3.8232878	4.4217971	3.9527094
12 N	1.9030512 *	5.0234160	5.3423551	4.5231316
13 C	2.8337022 *	6.1869191	6.6038202	5.8132639
14 C	3.1814960	7.4602405	7.7184951	6.7544666
15 C	2.9225749 *	7.9156817	7.9263084	6.7745613
16 C	4.1813351	9.2942641	9.2469690	8.0401608
17 C	5.3183146	10.1995331	10.2997450	9.1754771
18 C	5.4955648	9.8968566	10.1889966	9.2077522
19 C	4.5990958	8.5932168	8.9793072	8.0960643
20 O	1.9084868 *	7.1801244	6.9771725	5.7158630

21 N	1.9251270 *	4.3288166	3.7830169	2.4186401 *
22 H	6.3790828	1.1124741 *	2.2023612 *	3.4676725
23 H	6.1227625	2.2117428 *	1.1085099 *	2.2021286 *
24 H	4.2870881	3.4690485	2.2416618 *	1.1188275 *
25 H	6.4311916	2.6327959 *	4.0366521	4.8654222
26 H	6.2521277	4.6860169	5.9687369	6.3080879
27 H	4.4950994	5.3986753	6.3094026	6.0618047
28 H	3.8621114	6.3989449	7.0207791	6.4174996
29 H	4.4808670	9.7305323	9.5317842	8.2400548
30 H	6.2977290	11.2754733	11.3333090	10.1716259
31 H	6.5660734	10.7735428	11.1461671	10.2190267
32 H	5.1451849	8.5143097	9.0640679	8.3305406
33 H	2.5274360 *	7.8117398	7.5056654	6.1997027
34 H	2.5398300 *	4.7929154	4.2086786	2.8788275 *
35 H	2.4795913 *	4.7201213	3.9246985	2.5022421 *

C C C C

1 CO	2.7407558 *	3.0339749	4.4749656	5.3743861
2 C	2.8220359 *	2.5329719 *	1.4410727 *	2.4907548 *
3 C	2.4743871 *	2.9558666 *	2.4988361 *	3.7988104
4 C	1.4048114 *	2.5407809 *	2.8646346 *	4.3123961
5 C	0.0000000	1.4833636 *	2.4848874 *	3.8343203
6 C	1.4833636 *	0.0000000	1.4741448 *	2.5349745 *
7 C	2.4848874 *	1.4741448 *	0.0000000	1.4487737 *
8 C	3.8343203	2.5349745 *	1.4487737 *	0.0000000
9 C	4.4396961	2.9656486 *	2.5127224 *	1.4065348 *
10 C	3.9610695	2.5387592 *	2.8545978 *	2.4144724 *
11 C	2.6953008 *	1.4754460 *	2.4794152 *	2.8159730 *
12 N	3.1225374	2.4962368 *	3.8029089	4.2633733
13 C	4.4119725	3.7008249	4.8780003	5.0620847
14 C	5.3620494	4.9313762	6.2182344	6.4971041
15 C	5.4641514	5.4150950	6.8294998	7.3581344
16 C	6.7749782	6.8057031	8.2270507	8.7475674
17 C	7.8492345	7.6701823	9.0204397	9.3471349
18 C	7.8230271	7.3789269	8.6103419	8.7253735
19 C	6.6942893	6.1034375	7.2710049	7.3247382
20 O	4.5248080	4.8211686	6.2853239	7.0683044
21 N	1.5186799 *	2.6653071 *	3.9333092	5.1856872
22 H	3.9334209	3.5068044	2.1661272 *	2.6358853 *
23 H	3.4656579	4.0639234	3.5155414	4.7019436
24 H	2.1596523 *	3.5280376	3.9823333	5.4304267
25 H	4.6599695	3.5153911	2.1754104 *	1.1237364 *
26 H	5.5319917	4.0581248	3.5102546	2.1956974 *
27 H	4.8612629	3.5230222	3.9590785	3.4210829
28 H	5.0535824	4.0754892	5.0032074	4.8721617

29 H	7.0743540	7.3173361	8.7742739	9.4294742
30 H	8.8705347	8.7506327	10.1139272	10.4531144
31 H	8.8243628	8.2832624	9.4436929	9.4313422
32 H	6.9325301	6.1242158	7.1277338	6.9679230
33 H	5.1212384	5.5540127	7.0009070	7.8371871
34 H	2.1501336 *	3.2103768	4.4320682	5.6524057
35 H	2.1132935 *	3.4427141	4.5658523	5.8955628

C C C N

1 CO	5.2806295	4.1453465	2.8506701 *	1.9030512 *
2 C	3.8028309	4.2941450	3.8232878	5.0234160
3 C	5.0070257	5.2277074	4.4217971	5.3423551
4 C	5.2474066	5.0704997	3.9527094	4.5231316
5 C	4.4396961	3.9610695	2.6953008 *	3.1225374
6 C	2.9656486 *	2.5387592 *	1.4754460 *	2.4962368 *
7 C	2.5127224 *	2.8545978 *	2.4794152 *	3.8029089
8 C	1.4065348 *	2.4144724 *	2.8159730 *	4.2633733
9 C	0.0000000	1.4197090 *	2.4800698 *	3.7954991
10 C	1.4197090 *	0.0000000	1.4169650 *	2.4808843 *
11 C	2.4800698 *	1.4169650 *	0.0000000	1.4483057 *
12 N	3.7954991	2.4808843 *	1.4483057 *	0.0000000
13 C	4.2705315	2.8541472 *	2.4040594 *	1.3122002 *
14 C	5.7119381	4.2934095	3.7714174	2.4430249 *
15 C	6.7665635	5.3635337	4.5449529	3.0976274
16 C	8.1097934	6.6961307	5.9376100	4.4924042
17 C	8.5256778	7.1115689	6.6048155	5.2182716
18 C	7.7493503	6.3752005	6.1349928	4.8906951
19 C	6.3339369	4.9649001	4.7956005	3.6508958
20 O	6.7489628	5.4402596	4.3289382	2.9774806 *
21 N	5.5458945	4.7457897	3.3350182	3.0580933
22 H	4.0421129	4.8432846	4.6453297	5.9484812
23 H	5.9881141	6.3057586	5.5301444	6.4297086
24 H	6.3368839	6.0644226	4.8502138	5.1840586
25 H	2.2153876 *	3.4554654	3.9382045	5.3856533
26 H	1.0926387 *	2.1838261 *	3.4640006	4.6637594
27 H	2.1876213 *	1.1053585 *	2.1735291 *	2.6825555 *
28 H	3.8418956	2.5002906 *	2.6327961 *	2.1024700 *
29 H	8.9080136	7.5134488	6.6204425	5.1781869
30 H	9.6243449	8.2120929	7.7072826	6.3125030
31 H	8.3556903	7.0368084	6.9700042	5.8193363
32 H	5.8400062	4.5651226	4.7103239	3.8345914
33 H	7.5632141	6.2777090	5.1595308	3.8541886
34 H	5.9861817	5.1685784	3.7933064	3.4382645
35 H	6.3669391	5.6317816	4.2349658	3.9499847

	C	C	C	C
1 CO	2.8337022 *	3.1814960	2.9225749 *	4.1813351
2 C	6.1869191	7.4602405	7.9156817	9.2942641
3 C	6.6038202	7.7184951	7.9263084	9.2469690
4 C	5.8132639	6.7544666	6.7745613	8.0401608
5 C	4.4119725	5.3620494	5.4641514	6.7749782
6 C	3.7008249	4.9313762	5.4150950	6.8057031
7 C	4.8780003	6.2182344	6.8294998	8.2270507
8 C	5.0620847	6.4971041	7.3581344	8.7475674
9 C	4.2705315	5.7119381	6.7665635	8.1097934
10 C	2.8541472 *	4.2934095	5.3635337	6.6961307
11 C	2.4040594 *	3.7714174	4.5449529	5.9376100
12 N	1.3122002 *	2.4430249 *	3.0976274	4.4924042
13 C	0.0000000	1.4516123 *	2.6112933 *	3.8839027
14 C	1.4516123 *	0.0000000	1.4403529 *	2.5085281 *
15 C	2.6112933 *	1.4403529 *	0.0000000	1.3995916 *
16 C	3.8839027	2.5085281 *	1.3995916 *	0.0000000
17 C	4.2989334	2.8541270 *	2.4114257 *	1.4317805 *
18 C	3.7343970	2.4714226 *	2.8130642 *	2.5030372 *
19 C	2.4069912 *	1.4324184 *	2.4586602 *	2.8933833 *
20 O	3.1379967	2.5521791 *	1.4830898 *	2.4199603 *
21 N	4.2177091	4.7832923	4.5224160	5.7064573
22 H	7.0428412	8.3750672	8.9208190	10.3099445
23 H	7.6979539	8.7835051	8.9250882	10.2176241
24 H	6.4534020	7.2220292	7.0284624	8.1928382
25 H	6.1729597	7.6125969	8.4811463	9.8710072
26 H	4.9197584	6.3188031	7.4882019	8.7808780
27 H	2.5238269 *	3.8498974	5.0970281	6.3303713
28 H	1.1101378 *	2.1754844 *	3.5429958	4.6809834
29 H	4.7713325	3.4886575	2.1631510 *	1.1002941 *
30 H	5.4057333	3.9613643	3.4100826	2.1831914 *
31 H	4.5878193	3.4697856	3.9289738	3.5227808
32 H	2.5268788 *	2.1678394 *	3.4450791	3.9954531
33 H	4.0287972	3.3266267	2.0745743 *	2.5195787 *
34 H	4.4413736	4.9059873	4.6042887	5.7079806
35 H	5.0981385	5.5368789	5.0767401	6.1416091

	C	C	C	O
1 CO	5.3183146	5.4955648	4.5990958	1.9084868 *
2 C	10.1995331	9.8968566	8.5932168	7.1801244
3 C	10.2997450	10.1889966	8.9793072	6.9771725
4 C	9.1754771	9.2077522	8.0960643	5.7158630
5 C	7.8492345	7.8230271	6.6942893	4.5248080
6 C	7.6701823	7.3789269	6.1034375	4.8211686

7 C	9.0204397	8.6103419	7.2710049	6.2853239
8 C	9.3471349	8.7253735	7.3247382	7.0683044
9 C	8.5256778	7.7493503	6.3339369	6.7489628
10 C	7.1115689	6.3752005	4.9649001	5.4402596
11 C	6.6048155	6.1349928	4.7956005	4.3289382
12 N	5.2182716	4.8906951	3.6508958	2.9774806 *
13 C	4.2989334	3.7343970	2.4069912 *	3.1379967
14 C	2.8541270 *	2.4714226 *	1.4324184 *	2.5521791 *
15 C	2.4114257 *	2.8130642 *	2.4586602 *	1.4830898 *
16 C	1.4317805 *	2.5030372 *	2.8933833 *	2.4199603 *
17 C	0.0000000	1.4376292 *	2.4747510 *	3.7310702
18 C	1.4376292 *	0.0000000	1.4214366 *	4.2883958
19 C	2.4747510 *	1.4214366 *	0.0000000	3.8329883
20 O	3.7310702	4.2883958	3.8329883	0.0000000
21 N	6.9172922	7.1327939	6.1977338	3.3752202
22 H	11.1599086	10.7753701	9.4343421	8.2442795
23 H	11.3147062	11.2531210	10.0630722	7.9037498
24 H	9.4256761	9.6182093	8.6139316	5.8242841
25 H	10.4622982	9.8121485	8.4045812	8.1643765
26 H	9.0511114	8.1402489	6.7361956	7.6171473
27 H	6.5395739	5.6457703	4.2402209	5.4625059
28 H	4.8131375	3.9376110	2.5162330 *	4.2328514
29 H	2.2395013 *	3.5201498	3.9928528	2.5790621 *
30 H	1.1072764 *	2.2156249 *	3.4805562	4.5967220
31 H	2.2396681 *	1.1160501 *	2.1809655 *	5.4037622
32 H	3.4957223	2.2246774 *	1.1032092 *	4.7094371
33 H	3.9013177	4.6987987	4.4728559	0.9889223 *
34 H	6.9069162	7.1573593	6.2774623	3.5575327
35 H	7.4432270	7.8045159	6.9684427	3.7469970

N H H H

1 CO	1.9251270 *	6.3790828	6.1227625	4.2870881
2 C	4.3288166	1.1124741 *	2.2117428 *	3.4690485
3 C	3.7830169	2.2023612 *	1.1085099 *	2.2416618 *
4 C	2.4186401 *	3.4676725	2.2021286 *	1.1188275 *
5 C	1.5186799 *	3.9334209	3.4656579	2.1596523 *
6 C	2.6653071 *	3.5068044	4.0639234	3.5280376
7 C	3.9333092	2.1661272 *	3.5155414	3.9823333
8 C	5.1856872	2.6358853 *	4.7019436	5.4304267
9 C	5.5458945	4.0421129	5.9881141	6.3368839
10 C	4.7457897	4.8432846	6.3057586	6.0644226
11 C	3.3350182	4.6453297	5.5301444	4.8502138
12 N	3.0580933	5.9484812	6.4297086	5.1840586
13 C	4.2177091	7.0428412	7.6979539	6.4534020
14 C	4.7832923	8.3750672	8.7835051	7.2220292

15 C	4.5224160	8.9208190	8.9250882	7.0284624
16 C	5.7064573	10.3099445	10.2176241	8.1928382
17 C	6.9172922	11.1599086	11.3147062	9.4256761
18 C	7.1327939	10.7753701	11.2531210	9.6182093
19 C	6.1977338	9.4343421	10.0630722	8.6139316
20 O	3.3752202	8.2442795	7.9037498	5.8242841
21 N	0.0000000	5.4410257	4.6186546	2.5106412 *
22 H	5.4410257	0.0000000	2.5908918 *	4.4219161
23 H	4.6186546	2.5908918 *	0.0000000	2.5676440 *
24 H	2.5106412 *	4.4219161	2.5676440 *	0.0000000
25 H	6.0973130	2.2842971 *	4.7442431	5.9683877
26 H	6.6233778	4.7324254	6.8964197	7.4065439
27 H	5.4268662	5.9279315	7.3952628	7.0066172
28 H	5.1034612	7.1289522	8.1262217	7.1712890
29 H	5.8449697	10.7854102	10.4393070	8.2465441
30 H	7.8648292	12.2471445	12.3312775	10.3618966
31 H	8.2002717	11.6049838	12.2236146	10.6707028
32 H	6.6639871	9.2607251	10.1656738	8.9655886
33 H	3.8827342	8.8858145	8.3730745	6.1829652
34 H	1.0535144 *	5.8810642	4.9754287	2.8251139 *
35 H	1.0491723 *	5.8137907	4.5853165	2.1987702 *

H H H H

1 CO	6.4311916	6.2521277	4.4950994	3.8621114
2 C	2.6327959 *	4.6860169	5.3986753	6.3989449
3 C	4.0366521	5.9687369	6.3094026	7.0207791
4 C	4.8654222	6.3080879	6.0618047	6.4174996
5 C	4.6599695	5.5319917	4.8612629	5.0535824
6 C	3.5153911	4.0581248	3.5230222	4.0754892
7 C	2.1754104 *	3.5102546	3.9590785	5.0032074
8 C	1.1237364 *	2.1956974 *	3.4210829	4.8721617
9 C	2.2153876 *	1.0926387 *	2.1876213 *	3.8418956
10 C	3.4554654	2.1838261 *	1.1053585 *	2.5002906 *
11 C	3.9382045	3.4640006	2.1735291 *	2.6327961 *
12 N	5.3856533	4.6637594	2.6825555 *	2.1024700 *
13 C	6.1729597	4.9197584	2.5238269 *	1.1101378 *
14 C	7.6125969	6.3188031	3.8498974	2.1754844 *
15 C	8.4811463	7.4882019	5.0970281	3.5429958
16 C	9.8710072	8.7808780	6.3303713	4.6809834
17 C	10.4622982	9.0511114	6.5395739	4.8131375
18 C	9.8121485	8.1402489	5.6457703	3.9376110
19 C	8.4045812	6.7361956	4.2402209	2.5162330 *
20 O	8.1643765	7.6171473	5.4625059	4.2328514
21 N	6.0973130	6.6233778	5.4268662	5.1034612
22 H	2.2842971 *	4.7324254	5.9279315	7.1289522

23 H	4.7442431	6.8964197	7.3952628	8.1262217
24 H	5.9683877	7.4065439	7.0066172	7.1712890
25 H	0.0000000	2.5854417 *	4.3821046	5.9276411
26 H	2.5854417 *	0.0000000	2.5145020 *	4.2869169
27 H	4.3821046	2.5145020 *	0.0000000	1.8252225 *
28 H	5.9276411	4.2869169	1.8252225 *	0.0000000
29 H	10.5468888	9.6446797	7.2468391	5.6570948
30 H	11.5682391	10.1307008	7.6168072	5.8929857
31 H	10.4875314	8.6243340	6.1956783	4.5734668
32 H	7.9960035	6.0883960	3.6821890	2.1342510 *
33 H	8.9154187	8.4345151	6.2989462	5.1095102
34 H	6.5517864	7.0462024	5.8073086	5.3040930
35 H	6.7336702	7.4501187	6.3280060	6.0309542

H H H H

1 CO	4.4808670	6.2977290	6.5660734	5.1451849
2 C	9.7305323	11.2754733	10.7735428	8.5143097
3 C	9.5317842	11.3333090	11.1461671	9.0640679
4 C	8.2400548	10.1716259	10.2190267	8.3305406
5 C	7.0743540	8.8705347	8.8243628	6.9325301
6 C	7.3173361	8.7506327	8.2832624	6.1242158
7 C	8.7742739	10.1139272	9.4436929	7.1277338
8 C	9.4294742	10.4531144	9.4313422	6.9679230
9 C	8.9080136	9.6243449	8.3556903	5.8400062
10 C	7.5134488	8.2120929	7.0368084	4.5651226
11 C	6.6204425	7.7072826	6.9700042	4.7103239
12 N	5.1781869	6.3125030	5.8193363	3.8345914
13 C	4.7713325	5.4057333	4.5878193	2.5268788 *
14 C	3.4886575	3.9613643	3.4697856	2.1678394 *
15 C	2.1631510 *	3.4100826	3.9289738	3.4450791
16 C	1.1002941 *	2.1831914 *	3.5227808	3.9954531
17 C	2.2395013 *	1.1072764 *	2.2396681 *	3.4957223
18 C	3.5201498	2.2156249 *	1.1160501 *	2.2246774 *
19 C	3.9928528	3.4805562	2.1809655 *	1.1032092 *
20 O	2.5790621 *	4.5967220	5.4037622	4.7094371
21 N	5.8449697	7.8648292	8.2002717	6.6639871
22 H	10.7854102	12.2471445	11.6049838	9.2607251
23 H	10.4393070	12.3312775	12.2236146	10.1656738
24 H	8.2465441	10.3618966	10.6707028	8.9655886
25 H	10.5468888	11.5682391	10.4875314	7.9960035
26 H	9.6446797	10.1307008	8.6243340	6.0883960
27 H	7.2468391	7.6168072	6.1956783	3.6821890
28 H	5.6570948	5.8929857	4.5734668	2.1342510 *
29 H	0.0000000	2.5657730 *	4.4638233	5.0942101
30 H	2.5657730 *	0.0000000	2.5923708 *	4.4232371

31 H	4.4638233	2.5923708 *	0.0000000	2.5487599 *
32 H	5.0942101	4.4232371	2.5487599 *	0.0000000
33 H	2.3091841 *	4.5988727	5.7923433	5.4162017
34 H	5.8155078	7.8233729	8.2126582	6.7693527
35 H	6.1139240	8.3245661	8.8976909	7.5095512

H H H

1 CO	2.5274360 *	2.5398300 *	2.4795913 *
2 C	7.8117398	4.7929154	4.7201213
3 C	7.5056654	4.2086786	3.9246985
4 C	6.1997027	2.8788275 *	2.5022421 *
5 C	5.1212384	2.1501336 *	2.1132935 *
6 C	5.5540127	3.2103768	3.4427141
7 C	7.0009070	4.4320682	4.5658523
8 C	7.8371871	5.6524057	5.8955628
9 C	7.5632141	5.9861817	6.3669391
10 C	6.2777090	5.1685784	5.6317816
11 C	5.1595308	3.7933064	4.2349658
12 N	3.8541886	3.4382645	3.9499847
13 C	4.0287972	4.4413736	5.0981385
14 C	3.3266267	4.9059873	5.5368789
15 C	2.0745743 *	4.6042887	5.0767401
16 C	2.5195787 *	5.7079806	6.1416091
17 C	3.9013177	6.9069162	7.4432270
18 C	4.6987987	7.1573593	7.8045159
19 C	4.4728559	6.2774623	6.9684427
20 O	0.9889223 *	3.5575327	3.7469970
21 N	3.8827342	1.0535144 *	1.0491723 *
22 H	8.8858145	5.8810642	5.8137907
23 H	8.3730745	4.9754287	4.5853165
24 H	6.1829652	2.8251139 *	2.1987702 *
25 H	8.9154187	6.5517864	6.7336702
26 H	8.4345151	7.0462024	7.4501187
27 H	6.2989462	5.8073086	6.3280060
28 H	5.1095102	5.3040930	6.0309542
29 H	2.3091841 *	5.8155078	6.1139240
30 H	4.5988727	7.8233729	8.3245661
31 H	5.7923433	8.2126582	8.8976909
32 H	5.4162017	6.7693527	7.5095512
33 H	0.0000000	4.1267870	4.0072556
34 H	4.1267870	0.0000000	1.6925612 *
35 H	4.0072556	1.6925612 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.76 , TOTAL = 991.5 SECONDS (16.5 MIN)
WALL CLOCK TIME: STEP = 0.76 , TOTAL = 914.9 SECONDS (15.2 MIN)

CPU UTILIZATION: STEP = 99.93% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.87 , TOTAL = 992.4 SECONDS (16.5 MIN)
WALL CLOCK TIME: STEP = 0.88 , TOTAL = 915.8 SECONDS (15.3 MIN)

CPU UTILIZATION: STEP = 99.28% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.604346056	-284.604346056	1.504082620	0.010716374	201149375
11133401						
2	1	-284.610006026	-0.005659971	0.831880540	0.003393200	187106771
12336197						
3	2	-284.610040410	-0.000034383	0.659374521	0.003704997	182705311
12745145						
4	3	-284.611221133	-0.001180724	0.356418590	0.001200365	180240682
12935552						
5	4	-284.611213332	0.000007802	0.007102610	0.001445930	173035249
13565369						
6	5	-284.611258277	-0.000044946	0.192047400	0.000611977	156651835
14916934						
7	6	-284.611256332	0.000001945	0.025453387	0.000537990	167607703
14029180						
8	7	-284.611266430	-0.000010097	0.070679655	0.000148925	173776281
13522856						
9	8	-284.611267150	-0.000000720	0.005155387	0.000132217	195386152
11677548						
10	9	-284.611268781	-0.000001631	0.057694836	0.000116015	181783644
12900944						

-----DISABLING FDIFF OPTION-----

11	10	-284.611270842	-0.000002060	0.018628025	0.000119014	201119509
11135244						
12	11	-284.611273110	-0.000002268	0.046400828	0.000135396	201126303
11134686						

13 12	-284.611275310	-0.000002200	0.016758531	0.000162433	201111361
11135917					
14 13	-284.611276668	-0.000001358	0.011363394	0.000134593	201105251
11136408					
15 14	-284.611277686	-0.000001018	0.001348702	0.000082507	201109180
11136132					
16 15	-284.611278217	-0.000000531	0.005552289	0.000050585	201109084
11136097					
17 16	-284.611278364	-0.000000147	0.006558067	0.000034937	201107208
11136244					
18 17	-284.611278440	-0.000000076	0.005890922	0.000029180	201109701
11136048					
19 18	-284.611278473	-0.000000034	0.000929003	0.000024389	201111693
11135897					
20 19	-284.611278517	-0.000000043	0.004002759	0.000021730	201111582
11135915					
21 20	-284.611278596	-0.000000079	0.001034384	0.000021874	201110085
11136042					
22 21	-284.611278610	-0.000000015	0.000261489	0.000013219	201110362
11135997					
23 22	-284.611278622	-0.000000011	0.000805495	0.000009834	201110287
11136005					
24 23	-284.611278627	-0.000000005	0.000393694	0.000005865	201110090
11136019					
25 24	-284.611278630	-0.000000004	0.000308920	0.000003950	201109998
11136040					
26 25	-284.611278632	-0.000000002	0.000243994	0.000003517	201110175
11136024					
27 26	-284.611278633	-0.000000001	0.000077703	0.000002203	201110386
11136014					
28 27	-284.611278633	0.000000000	0.000070710	0.000001537	201110399
11136016					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 97.6 SECONDS (3.5 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 30.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 3.6 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6112786328 AFTER 28 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6103316216
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999900829

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 102.21 , TOTAL = 1094.6 SECONDS (18.2 MIN)
WALL CLOCK TIME: STEP = 93.55 , TOTAL = 1009.4 SECONDS (16.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.85 , TOTAL = 1098.5 SECONDS (18.3 MIN)
WALL CLOCK TIME: STEP = 3.84 , TOTAL = 1013.2 SECONDS (16.9 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.83 , TOTAL = 1101.3 SECONDS (18.4 MIN)
WALL CLOCK TIME: STEP = 2.74 , TOTAL = 1015.9 SECONDS (16.9 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 6 ENERGY= -284.6112786

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0030060	0.0005716	0.0006725
2 C	6.0	-0.0096863	-0.0062330	-0.0007890
3 C	6.0	0.0036309	0.0045407	0.0005311
4 C	6.0	-0.0058141	-0.0053072	0.0007600
5 C	6.0	0.0029637	-0.0037414	0.0006802

6 C	6.0	-0.0047337	-0.0008518	0.0007770
7 C	6.0	0.0119625	0.0047732	0.0008010
8 C	6.0	-0.0187701	-0.0052108	-0.0001277
9 C	6.0	-0.0082361	0.0123876	0.0025490
10 C	6.0	0.0056431	0.0082848	0.0005401
11 C	6.0	-0.0093926	0.0120212	0.0015412
12 N	7.0	-0.0148002	-0.0112145	-0.0024262
13 C	6.0	0.0105266	0.0048853	-0.0009107
14 C	6.0	-0.0000324	0.0005122	-0.0020886
15 C	6.0	-0.0015645	0.0074060	-0.0058140
16 C	6.0	0.0028370	-0.0168035	-0.0010172
17 C	6.0	0.0056403	-0.0033826	0.0018850
18 C	6.0	0.0020387	-0.0025672	0.0022304
19 C	6.0	0.0118526	0.0134542	0.0014117
20 O	8.0	0.0018951	-0.0116893	-0.0072404
21 N	7.0	-0.0003784	0.0039447	0.0010947
22 H	1.0	-0.0000038	0.0065708	0.0012570
23 H	1.0	0.0015016	-0.0039982	-0.0014171
24 H	1.0	-0.0051433	-0.0081497	-0.0019434
25 H	1.0	0.0123134	0.0014549	-0.0003809
26 H	1.0	-0.0013062	-0.0076217	-0.0012311
27 H	1.0	-0.0048824	-0.0030873	-0.0008115
28 H	1.0	0.0003367	0.0053416	0.0032557
29 H	1.0	0.0062888	0.0028612	-0.0002039
30 H	1.0	0.0001449	-0.0026018	0.0008745
31 H	1.0	-0.0027787	0.0087071	-0.0014572
32 H	1.0	0.0059548	-0.0016856	0.0018061
33 H	1.0	0.0085836	0.0047714	0.0055884
34 H	1.0	-0.0012446	-0.0028376	-0.0078891
35 H	1.0	-0.0023410	-0.0055051	0.0074923

MAXIMUM GRADIENT = 0.0187701 RMS GRADIENT = 0.0060075
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0071379892
 PREDICTED ENERGY CHANGE WAS -0.0067418939 RATIO= 1.059
 GDIIS STEP HAS LENGTH = 0.305429
 RADIUS OF STEP TAKEN= 0.30543 CURRENT TRUST RADIUS= 0.50000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 1101.3 SECONDS (18.4 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1016.0 SECONDS (16.9 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 7

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1275785308	-1.5725122561	0.9911019249
C	6.0	4.9299748949	0.6477647382	0.4366254791
C	6.0	5.1526681303	-0.7246766015	0.1860203849
C	6.0	4.0223591212	-1.5875723196	0.0624913445
C	6.0	2.6982239275	-1.0865534359	0.1806240357
C	6.0	2.3999455964	0.3567285406	0.4712321539
C	6.0	3.5886150260	1.2030586537	0.5832780361
C	6.0	3.4783730752	2.6350656567	0.8378914262
C	6.0	2.2268754270	3.2525982644	0.9971734721
C	6.0	1.0616148366	2.4350733618	0.9130846048
C	6.0	1.1295401512	1.0570054085	0.6537507484
N	7.0	-0.0789457654	0.2736225768	0.6273932709
C	6.0	-1.2741776456	0.8060569585	0.5068399997
C	6.0	-2.5405285342	0.0974236622	0.4981478273
C	6.0	-2.7705726889	-1.3190312017	0.5590067964
C	6.0	-4.0455355350	-1.8796424097	0.5134757048
C	6.0	-5.1826800784	-1.0183377749	0.5213781161
C	6.0	-4.9969094340	0.4094529554	0.5229582927
C	6.0	-3.6989221604	0.9508421196	0.4916259323
O	8.0	-1.6464649820	-2.2570557726	0.7668456066
N	7.0	1.6458492856	-2.1744236182	-0.0315410920
H	1.0	5.7702195822	1.3408306955	0.5230412622
H	1.0	6.1652936156	-1.1578212038	0.0568997365
H	1.0	4.1217337725	-2.6675018919	-0.1620588002
H	1.0	4.4039520230	3.1881498333	0.9004886562
H	1.0	2.1316667051	4.3314449459	1.2004760069
H	1.0	0.0808468014	2.8988244894	1.0837060295
H	1.0	-1.3583998519	1.9084556420	0.4220850912
H	1.0	-4.1400382853	-2.9970946246	0.5180082187
H	1.0	-6.1865209749	-1.4599533139	0.5460426859
H	1.0	-5.8757966104	1.0967393838	0.5303326620
H	1.0	-3.5129623298	2.0451713241	0.5053304134
H	1.0	-1.9540646225	-3.1083061106	1.1829118466
H	1.0	1.4459016604	-2.3220150457	-1.0432540506
H	1.0	2.0172843358	-3.0807066297	0.3094731763

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.000000	5.3197824	5.1593127	4.0039806

2 C	5.3197824	0.0000000	1.4127953 *	2.4414083 *
3 C	5.1593127	1.4127953 *	0.0000000	1.4273916 *
4 C	4.0039806	2.4414083 *	1.4273916 *	0.0000000
5 C	2.7388407 *	2.8379762 *	2.4809837 *	1.4206721 *
6 C	3.0258696	2.5469488 *	2.9712395 *	2.5650732 *
7 C	4.4552091	1.4591452 *	2.5140085 *	2.8717545 *
8 C	5.3809859	2.4934970 *	3.8099958	4.3275672
9 C	5.2620125	3.7955393	5.0036934	5.2463934
10 C	4.1157324	4.2878544	5.2200919	5.0666748
11 C	2.8340953 *	3.8285670	4.4247849	3.9638089
12 N	1.8929210 *	5.0264959	5.3442675	4.5391478
13 C	2.8030379 *	6.2065687	6.6144098	5.8292545
14 C	3.1859826	7.4910001	7.7432905	6.7897351
15 C	2.9411289 *	7.9486915	7.9542518	6.8163454
16 C	4.2115718	9.3248850	9.2762128	8.0857663
17 C	5.3597198	10.2493352	10.3449565	9.2340323
18 C	5.5143197	9.9301198	10.2183023	9.2491808
19 C	4.6107376	8.6343932	9.0139563	8.1391578
20 O	1.9147118 *	7.1969847	6.9938369	5.7515120
21 N	1.9269775 *	4.3553884	3.8009049	2.4497011 *
22 H	6.3675777	1.0926204 *	2.1820342 *	3.4413176
23 H	6.1236187	2.2204379 *	1.1089169 *	2.1856087 *
24 H	4.2990764	3.4644869	2.2267813 *	1.1074954 *
25 H	6.3999597	2.6354175 *	4.0473759	4.8636791
26 H	6.2383425	4.6886561	5.9766157	6.3170003
27 H	4.4725397	5.3851673	6.2975369	6.0585605
28 H	3.8274077	6.4135178	7.0273123	6.4268255
29 H	4.5239149	9.7753139	9.5722773	8.2957206
30 H	6.3307661	11.3150753	11.3687052	10.2211223
31 H	6.5861769	10.8155008	11.1831633	10.2663475
32 H	5.1553027	8.5580754	9.1031405	8.3769924
33 H	2.5939722 *	7.8775003	7.5618207	6.2678237
34 H	2.5373873 *	4.8112786	4.2193274	2.8983119 *
35 H	2.5120223 *	4.7330152	3.9238692	2.5121256 *

C C C C

1 CO	2.7388407 *	3.0258696	4.4552091	5.3809859
2 C	2.8379762 *	2.5469488 *	1.4591452 *	2.4934970 *
3 C	2.4809837 *	2.9712395 *	2.5140085 *	3.8099958
4 C	1.4206721 *	2.5650732 *	2.8717545 *	4.3275672
5 C	0.0000000	1.5021604 *	2.4894277 *	3.8588964
6 C	1.5021604 *	0.0000000	1.4634767 *	2.5472073 *
7 C	2.4894277 *	1.4634767 *	0.0000000	1.4586382 *
8 C	3.8588964	2.5472073 *	1.4586382 *	0.0000000
9 C	4.4404009	2.9483265 *	2.4952468 *	1.4046222 *

10 C	3.9518152	2.5111511 *	2.8306117 *	2.4261845 *
11 C	2.6980478 *	1.4620639 *	2.4644162 *	2.8357006 *
12 N	3.1244764	2.4851952 *	3.7837547	4.2749550
13 C	4.4122970	3.7016679	4.8795702	5.1030977
14 C	5.3802556	4.9473476	6.2286497	6.5408126
15 C	5.4867983	5.4360035	6.8411106	7.4001339
16 C	6.7983875	6.8225630	8.2333573	8.7804917
17 C	7.8885623	7.7064605	9.0484281	9.4053910
18 C	7.8466748	7.3972238	8.6223360	8.7682922
19 C	6.7209509	6.1277708	7.2924764	7.3803845
20 O	4.5376264	4.8262505	6.2779098	7.0853274
21 N	1.5283874 *	2.6885263 *	3.9445821	5.2196976
22 H	3.9302164	3.5113940	2.1867803 *	2.6507990 *
23 H	3.4700085	4.0796296	3.5341336	4.7133301
24 H	2.1548109 *	3.5371714	3.9775597	5.4342466
25 H	4.6584119	3.4953182	2.1693280 *	1.0800541 *
26 H	5.5421829	4.0499556	3.5057713	2.1960848 *
27 H	4.8527783	3.4950816	3.9281660	3.4166033
28 H	5.0482254	4.0663784	4.9996524	4.9086892
29 H	7.1081521	7.3499461	8.7964555	9.4796491
30 H	8.9000927	8.7768638	10.1314512	10.5006920
31 H	8.8545407	8.3089721	9.4651569	9.4848052
32 H	6.9636175	6.1493481	7.1517572	7.0240546
33 H	5.1706724	5.6098447	7.0476042	7.9130738
34 H	2.1430245 *	3.2217287	4.4342950	5.6782301
35 H	2.1111437 *	3.4624494	4.5710715	5.9231798

C C C N

1 CO	5.2620125	4.1157324	2.8340953 *	1.8929210 *
2 C	3.7955393	4.2878544	3.8285670	5.0264959
3 C	5.0036934	5.2200919	4.4247849	5.3442675
4 C	5.2463934	5.0666748	3.9638089	4.5391478
5 C	4.4404009	3.9518152	2.6980478 *	3.1244764
6 C	2.9483265 *	2.5111511 *	1.4620639 *	2.4851952 *
7 C	2.4952468 *	2.8306117 *	2.4644162 *	3.7837547
8 C	1.4046222 *	2.4261845 *	2.8357006 *	4.2749550
9 C	0.0000000	1.4259208 *	2.4784495 *	3.7852140
10 C	1.4259208 *	0.0000000	1.4039014 *	2.4605624 *
11 C	2.4784495 *	1.4039014 *	0.0000000	1.4404241 *
12 N	3.7852140	2.4605624 *	1.4404241 *	0.0000000
13 C	4.2992283	2.8765701 *	2.4212429 *	1.3140010 *
14 C	5.7386666	4.3141877	3.7966319	2.4712629 *
15 C	6.7872140	5.3762750	4.5678667	3.1282708
16 C	8.1189283	6.6977193	5.9518893	4.5147937
17 C	8.5655583	7.1463768	6.6459534	5.2657862

18 C	7.7776232	6.4000823	6.1619652	4.9209474
19 C	6.3772045	5.0043264	4.8323497	3.6852799
20 O	6.7388504	5.4195164	4.3245805	2.9800833 *
21 N	5.5541346	4.7414249	3.3434015	3.0662750
22 H	4.0540035	4.8497896	4.6511877	5.9466426
23 H	5.9872408	6.2999588	5.5335794	6.4315643
24 H	6.3231237	6.0462001	4.8467229	5.1883674
25 H	2.1801752 *	3.4261495	3.9146429	5.3540100
26 H	1.1019559 *	2.1963219 *	3.4677255	4.6563026
27 H	2.1767137 *	1.0982180 *	2.1626180 *	2.6693520 *
28 H	3.8719046	2.5248520 *	2.6397882 *	2.0861048 *
29 H	8.9345314	7.5313830	6.6500083	5.2155564
30 H	9.6538542	8.2365906	7.7376633	6.3493605
31 H	8.3975569	7.0756847	7.0065365	5.8558024
32 H	5.8860451	4.6092346	4.7488240	3.8659739
33 H	7.6141883	6.3163427	5.2094577	3.9066755
34 H	5.9874517	5.1579868	3.7944287	3.4428995
35 H	6.3739792	5.6304067	4.2458542	3.9682210

C C C C

1 CO	2.8030379 *	3.1859826	2.9411289 *	4.2115718
2 C	6.2065687	7.4910001	7.9486915	9.3248850
3 C	6.6144098	7.7432905	7.9542518	9.2762128
4 C	5.8292545	6.7897351	6.8163454	8.0857663
5 C	4.4122970	5.3802556	5.4867983	6.7983875
6 C	3.7016679	4.9473476	5.4360035	6.8225630
7 C	4.8795702	6.2286497	6.8411106	8.2333573
8 C	5.1030977	6.5408126	7.4001339	8.7804917
9 C	4.2992283	5.7386666	6.7872140	8.1189283
10 C	2.8765701 *	4.3141877	5.3762750	6.6977193
11 C	2.4212429 *	3.7966319	4.5678667	5.9518893
12 N	1.3140010 *	2.4712629 *	3.1282708	4.5147937
13 C	0.0000000	1.4511655 *	2.5995998 *	3.8592032
14 C	1.4511655 *	0.0000000	1.4363038 *	2.4847679 *
15 C	2.5995998 *	1.4363038 *	0.0000000	1.3935165 *
16 C	3.8592032	2.4847679 *	1.3935165 *	0.0000000
17 C	4.3133535	2.8681750 *	2.4310686 *	1.4265363 *
18 C	3.7438331	2.4762441 *	2.8187821 *	2.4789433 *
19 C	2.4291110 *	1.4388333 *	2.4533034 *	2.8517119 *
20 O	3.0965885	2.5328090 *	1.4787512 *	2.4417569 *
21 N	4.2070983	4.7924545	4.5370945	5.7250153
22 H	7.0646853	8.4032860	8.9454621	10.3305657
23 H	7.7074637	8.8069109	8.9514137	10.2464882
24 H	6.4520459	7.2433711	7.0599006	8.2329434
25 H	6.1701282	7.6118511	8.4796872	9.8603315

26 H	4.9506835	6.3442580	7.5080833	8.7867743
27 H	2.5590118 *	3.8810222	5.1182232	6.3392381
28 H	1.1088551 *	2.1640357 *	3.5255710	4.6452919
29 H	4.7620630	3.4835139	2.1663365 *	1.1214503 *
30 H	5.4099405	3.9649688	3.4188784	2.1819758 *
31 H	4.6108508	3.4819077	3.9343596	3.4941363
32 H	2.5588207 *	2.1770163 *	3.4455598	3.9607908
33 H	4.0300816	3.3300969	2.0633583 *	2.5163485 *
34 H	4.4256590	4.9113368	4.6208086	5.7249440
35 H	5.0970194	5.5596554	5.1077727	6.1840082

C C C O

1 CO	5.3597198	5.5143197	4.6107376	1.9147118 *
2 C	10.2493352	9.9301198	8.6343932	7.1969847
3 C	10.3449565	10.2183023	9.0139563	6.9938369
4 C	9.2340323	9.2491808	8.1391578	5.7515120
5 C	7.8885623	7.8466748	6.7209509	4.5376264
6 C	7.7064605	7.3972238	6.1277708	4.8262505
7 C	9.0484281	8.6223360	7.2924764	6.2779098
8 C	9.4053910	8.7682922	7.3803845	7.0853274
9 C	8.5655583	7.7776232	6.3772045	6.7388504
10 C	7.1463768	6.4000823	5.0043264	5.4195164
11 C	6.6459534	6.1619652	4.8323497	4.3245805
12 N	5.2657862	4.9209474	3.6852799	2.9800833 *
13 C	4.3133535	3.7438331	2.4291110 *	3.0965885
14 C	2.8681750 *	2.4762441 *	1.4388333 *	2.5328090 *
15 C	2.4310686 *	2.8187821 *	2.4533034 *	1.4787512 *
16 C	1.4265363 *	2.4789433 *	2.8517119 *	2.4417569 *
17 C	0.0000000	1.4398262 *	2.4657843 *	3.7549293
18 C	1.4398262 *	0.0000000	1.4067178 *	4.2889658
19 C	2.4657843 *	1.4067178 *	0.0000000	3.8182372
20 O	3.7549293	4.2889658	3.8182372	0.0000000
21 N	6.9477383	7.1491350	6.2134991	3.3887435
22 H	11.2040925	10.8073369	9.4772213	8.2469047
23 H	11.3583319	11.2813269	10.0964450	7.9206005
24 H	9.4741198	9.6481373	8.6418966	5.8569144
25 H	10.4757710	9.8101927	8.4160136	8.1409871
26 H	9.0874099	8.1644136	6.7769248	7.6072765
27 H	6.5852174	5.6828705	4.2932328	5.4467520
28 H	4.8167518	3.9364878	2.5298032 *	4.1896690
29 H	2.2366475 *	3.5126655	3.9725916	2.6129457 *
30 H	1.0969636 *	2.2159396 *	3.4645409	4.6147844
31 H	2.2257678 *	1.1157328 *	2.1821014 *	5.4028813
32 H	3.4890261	2.2086159 *	1.1101015 *	4.6969523
33 H	3.9025059	4.6977731	4.4720340	0.9961706 *

34 H	6.9343885	7.1710357	6.2878186	3.5837706
35 H	7.4925134	7.8374552	6.9972553	3.7829419

	N	H	H	H
--	---	---	---	---

1 CO	1.9269775 *	6.3675777	6.1236187	4.2990764
2 C	4.3553884	1.0926204 *	2.2204379 *	3.4644869
3 C	3.8009049	2.1820342 *	1.1089169 *	2.2267813 *
4 C	2.4497011 *	3.4413176	2.1856087 *	1.1074954 *
5 C	1.5283874 *	3.9302164	3.4700085	2.1548109 *
6 C	2.6885263 *	3.5113940	4.0796296	3.5371714
7 C	3.9445821	2.1867803 *	3.5341336	3.9775597
8 C	5.2196976	2.6507990 *	4.7133301	5.4342466
9 C	5.5541346	4.0540035	5.9872408	6.3231237
10 C	4.7414249	4.8497896	6.2999588	6.0462001
11 C	3.3434015	4.6511877	5.5335794	4.8467229
12 N	3.0662750	5.9466426	6.4315643	5.1883674
13 C	4.2070983	7.0646853	7.7074637	6.4520459
14 C	4.7924545	8.4032860	8.8069109	7.2433711
15 C	4.5370945	8.9454621	8.9514137	7.0599006
16 C	5.7250153	10.3305657	10.2464882	8.2329434
17 C	6.9477383	11.2040925	11.3583319	9.4741198
18 C	7.1491350	10.8073369	11.2813269	9.6481373
19 C	6.2134991	9.4772213	10.0964450	8.6418966
20 O	3.3887435	8.2469047	7.9206005	5.8569144
21 N	0.0000000	5.4474769	4.6332148	2.5278776 *
22 H	5.4474769	0.0000000	2.5722816 *	4.3878922
23 H	4.6332148	2.5722816 *	0.0000000	2.5501403 *
24 H	2.5278776 *	4.3878922	2.5501403 *	0.0000000
25 H	6.1018853	2.3284634 *	4.7646018	5.9579620
26 H	6.6392929	4.7583357	6.9072394	7.4028457
27 H	5.4250212	5.9254242	7.3845243	6.9903281
28 H	5.0893214	7.1518952	8.1327349	7.1632727
29 H	5.8698626	10.8180790	10.4783307	8.2962642
30 H	7.8860697	12.2804139	12.3651878	10.4028697
31 H	8.2213969	11.6485762	12.2594876	10.7051171
32 H	6.6862957	9.3098805	10.2043564	8.9968484
33 H	3.9123411	8.9383899	8.4259286	6.2384758
34 H	1.0417895 *	5.8795787	4.9838084	2.8382994 *
35 H	1.0371131 *	5.8034582	4.5790024	2.1958570 *

	H	H	H	H
--	---	---	---	---

1 CO	6.3999597	6.2383425	4.4725397	3.8274077
2 C	2.6354175 *	4.6886561	5.3851673	6.4135178
3 C	4.0473759	5.9766157	6.2975369	7.0273123

4 C	4.8636791	6.3170003	6.0585605	6.4268255
5 C	4.6584119	5.5421829	4.8527783	5.0482254
6 C	3.4953182	4.0499556	3.4950816	4.0663784
7 C	2.1693280 *	3.5057713	3.9281660	4.9996524
8 C	1.0800541 *	2.1960848 *	3.4166033	4.9086892
9 C	2.1801752 *	1.1019559 *	2.1767137 *	3.8719046
10 C	3.4261495	2.1963219 *	1.0982180 *	2.5248520 *
11 C	3.9146429	3.4677255	2.1626180 *	2.6397882 *
12 N	5.3540100	4.6563026	2.6693520 *	2.0861048 *
13 C	6.1701282	4.9506835	2.5590118 *	1.1088551 *
14 C	7.6118511	6.3442580	3.8810222	2.1640357 *
15 C	8.4796872	7.5080833	5.1182232	3.5255710
16 C	9.8603315	8.7867743	6.3392381	4.6452919
17 C	10.4757710	9.0874099	6.5852174	4.8167518
18 C	9.8101927	8.1644136	5.6828705	3.9364878
19 C	8.4160136	6.7769248	4.2932328	2.5298032 *
20 O	8.1409871	7.6072765	5.4467520	4.1896690
21 N	6.1018853	6.6392929	5.4250212	5.0893214
22 H	2.3284634 *	4.7583357	5.9254242	7.1518952
23 H	4.7646018	6.9072394	7.3845243	8.1327349
24 H	5.9579620	7.4028457	6.9903281	7.1632727
25 H	0.0000000	2.5613271 *	4.3366481	5.9220931
26 H	2.5613271 *	0.0000000	2.5043759 *	4.3194136
27 H	4.3366481	2.5043759 *	0.0000000	1.8681551 *
28 H	5.9220931	4.3194136	1.8681551 *	0.0000000
29 H	10.5547767	9.6699296	7.2730837	5.6401363
30 H	11.5710247	10.1568117	7.6529684	5.8883188
31 H	10.4968683	8.6620945	6.2478263	4.5910211
32 H	8.0087504	6.1296094	3.7388108	2.1605000 *
33 H	8.9526251	8.4878386	6.3432109	5.1089698
34 H	6.5490545	7.0550073	5.8003879	5.2828220
35 H	6.7337986	7.4663887	6.3327734	6.0249204

H H H H

1 CO	4.5239149	6.3307661	6.5861769	5.1553027
2 C	9.7753139	11.3150753	10.8155008	8.5580754
3 C	9.5722773	11.3687052	11.1831633	9.1031405
4 C	8.2957206	10.2211223	10.2663475	8.3769924
5 C	7.1081521	8.9000927	8.8545407	6.9636175
6 C	7.3499461	8.7768638	8.3089721	6.1493481
7 C	8.7964555	10.1314512	9.4651569	7.1517572
8 C	9.4796491	10.5006920	9.4848052	7.0240546
9 C	8.9345314	9.6538542	8.3975569	5.8860451
10 C	7.5313830	8.2365906	7.0756847	4.6092346
11 C	6.6500083	7.7376633	7.0065365	4.7488240

12 N	5.2155564	6.3493605	5.8558024	3.8659739
13 C	4.7620630	5.4099405	4.6108508	2.5588207 *
14 C	3.4835139	3.9649688	3.4819077	2.1770163 *
15 C	2.1663365 *	3.4188784	3.9343596	3.4455598
16 C	1.1214503 *	2.1819758 *	3.4941363	3.9607908
17 C	2.2366475 *	1.0969636 *	2.2257678 *	3.4890261
18 C	3.5126655	2.2159396 *	1.1157328 *	2.2086159 *
19 C	3.9725916	3.4645409	2.1821014 *	1.1101015 *
20 O	2.6129457 *	4.6147844	5.4028813	4.6969523
21 N	5.8698626	7.8860697	8.2213969	6.6862957
22 H	10.8180790	12.2804139	11.6485762	9.3098805
23 H	10.4783307	12.3651878	12.2594876	10.2043564
24 H	8.2962642	10.4028697	10.7051171	8.9968484
25 H	10.5547767	11.5710247	10.4968683	8.0087504
26 H	9.6699296	10.1568117	8.6620945	6.1296094
27 H	7.2730837	7.6529684	6.2478263	3.7388108
28 H	5.6401363	5.8883188	4.5910211	2.1605000 *
29 H	0.0000000	2.5596251 *	4.4466263	5.0811250
30 H	2.5596251 *	0.0000000	2.5755531 *	4.4085680
31 H	4.4466263	2.5755531 *	0.0000000	2.5461999 *
32 H	5.0811250	4.4085680	2.5461999 *	0.0000000
33 H	2.2875633 *	4.5865407	5.7869032	5.4265651
34 H	5.8391778	7.8436528	8.2323340	6.7868080
35 H	6.1614203	8.3657174	8.9331160	7.5429844

H H H

1 CO	2.5939722 *	2.5373873 *	2.5120223 *
2 C	7.8775003	4.8112786	4.7330152
3 C	7.5618207	4.2193274	3.9238692
4 C	6.2678237	2.8983119 *	2.5121256 *
5 C	5.1706724	2.1430245 *	2.1111437 *
6 C	5.6098447	3.2217287	3.4624494
7 C	7.0476042	4.4342950	4.5710715
8 C	7.9130738	5.6782301	5.9231798
9 C	7.6141883	5.9874517	6.3739792
10 C	6.3163427	5.1579868	5.6304067
11 C	5.2094577	3.7944287	4.2458542
12 N	3.9066755	3.4428995	3.9682210
13 C	4.0300816	4.4256590	5.0970194
14 C	3.3300969	4.9113368	5.5596554
15 C	2.0633583 *	4.6208086	5.1077727
16 C	2.5163485 *	5.7249440	6.1840082
17 C	3.9025059	6.9343885	7.4925134
18 C	4.6977731	7.1710357	7.8374552
19 C	4.4720340	6.2878186	6.9972553

20	O	0.9961706 *	3.5837706	3.7829419
21	N	3.9123411	1.0417895 *	1.0371131 *
22	H	8.9383899	5.8795787	5.8034582
23	H	8.4259286	4.9838084	4.5790024
24	H	6.2384758	2.8382994 *	2.1958570 *
25	H	8.9526251	6.5490545	6.7337986
26	H	8.4878386	7.0550073	7.4663887
27	H	6.3432109	5.8003879	6.3327734
28	H	5.1089698	5.2828220	6.0249204
29	H	2.2875633 *	5.8391778	6.1614203
30	H	4.5865407	7.8436528	8.3657174
31	H	5.7869032	8.2323340	8.9331160
32	H	5.4265651	6.7868080	7.5429844
33	H	0.0000000	4.1393042	4.0663582
34	H	4.1393042	0.0000000	1.6528648 *
35	H	4.0663582	1.6528648 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.81 , TOTAL = 1102.1 SECONDS (18.4 MIN)
WALL CLOCK TIME: STEP = 0.81 , TOTAL = 1016.8 SECONDS (16.9 MIN)
CPU UTILIZATION: STEP = 99.89% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.95 , TOTAL = 1103.1 SECONDS (18.4 MIN)
WALL CLOCK TIME: STEP = 0.95 , TOTAL = 1017.7 SECONDS (17.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.610297872	-284.610297872	0.958953264	0.007425244	200483171
11191301						
2	1	-284.616125644	-0.005827773	0.627847611	0.002153740	185292632
12493251						
3	2	-284.615925264	0.000200380	0.224193974	0.002666710	180261359
12944405						

4 3	-284.616585179	-0.000659915	0.176487539	0.000943838	173724645
13484117					
5 4	-284.616524448	0.000060731	0.019308873	0.001254659	169509239
13866081					
6 5	-284.616637895	-0.000113447	0.060544780	0.000313288	158968907
14691791					
7 6	-284.616636727	0.000001169	0.004935768	0.000387164	159735098
14694504					
8 7	-284.616642656	-0.000005929	0.024350928	0.000243173	165000877
14259502					
9 8	-284.616644310	-0.000001655	0.016208054	0.000190428	190167142
12163166					
10 9	-284.616647281	-0.000002970	0.024926855	0.000159796	188246951
12384961					

-----DISABLING FDIFF OPTION-----

11 10	-284.616649266	-0.000001985	0.008089531	0.000159700	200420510
11194775					
12 11	-284.616650364	-0.000001098	0.019543908	0.000138886	200424510
11194493					
13 12	-284.616651229	-0.000000865	0.019195208	0.000105745	200416170
11195187					
14 13	-284.616652228	-0.000000999	0.019875064	0.000088983	200407586
11195863					
15 14	-284.616652703	-0.000000475	0.012218600	0.000100332	200417038
11195126					
16 15	-284.616652936	-0.000000233	0.002689627	0.000088132	200422085
11194684					
17 16	-284.616653200	-0.000000264	0.005659852	0.000057634	200420680
11194789					
18 17	-284.616653479	-0.000000279	0.002308108	0.000037581	200418409
11194976					
19 18	-284.616653566	-0.000000087	0.000337274	0.000032593	200419844
11194894					
20 19	-284.616653622	-0.000000057	0.003469062	0.000027091	200419794
11194891					
21 20	-284.616653675	-0.000000052	0.003107374	0.000019996	200418255
11195030					
22 21	-284.616653747	-0.000000072	0.001528007	0.000014918	200416651
11195142					
23 22	-284.616653816	-0.000000069	0.003044158	0.000018759	200416616
11195103					
24 23	-284.616653827	-0.000000011	0.001002084	0.000009907	200418318
11194987					
25 24	-284.616653833	-0.000000006	0.000415838	0.000006174	200418825
11194934					

26 25 -284.616653835 -0.000000002 0.000058215 0.000003274 200418602
11194949
27 26 -284.616653836 -0.000000001 0.000074414 0.000001477 200418506
11194955

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 92.4 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 29.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 3.9 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6166538361 AFTER 27 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6259488131
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000179004

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 97.75 , TOTAL = 1200.8 SECONDS (20.0 MIN)
WALL CLOCK TIME: STEP = 90.87 , TOTAL = 1108.6 SECONDS (18.5
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.69 , TOTAL = 1204.5 SECONDS (20.1 MIN)
WALL CLOCK TIME: STEP = 3.65 , TOTAL = 1112.2 SECONDS (18.5
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84, TOTAL = 1207.4 SECONDS (20.1 MIN)
 WALL CLOCK TIME: STEP = 2.70, TOTAL = 1114.9 SECONDS (18.6 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 7 ENERGY= -284.6166538

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0024831	0.0070918	-0.0019326
2 C	6.0	0.0112743	0.0099585	0.0014875
3 C	6.0	-0.0016961	-0.0062088	-0.0002744
4 C	6.0	0.0177415	-0.0096732	-0.0011027
5 C	6.0	-0.0047430	-0.0082219	-0.0021036
6 C	6.0	-0.0109247	0.0172709	0.0045060
7 C	6.0	-0.0116706	-0.0016404	0.0003891
8 C	6.0	0.0139260	0.0181983	0.0027758
9 C	6.0	-0.0051828	0.0049265	0.0012780
10 C	6.0	-0.0011825	-0.0045538	-0.0010776
11 C	6.0	-0.0032368	0.0109510	0.0022617
12 N	7.0	-0.0062193	-0.0010253	-0.0012339
13 C	6.0	0.0078284	-0.0071729	-0.0009579
14 C	6.0	0.0002019	0.0017554	-0.0035111
15 C	6.0	-0.0068019	-0.0009727	-0.0033099
16 C	6.0	0.0075193	0.0139923	-0.0029873
17 C	6.0	-0.0064943	-0.0120167	0.0013476
18 C	6.0	0.0153011	0.0046772	0.0023384
19 C	6.0	-0.0034299	0.0007021	0.0001044
20 O	8.0	0.0113534	-0.0038883	-0.0065316
21 N	7.0	-0.0056644	-0.0061867	0.0003402
22 H	1.0	-0.0079114	-0.0044230	-0.0005653
23 H	1.0	0.0011183	-0.0048378	-0.0018320
24 H	1.0	-0.0065420	-0.0008705	-0.0002241
25 H	1.0	-0.0139547	-0.0118827	-0.0017174
26 H	1.0	-0.0007671	-0.0013141	-0.0002070
27 H	1.0	0.0006561	-0.0039180	-0.0013408
28 H	1.0	0.0011552	0.0031169	0.0032365
29 H	1.0	0.0044939	-0.0097366	-0.0003858
30 H	1.0	0.0058662	0.0007973	0.0014230
31 H	1.0	-0.0045815	0.0061763	-0.0009376
32 H	1.0	0.0053727	0.0026664	0.0025654
33 H	1.0	0.0020662	-0.0014017	0.0068141

34 H 1.0 0.0019610 -0.0038587 0.0014394
35 H 1.0 -0.0043492 0.0015228 -0.0000744

MAXIMUM GRADIENT = 0.0181983 RMS GRADIENT = 0.0063611
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0053752033
PREDICTED ENERGY CHANGE WAS -0.0058273289 RATIO= 0.922
GDIIS STEP HAS LENGTH = 0.300309
RADIUS OF STEP TAKEN= 0.30031 CURRENT TRUST RADIUS= 0.50000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.01 , TOTAL = 1207.4 SECONDS (20.1 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1115.0 SECONDS (18.6 MIN)
CPU UTILIZATION: STEP = 57.72% , TOTAL = 100.00%

INSERCH= 8

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1425372378	-1.5684599882	1.0027176885
C	6.0	4.9310757596	0.6426257975	0.4360842171
C	6.0	5.1695653697	-0.7152464906	0.1881606699
C	6.0	4.0213798391	-1.5716105164	0.0608246767
C	6.0	2.7134251305	-1.0750154318	0.1755481317
C	6.0	2.4208812581	0.3441737285	0.4639327107
C	6.0	3.6034916607	1.2090109976	0.5820431207
C	6.0	3.4867009452	2.6276997618	0.8361830198
C	6.0	2.2457694720	3.2513623564	0.9967376747
C	6.0	1.0729205584	2.4297450371	0.9139805078
C	6.0	1.1495620677	1.0492691547	0.6530562084
N	7.0	-0.0684959023	0.2843091467	0.6362652387
C	6.0	-1.2781536333	0.7977406519	0.5079599928
C	6.0	-2.5548976779	0.0821755433	0.5037927990
C	6.0	-2.7732472960	-1.3185912520	0.5829822545
C	6.0	-4.0694839045	-1.8795070884	0.5154363011
C	6.0	-5.2025190338	-0.9993983952	0.5125233824
C	6.0	-5.0313719280	0.4037222401	0.5154957035
C	6.0	-3.7177798685	0.9393466579	0.4828726011
O	8.0	-1.6648839583	-2.2337759252	0.8259857702
N	7.0	1.6548911469	-2.1746114462	-0.0311961964
H	1.0	5.7988579723	1.3319622231	0.5198414137
H	1.0	6.1765067359	-1.1540055279	0.0597629937
H	1.0	4.1497960935	-2.6557213873	-0.1586567643

H	1.0	4.4089210413	3.2101031873	0.9049332938
H	1.0	2.1401829554	4.3419997463	1.2012239244
H	1.0	0.0990714008	2.9045086006	1.0867766301
H	1.0	-1.3635713716	1.8825328171	0.4068530038
H	1.0	-4.1698847356	-2.9814610553	0.5187180579
H	1.0	-6.2125895223	-1.4575732491	0.5424731807
H	1.0	-5.8907429121	1.0790552288	0.5362225716
H	1.0	-3.5439632395	2.0364373895	0.4976295815
H	1.0	-1.9915447963	-3.1317076325	1.1447504548
H	1.0	1.4445029778	-2.3223094528	-1.0347017027
H	1.0	2.0390871568	-3.0876804275	0.2756738880

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3047220	5.1635732	3.9915651
2 C	5.3047220	0.0000000	1.4007714 *	2.4230577 *
3 C	5.1635732	1.4007714 *	0.0000000	1.4380208 *
4 C	3.9915651	2.4230577 *	1.4380208 *	0.0000000
5 C	2.7453891 *	2.8171164 *	2.4823814 *	1.4037499 *
6 C	3.0231289	2.5280280 *	2.9586628 *	2.5286995 *
7 C	4.4575237	1.4507156 *	2.5120703 *	2.8597474 *
8 C	5.3683257	2.4873312 *	3.7983227	4.3036344
9 C	5.2587364	3.7855922	4.9936324	5.2239633
10 C	4.1059872	4.2787313	5.2153892	5.0430282
11 C	2.8264586 *	3.8094988	4.4147559	3.9328216
12 N	1.9004147 *	5.0163911	5.3513732	4.5279856
13 C	2.8039353 *	6.2115824	6.6305718	5.8222685
14 C	3.2015120	7.5072290	7.7719261	6.7954878
15 C	2.9564187 *	7.9513864	7.9754738	6.8193567
16 C	4.2515074	9.3475946	9.3178669	8.1094727
17 C	5.3975687	10.2660523	10.3810447	9.2526628
18 C	5.5584372	9.9656282	10.2673444	9.2769057
19 C	4.6326430	8.6540705	9.0448570	8.1472464
20 O	1.9340762 *	7.2064134	7.0301102	5.7755978
21 N	1.9296663 *	4.3460974	3.8119284	2.4438385 *
22 H	6.3749183	1.1114162 *	2.1672759 *	3.4352379
23 H	6.1212518	2.2182426 *	1.1058600 *	2.1952146 *
24 H	4.3115022	3.4413964	2.2193816 *	1.1135346 *
25 H	6.4067354	2.6616546 *	4.0621070	4.8710875
26 H	6.2420772	4.6967956	5.9815712	6.3095324
27 H	4.4739695	5.3747354	6.2944457	6.0392651
28 H	3.8121869	6.4156688	7.0340713	6.4069136
29 H	4.5637497	9.7963420	9.6161492	8.3243114

30 H	6.3727354	11.3403453	11.4118376	10.2459318
31 H	6.6051059	10.8310783	11.2103115	10.2714268
32 H	5.1807996	8.5891085	9.1429271	8.3930462
33 H	2.6491928 *	7.9164687	7.6181262	6.3058751
34 H	2.5326827 *	4.8073113	4.2372318	2.8989690 *
35 H	2.5364394 *	4.7227655	3.9288669	2.5048178 *

C C C C

1 CO	2.7453891 *	3.0231289	4.4575237	5.3683257
2 C	2.8171164 *	2.5280280 *	1.4507156 *	2.4873312 *
3 C	2.4823814 *	2.9586628 *	2.5120703 *	3.7983227
4 C	1.4037499 *	2.5286995 *	2.8597474 *	4.3036344
5 C	0.0000000	1.4774456 *	2.4848005 *	3.8398560
6 C	1.4774456 *	0.0000000	1.4698507 *	2.5473581 *
7 C	2.4848005 *	1.4698507 *	0.0000000	1.4459962 *
8 C	3.8398560	2.5473581 *	1.4459962 *	0.0000000
9 C	4.4283856	2.9607923 *	2.4872837 *	1.3980857 *
10 C	3.9395283	2.5237172 *	2.8291631 *	2.4231332 *
11 C	2.6807213 *	1.4660081 *	2.4601485 *	2.8261629 *
12 N	3.1303527	2.4960531 *	3.7870181	4.2627305
13 C	4.4215850	3.7269989	4.8994992	5.1147160
14 C	5.4038931	4.9828313	6.2611213	6.5643805
15 C	5.5071686	5.4550831	6.8594150	7.4043417
16 C	6.8389024	6.8609219	8.2715134	8.8041877
17 C	7.9234741	7.7410451	9.0789718	9.4214192
18 C	7.8920283	7.4526695	8.6725883	8.8094541
19 C	6.7462953	6.1674752	7.3269073	7.4080975
20 O	4.5755202	4.8446243	6.2982594	7.0832815
21 N	1.5402431 *	2.6788379 *	3.9524685	5.2124914
22 H	3.9283553	3.5198833	2.1996862 *	2.6692842 *
23 H	3.4659169	4.0635719	3.5322840	4.7052288
24 H	2.1618246 *	3.5179731	3.9728128	5.4170047
25 H	4.6657208	3.5157269	2.1811338 *	1.0928908 *
26 H	5.5429839	4.0749236	3.5128729	2.2102466 *
27 H	4.8478649	3.5119866	3.9256120	3.4081453
28 H	5.0420724	4.0855708	5.0155796	4.9259253
29 H	7.1506822	7.3824823	8.8311634	9.4966717
30 H	8.9417404	8.8198230	10.1719068	10.5286256
31 H	8.8770386	8.3443617	9.4952345	9.5091918
32 H	6.9956976	6.2003437	7.1956842	7.0636003
33 H	5.2255218	5.6581594	7.1037251	7.9546945
34 H	2.1518853 *	3.2108180	4.4435706	5.6721577
35 H	2.1249888 *	3.4581543	4.5828791	5.9224426

C C C N

1	CO	5.2587364	4.1059872	2.8264586 *	1.9004147 *
2	C	3.7855922	4.2787313	3.8094988	5.0163911
3	C	4.9936324	5.2153892	4.4147559	5.3513732
4	C	5.2239633	5.0430282	3.9328216	4.5279856
5	C	4.4283856	3.9395283	2.6807213 *	3.1303527
6	C	2.9607923 *	2.5237172 *	1.4660081 *	2.4960531 *
7	C	2.4872837 *	2.8291631 *	2.4601485 *	3.7870181
8	C	1.3980857 *	2.4231332 *	2.8261629 *	4.2627305
9	C	0.0000000	1.4343913 *	2.4837476 *	3.7801018
10	C	1.4343913 *	0.0000000	1.4070071 *	2.4459870 *
11	C	2.4837476 *	1.4070071 *	0.0000000	1.4384405 *
12	N	3.7801018	2.4459870 *	1.4384405 *	0.0000000
13	C	4.3217123	2.8906471 *	2.4450200 *	1.3203583 *
14	C	5.7734864	4.3405531	3.8315234	2.4981194 *
15	C	6.8004558	5.3807613	4.5825873	3.1444886
16	C	8.1510673	6.7210725	5.9862434	4.5502313
17	C	8.5895537	7.1624950	6.6757563	5.2935253
18	C	7.8292678	6.4440628	6.2160758	4.9657812
19	C	6.4166498	5.0356680	4.8715565	3.7107785
20	O	6.7386281	5.4084882	4.3277472	2.9875075 *
21	N	5.5540055	4.7362588	3.3342113	3.0760134
22	H	4.0664438	4.8677466	4.6597869	5.9612895
23	H	5.9779497	6.2944061	5.5205606	6.4343735
24	H	6.3129939	6.0398413	4.8360353	5.2028519
25	H	2.1654919 *	3.4260677	3.9186818	5.3553446
26	H	1.1146538 *	2.2086819 *	3.4819380	4.6542769
27	H	2.1764023 *	1.0971058 *	2.1756740 *	2.6639228 *
28	H	3.9049967	2.5481586 *	2.6590946 *	2.0698235 *
29	H	8.9575225	7.5448255	6.6754286	5.2440884
30	H	9.6914533	8.2660703	7.7780308	6.3869271
31	H	8.4340872	7.1034972	7.0413373	5.8770903
32	H	5.9368473	4.6522742	4.7987330	3.8946176
33	H	7.6629187	6.3540506	5.2525120	3.9529539
34	H	5.9862001	5.1495104	3.7819386	3.4461220
35	H	6.3832683	5.6376322	4.2482966	3.9927742

C C C C

1	CO	2.8039353 *	3.2015120	2.9564187 *	4.2515074
2	C	6.2115824	7.5072290	7.9513864	9.3475946
3	C	6.6305718	7.7719261	7.9754738	9.3178669
4	C	5.8222685	6.7954878	6.8193567	8.1094727
5	C	4.4215850	5.4038931	5.5071686	6.8389024
6	C	3.7269989	4.9828313	5.4550831	6.8609219
7	C	4.8994992	6.2611213	6.8594150	8.2715134

8 C	5.1147160	6.5643805	7.4043417	8.8041877
9 C	4.3217123	5.7734864	6.8004558	8.1510673
10 C	2.8906471 *	4.3405531	5.3807613	6.7210725
11 C	2.4450200 *	3.8315234	4.5825873	5.9862434
12 N	1.3203583 *	2.4981194 *	3.1444886	4.5502313
13 C	0.0000000	1.4636004 *	2.5922566 *	3.8677172
14 C	1.4636004 *	0.0000000	1.4198927 *	2.4783676 *
15 C	2.5922566 *	1.4198927 *	0.0000000	1.4140079 *
16 C	3.8677172	2.4783676 *	1.4140079 *	0.0000000
17 C	4.3162916	2.8600310 *	2.4511650 *	1.4347015 *
18 C	3.7738515	2.4972893 *	2.8407825 *	2.4775723 *
19 C	2.4438612 *	1.4448097 *	2.4495811 *	2.8408964 *
20 O	3.0725874	2.5019121 *	1.4577664 *	2.4503160 *
21 N	4.2105009	4.8064147	4.5517465	5.7579826
22 H	7.0971563	8.4467424	8.9727593	10.3777515
23 H	7.7189478	8.8296506	8.9665458	10.2817467
24 H	6.4678757	7.2724025	7.0898854	8.2833250
25 H	6.1903069	7.6445808	8.4968387	9.8964231
26 H	4.9726665	6.3777970	7.5210578	8.8168824
27 H	2.5826825 *	3.9177782	5.1321142	6.3710352
28 H	1.0928371 *	2.1610049 *	3.5021997	4.6353746
29 H	4.7586332	3.4632752	2.1725243 *	1.1065232 *
30 H	5.4255220	3.9687570	3.4423875	2.1844132 *
31 H	4.6212462	3.4817645	3.9331506	3.4742636
32 H	2.5823186 *	2.1903032 *	3.4434729	3.9510897
33 H	4.0441307	3.3252426	2.0528111 *	2.5063666 *
34 H	4.4189792	4.9136259	4.6275014	5.7448284
35 H	5.1141510	5.5861187	5.1364071	6.2315174

C C C O

1 CO	5.3975687	5.5584372	4.6326430	1.9340762 *
2 C	10.2660523	9.9656282	8.6540705	7.2064134
3 C	10.3810447	10.2673444	9.0448570	7.0301102
4 C	9.2526628	9.2769057	8.1472464	5.7755978
5 C	7.9234741	7.8920283	6.7462953	4.5755202
6 C	7.7410451	7.4526695	6.1674752	4.8446243
7 C	9.0789718	8.6725883	7.3269073	6.2982594
8 C	9.4214192	8.8094541	7.4080975	7.0832815
9 C	8.5895537	7.8292678	6.4166498	6.7386281
10 C	7.1624950	6.4440628	5.0356680	5.4084882
11 C	6.6757563	6.2160758	4.8715565	4.3277472
12 N	5.2935253	4.9657812	3.7107785	2.9875075 *
13 C	4.3162916	3.7738515	2.4438612 *	3.0725874
14 C	2.8600310 *	2.4972893 *	1.4448097 *	2.5019121 *
15 C	2.4511650 *	2.8407825 *	2.4495811 *	1.4577664 *

16 C	1.4347015 *	2.4775723 *	2.8408964 *	2.4503160 *
17 C	0.0000000	1.4135231 *	2.4421429 *	3.7598947
18 C	1.4135231 *	0.0000000	1.4189721 *	4.2878948
19 C	2.4421429 *	1.4189721 *	0.0000000	3.7948406
20 O	3.7598947	4.2878948	3.7948406	0.0000000
21 N	6.9785981	7.1869876	6.2310991	3.4291643
22 H	11.2456921	10.8699369	9.5248050	8.2774185
23 H	11.3890791	11.3247849	10.1221565	7.9523839
24 H	9.5215381	9.7009548	8.6738011	5.9125344
25 H	10.5001747	9.8562958	8.4485347	8.1567861
26 H	9.1060483	8.2104478	6.8124742	7.6065869
27 H	6.6088666	5.7360041	4.3353103	5.4388894
28 H	4.8014803	3.9561907	2.5372577 *	4.1485490
29 H	2.2349372 *	3.4930841	3.9469503	2.6321997 *
30 H	1.1095330 *	2.2046369 *	3.4601810	4.6221744
31 H	2.1895623 *	1.0931710 *	2.1781031 *	5.3774247
32 H	3.4593826	2.2087242 *	1.1108727 *	4.6769091
33 H	3.9059966	4.7048672	4.4711803	1.0072733 *
34 H	6.9517552	7.1952287	6.2921059	3.6246770
35 H	7.5404164	7.8891570	7.0286127	3.8407549

N H H H

1 CO	1.9296663 *	6.3749183	6.1212518	4.3115022
2 C	4.3460974	1.1114162 *	2.2182426 *	3.4413964
3 C	3.8119284	2.1672759 *	1.1058600 *	2.2193816 *
4 C	2.4438385 *	3.4352379	2.1952146 *	1.1135346 *
5 C	1.5402431 *	3.9283553	3.4659169	2.1618246 *
6 C	2.6788379 *	3.5198833	4.0635719	3.5179731
7 C	3.9524685	2.1996862 *	3.5322840	3.9728128
8 C	5.2124914	2.6692842 *	4.7052288	5.4170047
9 C	5.5540055	4.0664438	5.9779497	6.3129939
10 C	4.7362588	4.8677466	6.2944061	6.0398413
11 C	3.3342113	4.6597869	5.5205606	4.8360353
12 N	3.0760134	5.9612895	6.4343735	5.2028519
13 C	4.2105009	7.0971563	7.7189478	6.4678757
14 C	4.8064147	8.4467424	8.8296506	7.2724025
15 C	4.5517465	8.9727593	8.9665458	7.0898854
16 C	5.7579826	10.3777515	10.2817467	8.2833250
17 C	6.9785981	11.2456921	11.3890791	9.5215381
18 C	7.1869876	10.8699369	11.3247849	9.7009548
19 C	6.2310991	9.5248050	10.1221565	8.6738011
20 O	3.4291643	8.2774185	7.9523839	5.9125344
21 N	0.0000000	5.4563873	4.6362612	2.5440644 *
22 H	5.4563873	0.0000000	2.5562329 *	4.3682245
23 H	4.6362612	2.5562329 *	0.0000000	2.5318795 *

24 H	2.5440644 *	4.3682245	2.5318795 *	0.0000000
25 H	6.1201447	2.3680443 *	4.7837346	5.9670987
26 H	6.6498563	4.7864925	6.9138207	7.4064783
27 H	5.4284343	5.9398556	7.3798045	6.9911110
28 H	5.0757682	7.1844477	8.1359581	7.1632935
29 H	5.9060500	10.8619268	10.5165607	8.3535640
30 H	7.9208896	12.3311350	12.4022122	10.4549595
31 H	8.2368018	11.6923479	12.2813716	10.7351682
32 H	6.7112351	9.3693696	10.2400288	9.0355408
33 H	3.9490985	9.0002908	8.4738167	6.2961497
34 H	1.0359060 *	5.8932769	4.9954626	2.8630804 *
35 H	1.0370491 *	5.8076446	4.5720845	2.1977998 *

H H H H

1 CO	6.4067354	6.2420772	4.4739695	3.8121869
2 C	2.6616546 *	4.6967956	5.3747354	6.4156688
3 C	4.0621070	5.9815712	6.2944457	7.0340713
4 C	4.8710875	6.3095324	6.0392651	6.4069136
5 C	4.6657208	5.5429839	4.8478649	5.0420724
6 C	3.5157269	4.0749236	3.5119866	4.0855708
7 C	2.1811338 *	3.5128729	3.9256120	5.0155796
8 C	1.0928908 *	2.2102466 *	3.4081453	4.9259253
9 C	2.1654919 *	1.1146538 *	2.1764023 *	3.9049967
10 C	3.4260677	2.2086819 *	1.0971058 *	2.5481586 *
11 C	3.9186818	3.4819380	2.1756740 *	2.6590946 *
12 N	5.3553446	4.6542769	2.6639228 *	2.0698235 *
13 C	6.1903069	4.9726665	2.5826825 *	1.0928371 *
14 C	7.6445808	6.3777970	3.9177782	2.1610049 *
15 C	8.4968387	7.5210578	5.1321142	3.5021997
16 C	9.8964231	8.8168824	6.3710352	4.6353746
17 C	10.5001747	9.1060483	6.6088666	4.8014803
18 C	9.8562958	8.2104478	5.7360041	3.9561907
19 C	8.4485347	6.8124742	4.3353103	2.5372577 *
20 O	8.1567861	7.6065869	5.4388894	4.1485490
21 N	6.1201447	6.6498563	5.4284343	5.0757682
22 H	2.3680443 *	4.7864925	5.9398556	7.1844477
23 H	4.7837346	6.9138207	7.3798045	8.1359581
24 H	5.9670987	7.4064783	6.9911110	7.1632935
25 H	0.0000000	2.5526752 *	4.3244952	5.9440891
26 H	2.5526752 *	0.0000000	2.4991229 *	4.3538830
27 H	4.3244952	2.4991229 *	0.0000000	1.9094645 *
28 H	5.9440891	4.3538830	1.9094645 *	0.0000000
29 H	10.5868096	9.6910189	7.2932377	5.6166133
30 H	11.6075436	10.1900838	7.6916245	5.8896246
31 H	10.5242762	8.6939522	6.2859578	4.5997386

32 H	8.0493326	6.1741543	3.7910873	2.1877010 *
33 H	9.0134366	8.5399453	6.3882661	5.1070002
34 H	6.5694405	7.0637349	5.7991795	5.2577619
35 H	6.7582659	7.4877908	6.3504235	6.0248081

H H H H

1 CO	4.5637497	6.3727354	6.6051059	5.1807996
2 C	9.7963420	11.3403453	10.8310783	8.5891085
3 C	9.6161492	11.4118376	11.2103115	9.1429271
4 C	8.3243114	10.2459318	10.2714268	8.3930462
5 C	7.1506822	8.9417404	8.8770386	6.9956976
6 C	7.3824823	8.8198230	8.3443617	6.2003437
7 C	8.8311634	10.1719068	9.4952345	7.1956842
8 C	9.4966717	10.5286256	9.5091918	7.0636003
9 C	8.9575225	9.6914533	8.4340872	5.9368473
10 C	7.5448255	8.2660703	7.1034972	4.6522742
11 C	6.6754286	7.7780308	7.0413373	4.7987330
12 N	5.2440884	6.3869271	5.8770903	3.8946176
13 C	4.7586332	5.4255220	4.6212462	2.5823186 *
14 C	3.4632752	3.9687570	3.4817645	2.1903032 *
15 C	2.1725243 *	3.4423875	3.9331506	3.4434729
16 C	1.1065232 *	2.1844132 *	3.4742636	3.9510897
17 C	2.2349372 *	1.1095330 *	2.1895623 *	3.4593826
18 C	3.4930841	2.2046369 *	1.0931710 *	2.2087242 *
19 C	3.9469503	3.4601810	2.1781031 *	1.1108727 *
20 O	2.6321997 *	4.6221744	5.3774247	4.6769091
21 N	5.9060500	7.9208896	8.2368018	6.7112351
22 H	10.8619268	12.3311350	11.6923479	9.3693696
23 H	10.5165607	12.4022122	12.2813716	10.2400288
24 H	8.3535640	10.4549595	10.7351682	9.0355408
25 H	10.5868096	11.6075436	10.5242762	8.0493326
26 H	9.6910189	10.1900838	8.6939522	6.1741543
27 H	7.2932377	7.6916245	6.2859578	3.7910873
28 H	5.6166133	5.8896246	4.5997386	2.1877010 *
29 H	0.0000000	2.5486155 *	4.4101533	5.0568298
30 H	2.5486155 *	0.0000000	2.5569725 *	4.3967815
31 H	4.4101533	2.5569725 *	0.0000000	2.5348461 *
32 H	5.0568298	4.3967815	2.5348461 *	0.0000000
33 H	2.2714875 *	4.5806858	5.7710117	5.4349325
34 H	5.8625032	7.8655143	8.2366812	6.7993756
35 H	6.2146347	8.4153787	8.9616838	7.5813125

H H H

1 CO	2.6491928 *	2.5326827 *	2.5364394 *
------	-------------	-------------	-------------

2 C	7.9164687	4.8073113	4.7227655
3 C	7.6181262	4.2372318	3.9288669
4 C	6.3058751	2.8989690 *	2.5048178 *
5 C	5.2255218	2.1518853 *	2.1249888 *
6 C	5.6581594	3.2108180	3.4581543
7 C	7.1037251	4.4435706	4.5828791
8 C	7.9546945	5.6721577	5.9224426
9 C	7.6629187	5.9862001	6.3832683
10 C	6.3540506	5.1495104	5.6376322
11 C	5.2525120	3.7819386	4.2482966
12 N	3.9529539	3.4461220	3.9927742
13 C	4.0441307	4.4189792	5.1141510
14 C	3.3252426	4.9136259	5.5861187
15 C	2.0528111 *	4.6275014	5.1364071
16 C	2.5063666 *	5.7448284	6.2315174
17 C	3.9059966	6.9517552	7.5404164
18 C	4.7048672	7.1952287	7.8891570
19 C	4.4711803	6.2921059	7.0286127
20 O	1.0072733 *	3.6246770	3.8407549
21 N	3.9490985	1.0359060 *	1.0370491 *
22 H	9.0002908	5.8932769	5.8076446
23 H	8.4738167	4.9954626	4.5720845
24 H	6.2961497	2.8630804 *	2.1977998 *
25 H	9.0134366	6.5694405	6.7582659
26 H	8.5399453	7.0637349	7.4877908
27 H	6.3882661	5.7991795	6.3504235
28 H	5.1070002	5.2577619	6.0248081
29 H	2.2714875 *	5.8625032	6.2146347
30 H	4.5806858	7.8655143	8.4153787
31 H	5.7710117	8.2366812	8.9616838
32 H	5.4349325	6.7993756	7.5813125
33 H	0.0000000	4.1486819	4.1234969
34 H	4.1486819	0.0000000	1.6298488 *
35 H	4.1234969	1.6298488 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.60 , TOTAL = 1208.0 SECONDS (20.1 MIN)
WALL CLOCK TIME: STEP = 0.61 , TOTAL = 1115.6 SECONDS (18.6 MIN)

CPU UTILIZATION: STEP = 98.31% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.96, TOTAL = 1208.9 SECONDS (20.1 MIN)
 WALL CLOCK TIME: STEP = 0.96, TOTAL = 1116.5 SECONDS (18.6 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
 INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.614323215	-284.614323215	0.539528548	0.009731180	199612137
11259110						
2	1	-284.620118215	-0.005795000	0.631636138	0.002002784	183896212
12604446						
3	2	-284.619854854	0.000263361	0.218070663	0.003033744	180394747
12931825						
4	3	-284.620655854	-0.000801000	0.124646522	0.000813007	173707511
13485109						
5	4	-284.620630485	0.000025370	0.017154465	0.001317199	167574299
14021770						
6	5	-284.620680608	-0.000050124	0.067055741	0.000375160	155599837
15002821						
7	6	-284.620678040	0.000002569	0.008132682	0.000458593	160371696
14637162						
8	7	-284.620684555	-0.000006516	0.017606994	0.000110963	166872160
14071724						
9	8	-284.620685160	-0.000000605	0.007250694	0.000101881	187651633
12371431						
10	9	-284.620686487	-0.000001327	0.019091828	0.000118158	183274746
12771738						

-----DISABLING FDIFF OPTION-----

11	10	-284.620687970	-0.000001483	0.005042331	0.000099843	199620260
11256635						
12	11	-284.620688273	-0.000000303	0.012672804	0.000082793	199623013
11256424						
13	12	-284.620688758	-0.000000485	0.007112558	0.000066591	199617986
11256834						
14	13	-284.620688963	-0.000000205	0.004373427	0.000042484	199615285
11257067						
15	14	-284.620689123	-0.000000160	0.004819445	0.000021277	199616896
11256920						
16	15	-284.620689158	-0.000000035	0.000328081	0.000026365	199618826
11256746						

17 16	-284.620689183	-0.000000025	0.000635281	0.000021750	199618669
11256765					
18 17	-284.620689194	-0.000000011	0.000481357	0.000015929	199618475
11256789					
19 18	-284.620689207	-0.000000013	0.000506948	0.000008643	199618536
11256777					
20 19	-284.620689213	-0.000000006	0.000714522	0.000003887	199618858
11256762					
21 20	-284.620689214	-0.000000001	0.000368246	0.000003288	199618707
11256776					
22 21	-284.620689215	-0.000000001	0.000094091	0.000003170	199618841
11256777					
23 22	-284.620689215	-0.000000001	0.000134370	0.000002935	199618797
11256784					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 79.8 SECONDS (3.5 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 25.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.2
TIME TO SOLVE SCF EQUATIONS= 2.1 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6206892154 AFTER 23 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6287222950
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000147076

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 83.24 , TOTAL = 1292.2 SECONDS (21.5 MIN)
WALL CLOCK TIME: STEP = 77.09 , TOTAL = 1193.6 SECONDS (19.9 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.81 , TOTAL = 1296.0 SECONDS (21.6 MIN)
WALL CLOCK TIME: STEP = 3.81 , TOTAL = 1197.4 SECONDS (20.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.83 , TOTAL = 1298.8 SECONDS (21.6 MIN)
WALL CLOCK TIME: STEP = 2.74 , TOTAL = 1200.2 SECONDS (20.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 8 ENERGY= -284.6206892

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0023180	0.0077022	-0.0025675
2 C	6.0	-0.0104682	-0.0085274	-0.0006455
3 C	6.0	0.0112878	0.0049674	0.0017420
4 C	6.0	-0.0052179	-0.0006164	0.0006073
5 C	6.0	0.0053663	0.0033141	0.0000538
6 C	6.0	-0.0044461	-0.0009171	0.0001272
7 C	6.0	-0.0058680	0.0099381	0.0023130
8 C	6.0	0.0003816	0.0034679	0.0007300
9 C	6.0	0.0085280	0.0004768	-0.0000405
10 C	6.0	-0.0102055	-0.0069379	-0.0007197
11 C	6.0	0.0013427	0.0048644	0.0019533
12 N	7.0	0.0013652	0.0090875	-0.0004788
13 C	6.0	0.0046753	0.0031948	-0.0022557
14 C	6.0	-0.0057103	-0.0156954	-0.0037804
15 C	6.0	0.0173987	0.0118657	-0.0009958
16 C	6.0	-0.0053990	-0.0065583	-0.0041648
17 C	6.0	0.0015086	0.0181454	0.0003710
18 C	6.0	-0.0120804	-0.0056704	0.0021665
19 C	6.0	0.0021253	0.0017955	-0.0009903
20 O	8.0	0.0065291	0.0098939	-0.0066536
21 N	7.0	-0.0075726	-0.0083616	-0.0025439
22 H	1.0	0.0033005	0.0013605	-0.0001993
23 H	1.0	-0.0003318	-0.0045027	-0.0017931

24 H	1.0	-0.0029932	-0.0043305	-0.0006948
25 H	1.0	-0.0074926	-0.0043681	-0.0006260
26 H	1.0	-0.0028003	0.0070299	0.0013364
27 H	1.0	0.0024900	-0.0022654	-0.0012251
28 H	1.0	0.0027875	-0.0084175	0.0040641
29 H	1.0	0.0055475	-0.0002791	-0.0008673
30 H	1.0	-0.0014965	-0.0028865	0.0021856
31 H	1.0	0.0067720	-0.0038026	-0.0002961
32 H	1.0	0.0034166	0.0032454	0.0029673
33 H	1.0	-0.0033481	-0.0109304	0.0074666
34 H	1.0	0.0030377	-0.0058057	0.0068521
35 H	1.0	-0.0047479	0.0005237	-0.0033981

MAXIMUM GRADIENT = 0.0181454 RMS GRADIENT = 0.0057328
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0040353794
 PREDICTED ENERGY CHANGE WAS -0.0048452233 RATIO= 0.833
 GDIIS STEP HAS LENGTH = 0.207841
 RADIUS OF STEP TAKEN= 0.20784 CURRENT TRUST RADIUS= 0.42470

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 1298.8 SECONDS (21.6 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1200.2 SECONDS (20.0
 MIN)
 CPU UTILIZATION: STEP = 96.68% , TOTAL = 100.00%

INSERCH= 9

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1470908038	-1.5790333063	1.0135092420
C	6.0	4.9420097238	0.6488835420	0.4363213252
C	6.0	5.1644574262	-0.7142449039	0.1871716848
C	6.0	4.0220513180	-1.5625688468	0.0590902955
C	6.0	2.7156959581	-1.0696134302	0.1738306611
C	6.0	2.4381698437	0.3354837763	0.4591714272
C	6.0	3.6213810111	1.1951952032	0.5775487528
C	6.0	3.4924114811	2.6189047645	0.8341550722
C	6.0	2.2457902514	3.2519947030	0.9967536894
C	6.0	1.0884083149	2.4316950662	0.9147718190
C	6.0	1.1642222053	1.0401060656	0.6499803869
N	7.0	-0.0670662253	0.2773830059	0.6415189413
C	6.0	-1.2855767913	0.7965971426	0.5114254966
C	6.0	-2.5571700114	0.0879353513	0.5124785629

C	6.0	-2.7972021857	-1.3313593787	0.5970008421
C	6.0	-4.0724644274	-1.8719969017	0.5227014200
C	6.0	-5.2163243983	-1.0116318381	0.5072701814
C	6.0	-5.0369998336	0.4076305776	0.5082874576
C	6.0	-3.7299466796	0.9331013679	0.4797462357
O	8.0	-1.6864849892	-2.2344106707	0.8666662842
N	7.0	1.6724796109	-2.1629600238	-0.0286213165
H	1.0	5.8119785266	1.3275544339	0.5187237099
H	1.0	6.1830602047	-1.1452942796	0.0639367904
H	1.0	4.1697949319	-2.6439913825	-0.1560101854
H	1.0	4.4226889218	3.2284514870	0.9082505718
H	1.0	2.1485784644	4.3386251981	1.1999409473
H	1.0	0.1043585956	2.9117529808	1.0904264845
H	1.0	-1.3696516555	1.8773879991	0.3931845059
H	1.0	-4.1939795609	-2.9734240653	0.5202896022
H	1.0	-6.2243699197	-1.4522335224	0.5374010916
H	1.0	-5.9060600336	1.0735868378	0.5398243678
H	1.0	-3.5654451975	2.0272636881	0.4891574294
H	1.0	-2.0063261398	-3.1290933677	1.1139224185
H	1.0	1.4390500382	-2.3139599327	-1.0400619684
H	1.0	2.0573874172	-3.0926123405	0.2631227730

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3186471	5.1579706	3.9908026
2 C	5.3186471	0.0000000	1.4034521 *	2.4246955 *
3 C	5.1579706	1.4034521 *	0.0000000	1.4286882 *
4 C	3.9908026	2.4246955 *	1.4286882 *	0.0000000
5 C	2.7499638 *	2.8246427 *	2.4744489 *	1.4009763 *
6 C	3.0367267	2.5234809 *	2.9340344 *	2.5042662 *
7 C	4.4673368	1.4361274 *	2.4858481 *	2.8345367 *
8 C	5.3708493	2.4780215 *	3.7847341	4.2855531
9 C	5.2672243	3.7894421	4.9905007	5.2167364
10 C	4.1208943	4.2728884	5.2000497	5.0291745
11 C	2.8331256 *	3.8039958	4.3924732	3.9102756
12 N	1.9053928 *	5.0270230	5.3440244	4.5216732
13 C	2.8192631 *	6.2297908	6.6325505	5.8259066
14 C	3.2160290	7.5205159	7.7699967	6.7982261
15 C	2.9839040 *	7.9901552	7.9960499	6.8443425
16 C	4.2580942	9.3607181	9.3152399	8.1136839
17 C	5.4170513	10.2934007	10.3899727	9.2656345
18 C	5.5746640	9.9821848	10.2679818	9.2816955
19 C	4.6504992	8.6767213	9.0504019	8.1546793

20	O	1.9527116 *	7.2412378	7.0503921	5.8043895
21	N	1.9374771 *	4.3373336	3.7867204	2.4266541 *
22	H	6.3862366	1.1064493 *	2.1675227 *	3.4304395
23	H	6.1255811	2.2131314 *	1.1128980 *	2.2009318 *
24	H	4.3225062	3.4336857	2.1979647 *	1.1124617 *
25	H	6.4345729	2.6733092 *	4.0761538	4.8821573
26	H	6.2497513	4.6904762	5.9709902	6.2956757
27	H	4.4916482	5.3806412	6.2903362	6.0358534
28	H	3.8252005	6.4302530	7.0323242	6.4043253
29	H	4.5861185	9.8282482	9.6330266	8.3490347
30	H	6.3904827	11.3627877	11.4180855	10.2581725
31	H	6.6258136	10.8568735	11.2194948	10.2833758
32	H	5.2022348	8.6185563	9.1552315	8.4048771
33	H	2.6551786 *	7.9379861	7.6230241	6.3172783
34	H	2.5350405 *	4.8196344	4.2360183	2.9059628 *
35	H	2.5501440 *	4.7275612	3.9136025	2.4985129 *

C C C C

1	CO	2.7499638 *	3.0367267	4.4673368	5.3708493
2	C	2.8246427 *	2.5234809 *	1.4361274 *	2.4780215 *
3	C	2.4744489 *	2.9340344 *	2.4858481 *	3.7847341
4	C	1.4009763 *	2.5042662 *	2.8345367 *	4.2855531
5	C	0.0000000	1.4603898 *	2.4723697 *	3.8268109
6	C	1.4603898 *	0.0000000	1.4673464 *	2.5428428 *
7	C	2.4723697 *	1.4673464 *	0.0000000	1.4523873 *
8	C	3.8268109	2.5428428 *	1.4523873 *	0.0000000
9	C	4.4242864	2.9718749 *	2.5096627 *	1.4075886 *
10	C	3.9314399	2.5344683 *	2.8387677 *	2.4126288 *
11	C	2.6617111 *	1.4682790 *	2.4631136 *	2.8190408 *
12	N	3.1268030	2.5125354 *	3.8014621	4.2649401
13	C	4.4279675	3.7525518	4.9235645	5.1238785
14	C	5.4090403	5.0017539	6.2773204	6.5655707
15	C	5.5353076	5.4960425	6.8979756	7.4310207
16	C	6.8443153	6.8749811	8.2828699	8.8029852
17	C	7.9392374	7.7722787	9.1093392	9.4408543
18	C	7.8992660	7.4756792	8.6944013	8.8174135
19	C	6.7565346	6.1970341	7.3566485	7.4249577
20	O	4.6060798	4.8768009	6.3260752	7.0976543
21	N	1.5246947 *	2.6582785 *	3.9297411	5.1887153
22	H	3.9309453	3.5171488	2.1953808 *	2.6734760 *
23	H	3.4699307	4.0463710	3.5076899	4.6906312
24	H	2.1683784 *	3.5006065	3.9469254	5.3979025
25	H	4.6825804	3.5368418	2.2103369 *	1.1146540 *
26	H	5.5338567	4.0813899	3.5267083	2.2129448 *
27	H	4.8487637	3.5330328	3.9470319	3.4103281

28 H	5.0421224	4.1086893	5.0408119	4.9380118
29 H	7.1755240	7.4120181	8.8577947	9.5106919
30 H	8.9556328	8.8454309	10.1955531	10.5393582
31 H	8.8916779	8.3771996	9.5282918	9.5292132
32 H	7.0101935	6.2375005	7.2353730	7.0910086
33 H	5.2366710	5.6732300	7.1174614	7.9595143
34 H	2.1567935 *	3.2039808	4.4377249	5.6623438
35 H	2.1292881 *	3.4547465	4.5749572	5.9166544

C C C N

1 CO	5.2672243	4.1208943	2.8331256 *	1.9053928 *
2 C	3.7894421	4.2728884	3.8039958	5.0270230
3 C	4.9905007	5.2000497	4.3924732	5.3440244
4 C	5.2167364	5.0291745	3.9102756	4.5216732
5 C	4.4242864	3.9314399	2.6617111 *	3.1268030
6 C	2.9718749 *	2.5344683 *	1.4682790 *	2.5125354 *
7 C	2.5096627 *	2.8387677 *	2.4631136 *	3.8014621
8 C	1.4075886 *	2.4126288 *	2.8190408 *	4.2649401
9 C	0.0000000	1.4209664 *	2.4864618 *	3.7846812
10 C	1.4209664 *	0.0000000	1.4185846 *	2.4598474 *
11 C	2.4864618 *	1.4185846 *	0.0000000	1.4484092 *
12 N	3.7846812	2.4598474 *	1.4484092 *	0.0000000
13 C	4.3284031	2.9106767 *	2.4657675 *	1.3308928 *
14 C	5.7718473	4.3526188	3.8437346	2.5006317 *
15 C	6.8263248	5.4184431	4.6173086	3.1691760
16 C	8.1486415	6.7312771	5.9932821	4.5472152
17 C	8.6082089	7.1952910	6.7038325	5.3098439
18 C	7.8337755	6.4639532	6.2350026	4.9734249
19 C	6.4307072	5.0647384	4.8982975	3.7246248
20 O	6.7513225	5.4290782	4.3469465	2.9970512 *
21 N	5.5409217	4.7267309	3.3133757	3.0708927
22 H	4.0804022	4.8670418	4.6584862	5.9733664
23 H	5.9756500	6.2828537	5.5052844	6.4359686
24 H	6.3081939	6.0335819	4.8224125	5.2078281
25 H	2.1788242 *	3.4281614	3.9335944	5.3793914
26 H	1.1097302 *	2.2003783 *	3.4859206	4.6598932
27 H	2.1703153 *	1.1089022 *	2.1955331 *	2.6778367 *
28 H	3.9147490	2.5732020 *	2.6809517 *	2.0780796 *
29 H	8.9695871	7.5679952	6.6959368	5.2548889
30 H	9.6997104	8.2887897	7.7984437	6.3964680
31 H	8.4502608	7.1349584	7.0712196	5.8939063
32 H	5.9605434	4.6907425	4.8342629	3.9145820
33 H	7.6689313	6.3670566	5.2583118	3.9481610
34 H	5.9815800	5.1444695	3.7658375	3.4367366
35 H	6.3896595	5.6463740	4.2457937	4.0016691

	C	C	C	C
1 CO	2.8192631 *	3.2160290	2.9839040 *	4.2580942
2 C	6.2297908	7.5205159	7.9901552	9.3607181
3 C	6.6325505	7.7699967	7.9960499	9.3152399
4 C	5.8259066	6.7982261	6.8443425	8.1136839
5 C	4.4279675	5.4090403	5.5353076	6.8443153
6 C	3.7525518	5.0017539	5.4960425	6.8749811
7 C	4.9235645	6.2773204	6.8979756	8.2828699
8 C	5.1238785	6.5655707	7.4310207	8.8029852
9 C	4.3284031	5.7718473	6.8263248	8.1486415
10 C	2.9106767 *	4.3526188	5.4184431	6.7312771
11 C	2.4657675 *	3.8437346	4.6173086	5.9932821
12 N	1.3308928 *	2.5006317 *	3.1691760	4.5472152
13 C	0.0000000	1.4557307 *	2.6116151 *	3.8585313
14 C	1.4557307 *	0.0000000	1.4419282 *	2.4774092 *
15 C	2.6116151 *	1.4419282 *	0.0000000	1.3871204 *
16 C	3.8585313	2.4774092 *	1.3871204 *	0.0000000
17 C	4.3267177	2.8775297 *	2.4418087 *	1.4313916 *
18 C	3.7715355	2.5003557 *	2.8370142 *	2.4753258 *
19 C	2.4483834 *	1.4459537 *	2.4518449 *	2.8262590 *
20 O	3.0779753	2.5053607 *	1.4566790 *	2.4377353 *
21 N	4.2190908	4.8217481	4.5892285	5.7786675
22 H	7.1173914	8.4604575	9.0107681	10.3893868
23 H	7.7299241	8.8381938	8.9979937	10.2914696
24 H	6.4841499	7.2912522	7.1294514	8.3061101
25 H	6.2173695	7.6640660	8.5449154	9.9161914
26 H	4.9813089	6.3784824	7.5480466	8.8165671
27 H	2.5963526 *	3.9232263	5.1639642	6.3759254
28 H	1.0904854 *	2.1509467 *	3.5178831	4.6238359
29 H	4.7615066	3.4714735	2.1571389 *	1.1081126 *
30 H	5.4267478	3.9775742	3.4298165	2.1925133 *
31 H	4.6288654	3.4910344	3.9309073	3.4697017
32 H	2.5909141 *	2.1858996 *	3.4470533	3.9322292
33 H	4.0365243	3.3188006	2.0308964 *	2.4897312 *
34 H	4.4165903	4.9141894	4.6466452	5.7458117
35 H	5.1344926	5.6100091	5.1749905	6.2555868

	C	C	C	O
1 CO	5.4170513	5.5746640	4.6504992	1.9527116 *
2 C	10.2934007	9.9821848	8.6767213	7.2412378
3 C	10.3899727	10.2679818	9.0504019	7.0503921
4 C	9.2656345	9.2816955	8.1546793	5.8043895
5 C	7.9392374	7.8992660	6.7565346	4.6060798

6 C	7.7722787	7.4756792	6.1970341	4.8768009
7 C	9.1093392	8.6944013	7.3566485	6.3260752
8 C	9.4408543	8.8174135	7.4249577	7.0976543
9 C	8.6082089	7.8337755	6.4307072	6.7513225
10 C	7.1952910	6.4639532	5.0647384	5.4290782
11 C	6.7038325	6.2350026	4.8982975	4.3469465
12 N	5.3098439	4.9734249	3.7246248	2.9970512 *
13 C	4.3267177	3.7715355	2.4483834 *	3.0779753
14 C	2.8775297 *	2.5003557 *	1.4459537 *	2.5053607 *
15 C	2.4418087 *	2.8370142 *	2.4518449 *	1.4566790 *
16 C	1.4313916 *	2.4753258 *	2.8262590 *	2.4377353 *
17 C	0.0000000	1.4305468 *	2.4478692 *	3.7528815
18 C	1.4305468 *	0.0000000	1.4090146 *	4.2819116
19 C	2.4478692 *	1.4090146 *	0.0000000	3.7892711
20 O	3.7528815	4.2819116	3.7892711	0.0000000
21 N	7.0048809	7.2050900	6.2474189	3.4769654
22 H	11.2736591	10.8879153	9.5501544	8.3087673
23 H	11.4087852	11.3357298	10.1370771	7.9850041
24 H	9.5500667	9.7220758	8.6951536	5.9589964
25 H	10.5380107	9.8794085	8.4804313	8.1955231
26 H	9.1294489	8.2197104	6.8317883	7.6173213
27 H	6.6364665	5.7483112	4.3577390	5.4534567
28 H	4.8121037	3.9525787	2.5436515 *	4.1510790
29 H	2.2122358 *	3.4845886	3.9341977	2.6369768 *
30 H	1.1005424 *	2.2067600 *	3.4518537	4.6165589
31 H	2.1965728 *	1.0953346 *	2.1814708 *	5.3716372
32 H	3.4584124	2.1883899 *	1.1064992 *	4.6727800
33 H	3.8930398	4.6968280	4.4580795	0.9817796 *
34 H	6.9558827	7.1933068	6.2906082	3.6620909
35 H	7.5694763	7.9146786	7.0531222	3.8881044

N H H H

1 CO	1.9374771 *	6.3862366	6.1255811	4.3225062
2 C	4.3373336	1.1064493 *	2.2131314 *	3.4336857
3 C	3.7867204	2.1675227 *	1.1128980 *	2.1979647 *
4 C	2.4266541 *	3.4304395	2.2009318 *	1.1124617 *
5 C	1.5246947 *	3.9309453	3.4699307	2.1683784 *
6 C	2.6582785 *	3.5171488	4.0463710	3.5006065
7 C	3.9297411	2.1953808 *	3.5076899	3.9469254
8 C	5.1887153	2.6734760 *	4.6906312	5.3979025
9 C	5.5409217	4.0804022	5.9756500	6.3081939
10 C	4.7267309	4.8670418	6.2828537	6.0335819
11 C	3.3133757	4.6584862	5.5052844	4.8224125
12 N	3.0708927	5.9733664	6.4359686	5.2078281
13 C	4.2190908	7.1173914	7.7299241	6.4841499

14 C	4.8217481	8.4604575	8.8381938	7.2912522
15 C	4.5892285	9.0107681	8.9979937	7.1294514
16 C	5.7786675	10.3893868	10.2914696	8.3061101
17 C	7.0048809	11.2736591	11.4087852	9.5500667
18 C	7.2050900	10.8879153	11.3357298	9.7220758
19 C	6.2474189	9.5501544	10.1370771	8.6951536
20 O	3.4769654	8.3087673	7.9850041	5.9589964
21 N	0.0000000	5.4423092	4.6248836	2.5464098 *
22 H	5.4423092	0.0000000	2.5415573 *	4.3503114
23 H	4.6248836	2.5415573 *	0.0000000	2.5194656 *
24 H	2.5464098 *	4.3503114	2.5194656 *	0.0000000
25 H	6.1244345	2.3864757 *	4.7897207	5.9734573
26 H	6.6337505	4.7907311	6.9022403	7.3946503
27 H	5.4280737	5.9509205	7.3799679	6.9962613
28 H	5.0751251	7.2037413	8.1417731	7.1714681
29 H	5.9475624	10.8911715	10.5467185	8.3975372
30 H	7.9489462	12.3531880	12.4202537	10.4852167
31 H	8.2603044	11.7208094	12.3002736	10.7623151
32 H	6.7276984	9.4035389	10.2605699	9.0592938
33 H	3.9714521	9.0189722	8.4914061	6.3239643
34 H	1.0489531 *	5.9002494	5.0090144	2.8891930 *
35 H	1.0476269 *	5.8051839	4.5664974	2.1998179 *

H H H H

1 CO	6.4345729	6.2497513	4.4916482	3.8252005
2 C	2.6733092 *	4.6904762	5.3806412	6.4302530
3 C	4.0761538	5.9709902	6.2903362	7.0323242
4 C	4.8821573	6.2956757	6.0358534	6.4043253
5 C	4.6825804	5.5338567	4.8487637	5.0421224
6 C	3.5368418	4.0813899	3.5330328	4.1086893
7 C	2.2103369 *	3.5267083	3.9470319	5.0408119
8 C	1.1146540 *	2.2129448 *	3.4103281	4.9380118
9 C	2.1788242 *	1.1097302 *	2.1703153 *	3.9147490
10 C	3.4281614	2.2003783 *	1.1089022 *	2.5732020 *
11 C	3.9335944	3.4859206	2.1955331 *	2.6809517 *
12 N	5.3793914	4.6598932	2.6778367 *	2.0780796 *
13 C	6.2173695	4.9813089	2.5963526 *	1.0904854 *
14 C	7.6640660	6.3784824	3.9232263	2.1509467 *
15 C	8.5449154	7.5480466	5.1639642	3.5178831
16 C	9.9161914	8.8165671	6.3759254	4.6238359
17 C	10.5380107	9.1294489	6.6364665	4.8121037
18 C	9.8794085	8.2197104	5.7483112	3.9525787
19 C	8.4804313	6.8317883	4.3577390	2.5436515 *
20 O	8.1955231	7.6173213	5.4534567	4.1510790
21 N	6.1244345	6.6337505	5.4280737	5.0751251

22 H	2.3864757 *	4.7907311	5.9509205	7.2037413
23 H	4.7897207	6.9022403	7.3799679	8.1417731
24 H	5.9734573	7.3946503	6.9962613	7.1714681
25 H	0.0000000	2.5473805 *	4.3337585	5.9700817
26 H	2.5473805 *	0.0000000	2.4953542 *	4.3688085
27 H	4.3337585	2.4953542 *	0.0000000	1.9310007 *
28 H	5.9700817	4.3688085	1.9310007 *	0.0000000
29 H	10.6235940	9.7034031	7.3099983	5.6145669
30 H	11.6364171	10.2019247	7.7073355	5.8885879
31 H	10.5575676	8.7162739	6.3092907	4.6094035
32 H	8.0888057	6.2046492	3.8224738	2.2029941 *
33 H	9.0439434	8.5461952	6.3990129	5.0980068
34 H	6.5891082	7.0553478	5.7990049	5.2450356
35 H	6.7798738	7.4906098	6.3679790	6.0384117

H H H H

1 CO	4.5861185	6.3904827	6.6258136	5.2022348
2 C	9.8282482	11.3627877	10.8568735	8.6185563
3 C	9.6330266	11.4180855	11.2194948	9.1552315
4 C	8.3490347	10.2581725	10.2833758	8.4048771
5 C	7.1755240	8.9556328	8.8916779	7.0101935
6 C	7.4120181	8.8454309	8.3771996	6.2375005
7 C	8.8577947	10.1955531	9.5282918	7.2353730
8 C	9.5106919	10.5393582	9.5292132	7.0910086
9 C	8.9695871	9.6997104	8.4502608	5.9605434
10 C	7.5679952	8.2887897	7.1349584	4.6907425
11 C	6.6959368	7.7984437	7.0712196	4.8342629
12 N	5.2548889	6.3964680	5.8939063	3.9145820
13 C	4.7615066	5.4267478	4.6288654	2.5909141 *
14 C	3.4714735	3.9775742	3.4910344	2.1858996 *
15 C	2.1571389 *	3.4298165	3.9309073	3.4470533
16 C	1.1081126 *	2.1925133 *	3.4697017	3.9322292
17 C	2.2122358 *	1.1005424 *	2.1965728 *	3.4584124
18 C	3.4845886	2.2067600 *	1.0953346 *	2.1883899 *
19 C	3.9341977	3.4518537	2.1814708 *	1.1064992 *
20 O	2.6369768 *	4.6165589	5.3716372	4.6727800
21 N	5.9475624	7.9489462	8.2603044	6.7276984
22 H	10.8911715	12.3531880	11.7208094	9.4035389
23 H	10.5467185	12.4202537	12.3002736	10.2605699
24 H	8.3975372	10.4852167	10.7623151	9.0592938
25 H	10.6235940	11.6364171	10.5575676	8.0888057
26 H	9.7034031	10.2019247	8.7162739	6.2046492
27 H	7.3099983	7.7073355	6.3092907	3.8224738
28 H	5.6145669	5.8885879	4.6094035	2.2029941 *
29 H	0.0000000	2.5370846 *	4.3943029	5.0401292

30 H	2.5370846 *	0.0000000	2.5457996 *	4.3793960
31 H	4.3943029	2.5457996 *	0.0000000	2.5279526 *
32 H	5.0401292	4.3793960	2.5279526 *	0.0000000
33 H	2.2721048 *	4.5756015	5.7619471	5.4230251
34 H	5.8822285	7.8714019	8.2414899	6.7992431
35 H	6.2577895	8.4471046	8.9916781	7.6079215

H H H

1 CO	2.6551786 *	2.5350405 *	2.5501440 *
2 C	7.9379861	4.8196344	4.7275612
3 C	7.6230241	4.2360183	3.9136025
4 C	6.3172783	2.9059628 *	2.4985129 *
5 C	5.2366710	2.1567935 *	2.1292881 *
6 C	5.6732300	3.2039808	3.4547465
7 C	7.1174614	4.4377249	4.5749572
8 C	7.9595143	5.6623438	5.9166544
9 C	7.6689313	5.9815800	6.3896595
10 C	6.3670566	5.1444695	5.6463740
11 C	5.2583118	3.7658375	4.2457937
12 N	3.9481610	3.4367366	4.0016691
13 C	4.0365243	4.4165903	5.1344926
14 C	3.3188006	4.9141894	5.6100091
15 C	2.0308964 *	4.6466452	5.1749905
16 C	2.4897312 *	5.7458117	6.2555868
17 C	3.8930398	6.9558827	7.5694763
18 C	4.6968280	7.1933068	7.9146786
19 C	4.4580795	6.2906082	7.0531222
20 O	0.9817796 *	3.6620909	3.8881044
21 N	3.9714521	1.0489531 *	1.0476269 *
22 H	9.0189722	5.9002494	5.8051839
23 H	8.4914061	5.0090144	4.5664974
24 H	6.3239643	2.8891930 *	2.1998179 *
25 H	9.0439434	6.5891082	6.7798738
26 H	8.5461952	7.0553478	7.4906098
27 H	6.3990129	5.7990049	6.3679790
28 H	5.0980068	5.2450356	6.0384117
29 H	2.2721048 *	5.8822285	6.2577895
30 H	4.5756015	7.8714019	8.4471046
31 H	5.7619471	8.2414899	8.9916781
32 H	5.4230251	6.7992431	7.6079215
33 H	0.0000000	4.1442380	4.1519825
34 H	4.1442380	0.0000000	1.6391861 *
35 H	4.1519825	1.6391861 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80 , TOTAL = 1299.6 SECONDS (21.7 MIN)
WALL CLOCK TIME: STEP = 0.80 , TOTAL = 1201.0 SECONDS (20.0 MIN)
CPU UTILIZATION: STEP = 99.70% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.16 , TOTAL = 1300.8 SECONDS (21.7 MIN)
WALL CLOCK TIME: STEP = 1.15 , TOTAL = 1202.1 SECONDS (20.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----
1 0 -284.619097122 -284.619097122 0.304348648 0.008977031 199079933
11299783
2 1 -284.622791437 -0.003694315 0.214784753 0.001542692 181045575
12824849
3 2 -284.622690665 0.000100771 0.125384023 0.002748089 175799163
13287910
4 3 -284.623243418 -0.000552753 0.021119186 0.001369297 171788350
13626008
5 4 -284.623180049 0.000063369 0.010605051 0.002086380 161995247
14434607
6 5 -284.623284899 -0.000104849 0.011024579 0.000288266 157258782
14813629
7 6 -284.623279923 0.000004976 0.001807244 0.000444773 151325043
15331886
8 7 -284.623288042 -0.000008119 0.001894883 0.000143200 164015861
14292555
9 8 -284.623288415 -0.000000373 0.001658004 0.000137780 176229629
13314735
10 9 -284.623289525 -0.000001110 0.006889073 0.000116516 174908987
13522902
-----DISABLING FDIFF OPTION-----
11 10 -284.623291839 -0.000002313 0.003060406 0.000152437 199079759
11299591

12 11	-284.623292766	-0.000000927	0.002131516	0.000141960	199082652
11299358					
13 12	-284.623293382	-0.000000615	0.003412036	0.000102101	199081084
11299464					
14 13	-284.623293963	-0.000000581	0.002699445	0.000051022	199078876
11299595					
15 14	-284.623294230	-0.000000267	0.002257077	0.000047517	199079936
11299527					
16 15	-284.623294326	-0.000000097	0.000837683	0.000052378	199081878
11299389					
17 16	-284.623294395	-0.000000069	0.001076706	0.000047262	199081400
11299437					
18 17	-284.623294483	-0.000000088	0.000571364	0.000032714	199080095
11299531					
19 18	-284.623294573	-0.000000090	0.000957973	0.000021659	199080484
11299513					
20 19	-284.623294625	-0.000000053	0.000347677	0.000015913	199080892
11299469					
21 20	-284.623294645	-0.000000019	0.000121880	0.000015148	199081124
11299464					
22 21	-284.623294654	-0.000000009	0.000122733	0.000010283	199080896
11299477					
23 22	-284.623294660	-0.000000006	0.000103721	0.000007243	199080999
11299468					
24 23	-284.623294664	-0.000000004	0.000081277	0.000005125	199080965
11299467					
25 24	-284.623294666	-0.000000002	0.000038279	0.000002718	199080932
11299472					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 85.1 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 27.1 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.8, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 3.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6232946661 AFTER 25 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6286763255
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000256833

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 89.80 , TOTAL = 1390.6 SECONDS (23.2 MIN)
WALL CLOCK TIME: STEP = 83.32 , TOTAL = 1285.5 SECONDS (21.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.64 , TOTAL = 1394.2 SECONDS (23.2 MIN)
WALL CLOCK TIME: STEP = 3.62 , TOTAL = 1289.1 SECONDS (21.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.90 , TOTAL = 1397.1 SECONDS (23.3 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 1291.8 SECONDS (21.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 9 ENERGY= -284.6232947

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0059597	0.0069314	-0.0020718
2 C	6.0	-0.0127770	0.0014607	0.0013772
3 C	6.0	-0.0012326	0.0007925	0.0012753
4 C	6.0	-0.0080421	0.0038298	0.0010283
5 C	6.0	0.0005910	0.0091013	0.0016783
6 C	6.0	0.0036537	-0.0067582	-0.0016595
7 C	6.0	0.0017299	-0.0056420	-0.0007226
8 C	6.0	-0.0067087	-0.0068556	-0.0007418
9 C	6.0	-0.0069566	0.0048640	0.0015139

10 C	6.0	0.0057389	0.0022632	0.0001584
11 C	6.0	0.0072363	-0.0019462	0.0000357
12 N	7.0	0.0024551	0.0051906	0.0000933
13 C	6.0	-0.0063018	0.0068242	-0.0027020
14 C	6.0	0.0050218	0.0018843	-0.0039470
15 C	6.0	-0.0100571	-0.0147671	-0.0021705
16 C	6.0	0.0158456	0.0104268	-0.0020580
17 C	6.0	-0.0061678	-0.0054148	0.0000402
18 C	6.0	-0.0003039	0.0123133	0.0007793
19 C	6.0	-0.0060002	-0.0020356	-0.0009509
20 O	8.0	-0.0019613	-0.0083351	0.0020157
21 N	7.0	0.0000289	0.0035407	0.0045757
22 H	1.0	0.0015619	-0.0009153	-0.0006065
23 H	1.0	0.0046700	-0.0045204	-0.0018547
24 H	1.0	-0.0010287	-0.0034174	-0.0003773
25 H	1.0	0.0037619	0.0049627	0.0006183
26 H	1.0	-0.0022986	0.0041461	0.0007357
27 H	1.0	-0.0036789	0.0021772	0.0001167
28 H	1.0	0.0021036	-0.0103174	0.0036992
29 H	1.0	0.0033662	-0.0006558	-0.0016382
30 H	1.0	0.0029693	0.0012228	0.0023099
31 H	1.0	0.0046228	-0.0040337	0.0006548
32 H	1.0	0.0021304	0.0000700	0.0028274
33 H	1.0	0.0024566	0.0087382	-0.0001518
34 H	1.0	0.0003028	-0.0079789	-0.0020480
35 H	1.0	-0.0026910	-0.0071464	-0.0018330

MAXIMUM GRADIENT = 0.0158456 RMS GRADIENT = 0.0049512
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0026054507
 PREDICTED ENERGY CHANGE WAS -0.0035303230 RATIO= 0.738
 GDIIS STEP HAS LENGTH = 0.177076
 RADIUS OF STEP TAKEN= 0.17708 CURRENT TRUST RADIUS= 0.20784

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.01 , TOTAL = 1397.1 SECONDS (23.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1291.8 SECONDS (21.5
 MIN)
 CPU UTILIZATION: STEP = 57.07% , TOTAL = 100.00%

INSERCH= 10

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM CHARGE X Y Z

CO	27.0	0.1425888042	-1.5953098142	1.0270694080
C	6.0	4.9679726317	0.6518636834	0.4348050553
C	6.0	5.1658649754	-0.7150142421	0.1848959396
C	6.0	4.0348595856	-1.5641953524	0.0565035593
C	6.0	2.7187045878	-1.0769023161	0.1702477764
C	6.0	2.4441452606	0.3405919940	0.4584214277
C	6.0	3.6319897793	1.1937394352	0.5755473136
C	6.0	3.5049559824	2.6270710160	0.8347372856
C	6.0	2.2553070231	3.2498179570	0.9954476125
C	6.0	1.0896358816	2.4334608855	0.9158229629
C	6.0	1.1645970319	1.0387090513	0.6482106366
N	7.0	-0.0673912045	0.2641937755	0.6452318233
C	6.0	-1.2866789864	0.7900568730	0.5157065727
C	6.0	-2.5658539558	0.0897604533	0.5220316918
C	6.0	-2.8034492006	-1.3208405420	0.6088462707
C	6.0	-4.0952122457	-1.8811581423	0.5292938084
C	6.0	-5.2198561731	-1.0157204694	0.5036186857
C	6.0	-5.0428896280	0.3961158574	0.5029209992
C	6.0	-3.7306854252	0.9334182925	0.4784194153
O	8.0	-1.6988108501	-2.2236308125	0.8950090332
N	7.0	1.6861939165	-2.1613544801	-0.0341607128
H	1.0	5.8214488315	1.3269026227	0.5187971256
H	1.0	6.1856700242	-1.1365607405	0.0682876411
H	1.0	4.1851566668	-2.6358825694	-0.1546147521
H	1.0	4.4294963102	3.2348941660	0.9096707732
H	1.0	2.1571673568	4.3344279792	1.1987167825
H	1.0	0.1121664749	2.9125402286	1.0925811807
H	1.0	-1.3758547120	1.8862738339	0.3794334854
H	1.0	-4.2151895438	-2.9702513637	0.5232485094
H	1.0	-6.2391292236	-1.4510857880	0.5312649696
H	1.0	-5.9260105188	1.0773712322	0.5413578151
H	1.0	-3.5820181381	2.0229751391	0.4801564806
H	1.0	-2.0211699659	-3.1435892198	1.0931645620
H	1.0	1.4343109088	-2.3009040812	-1.0432125111
H	1.0	2.0739647384	-3.0906795424	0.2554083729

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3558281	5.1688954	4.0115755
2 C	5.3558281	0.0000000	1.4035566 *	2.4340768 *
3 C	5.1688954	1.4035566 *	0.0000000	1.4201290 *
4 C	4.0115755	2.4340768 *	1.4201290 *	0.0000000
5 C	2.7639215 *	2.8491804 *	2.4738172 *	1.4080683 *

6 C	3.0607578	2.5430597 *	2.9320435 *	2.5139859 *
7 C	4.4898315	1.4485468 *	2.4796617 *	2.8351217 *
8 C	5.4010188	2.4903429 *	3.7881983	4.2957141
9 C	5.2858151	3.7976626	4.9848005	5.2175806
10 C	4.1400806	4.2949928	5.2021912	5.0392487
11 C	2.8506298 *	3.8289499	4.3932165	3.9196474
12 N	1.9098809 *	5.0546470	5.3439431	4.5296876
13 C	2.8274145 *	6.2567011	6.6340032	5.8371349
14 C	3.2295800	7.5552705	7.7807969	6.8206822
15 C	2.9882075 *	8.0197787	8.0035447	6.8648941
16 C	4.2764995	9.4109749	9.3405596	8.1499733
17 C	5.4190166	10.3236344	10.3949609	9.2817294
18 C	5.5793991	10.0143602	10.2739681	9.2977223
19 C	4.6580829	8.7033228	9.0527396	8.1682174
20 O	1.9501230 *	7.2750435	7.0642734	5.8320599
21 N	1.9568681 *	4.3478957	3.7746518	2.4250875 *
22 H	6.4068024	1.0914000 *	2.1704158 *	3.4298781
23 H	6.1358409	2.1944439 *	1.1096402 *	2.1929423 *
24 H	4.3383780	3.4306693	2.1832983 *	1.1025759 *
25 H	6.4592746	2.6809514 *	4.0828071	4.8902855
26 H	6.2649645	4.6952601	5.9646426	6.2947706
27 H	4.5084287	5.3964971	6.2867251	6.0417001
28 H	3.8531192	6.4630473	7.0426303	6.4254066
29 H	4.5972309	9.8720822	9.6542613	8.3820138
30 H	6.4025735	11.4031063	11.4339698	10.2855743
31 H	6.6488373	10.9028106	11.2414151	10.3165833
32 H	5.2214746	8.6593502	9.1711081	8.4299526
33 H	2.6614638 *	7.9804144	7.6404450	6.3438667
34 H	2.5401725 *	4.8363352	4.2364835	2.9180419 *
35 H	2.5616019 *	4.7343526	3.8998211	2.4929552 *

C C C C

1 CO	2.7639215 *	3.0607578	4.4898315	5.4010188
2 C	2.8491804 *	2.5430597 *	1.4485468 *	2.4903429 *
3 C	2.4738172 *	2.9320435 *	2.4796617 *	3.7881983
4 C	1.4080683 *	2.5139859 *	2.8351217 *	4.2957141
5 C	0.0000000	1.4723169 *	2.4807603 *	3.8443668
6 C	1.4723169 *	0.0000000	1.4671584 *	2.5485132 *
7 C	2.4807603 *	1.4671584 *	0.0000000	1.4621069 *
8 C	3.8443668	2.5485132 *	1.4621069 *	0.0000000
9 C	4.4290180	2.9643975 *	2.5097870 *	1.4054409 *
10 C	3.9411162	2.5345635 *	2.8489051 *	2.4244238 *
11 C	2.6682410 *	1.4699085 *	2.4733260 *	2.8346015 *
12 N	3.1283348	2.5196330 *	3.8150139	4.2872795
13 C	4.4326037	3.7582376	4.9355692	5.1416113

14 C	5.4232290	5.0166777	6.2956255	6.5871438
15 C	5.5449127	5.5063811	6.9093485	7.4453347
16 C	6.8706043	6.9068367	8.3166571	8.8419445
17 C	7.9457930	7.7832220	9.1237089	9.4605453
18 C	7.9071359	7.4873730	8.7117743	8.8404144
19 C	6.7624692	6.2032554	7.3679161	7.4397533
20 O	4.6211154	4.8918230	6.3401822	7.1142203
21 N	1.5112570 *	2.6602375 *	3.9261330	5.1953727
22 H	3.9404044	3.5188966	2.1942388 *	2.6751440 *
23 H	3.4689774	4.0414344	3.4941228	4.6838656
24 H	2.1648180 *	3.5023328	3.9376560	5.3981637
25 H	4.6973550	3.5386763	2.2167471 *	1.1089810 *
26 H	5.5367471	4.0719921	3.5252469	2.2054666 *
27 H	4.8539048	3.5291927	3.9510450	3.4145273
28 H	5.0586152	4.1216224	5.0593054	4.9576602
29 H	7.1964066	7.4372459	8.8836804	9.5408433
30 H	8.9729111	8.8664915	10.2193959	10.5674337
31 H	8.9168221	8.4029298	9.5587698	9.5619438
32 H	7.0288257	6.2566389	7.2621375	7.1215070
33 H	5.2525595	5.6992506	7.1441278	7.9940836
34 H	2.1494961 *	3.2019012	4.4342653	5.6656160
35 H	2.1161854 *	3.4571480	4.5701397	5.9225020

C C C N

1 CO	5.2858151	4.1400806	2.8506298 *	1.9098809 *
2 C	3.7976626	4.2949928	3.8289499	5.0546470
3 C	4.9848005	5.2021912	4.3932165	5.3439431
4 C	5.2175806	5.0392487	3.9196474	4.5296876
5 C	4.4290180	3.9411162	2.6682410 *	3.1283348
6 C	2.9643975 *	2.5345635 *	1.4699085 *	2.5196330 *
7 C	2.5097870 *	2.8489051 *	2.4733260 *	3.8150139
8 C	1.4054409 *	2.4244238 *	2.8346015 *	4.2872795
9 C	0.0000000	1.4253309 *	2.4898242 *	3.7988854
10 C	1.4253309 *	0.0000000	1.4221702 *	2.4733886 *
11 C	2.4898242 *	1.4221702 *	0.0000000	1.4552243 *
12 N	3.7988854	2.4733886 *	1.4552243 *	0.0000000
13 C	4.3389216	2.9168034 *	2.4674155 *	1.3341557 *
14 C	5.7839156	4.3601157	3.8513230	2.5075728 *
15 C	6.8287183	5.4171141	4.6167537	3.1622256
16 C	8.1776103	6.7563298	6.0170889	4.5650103
17 C	8.6206020	7.2025311	6.7084149	5.3109444
18 C	7.8517433	6.4752708	6.2423494	4.9792811
19 C	6.4393424	5.0672426	4.8993577	3.7276551
20 O	6.7530569	5.4281094	4.3477437	2.9854966 *
21 N	5.5375780	4.7297652	3.3133217	3.0691887

22 H	4.0794812	4.8756696	4.6675553	5.9852964
23 H	5.9621889	6.2795648	5.5026615	6.4339531
24 H	6.2998757	6.0354228	4.8239955	5.2090652
25 H	2.1759319 *	3.4346762	3.9434956	5.3960158
26 H	1.1078487 *	2.1984832 *	3.4856873	4.6713823
27 H	2.1716912 *	1.1028177 *	2.1946113 *	2.6918583 *
28 H	3.9273479	2.5818155 *	2.6915613 *	2.1009210 *
29 H	8.9877450	7.5825717	6.7104011	5.2612495
30 H	9.7195375	8.3035165	7.8120367	6.4066780
31 H	8.4770088	7.1553126	7.0915180	5.9156967
32 H	5.9870722	4.7098466	4.8505028	3.9335943
33 H	7.6924287	6.3884310	5.2762405	3.9535908
34 H	5.9699820	5.1352539	3.7532218	3.4184325
35 H	6.3861140	5.6498830	4.2465390	3.9990677

C C C C

1 CO	2.8274145 *	3.2295800	2.9882075 *	4.2764995
2 C	6.2567011	7.5552705	8.0197787	9.4109749
3 C	6.6340032	7.7807969	8.0035447	9.3405596
4 C	5.8371349	6.8206822	6.8648941	8.1499733
5 C	4.4326037	5.4232290	5.5449127	6.8706043
6 C	3.7582376	5.0166777	5.5063811	6.9068367
7 C	4.9355692	6.2956255	6.9093485	8.3166571
8 C	5.1416113	6.5871438	7.4453347	8.8419445
9 C	4.3389216	5.7839156	6.8287183	8.1776103
10 C	2.9168034 *	4.3601157	5.4171141	6.7563298
11 C	2.4674155 *	3.8513230	4.6167537	6.0170889
12 N	1.3341557 *	2.5075728 *	3.1622256	4.5650103
13 C	0.0000000	1.4583359 *	2.6009911 *	3.8760074
14 C	1.4583359 *	0.0000000	1.4331027 *	2.4946963 *
15 C	2.6009911 *	1.4331027 *	0.0000000	1.4102965 *
16 C	3.8760074	2.4946963 *	1.4102965 *	0.0000000
17 C	4.3279164	2.8750922 *	2.4378666 *	1.4193187 *
18 C	3.7768335	2.4959817 *	2.8238720 *	2.4667316 *
19 C	2.4484914 *	1.4389208 *	2.4409959 *	2.8385399 *
20 O	3.0652955	2.4985306 *	1.4550413 *	2.4482187 *
21 N	4.2250629	4.8432200	4.6126800	5.8155523
22 H	7.1283725	8.4780528	9.0226115	10.4226643
23 H	7.7296856	8.8486677	9.0072430	10.3181148
24 H	6.4905606	7.3118482	7.1521200	8.3427723
25 H	6.2295343	7.6796520	8.5534037	9.9493384
26 H	4.9889024	6.3860814	7.5457091	8.8415999
27 H	2.6066240 *	3.9326080	5.1629766	6.4030362
28 H	1.1082483 *	2.1596048 *	3.5179879	4.6487533
29 H	4.7661461	3.4762022	2.1727618 *	1.0956985 *

30 H	5.4359660	3.9833709	3.4390231	2.1866289 *
31 H	4.6482905	3.5023422	3.9378120	3.4792045
32 H	2.6057500 *	2.1844135 *	3.4356708	3.9380248
33 H	4.0430813	3.3282764	2.0417977 *	2.4926560 *
34 H	4.4031868	4.9159521	4.6527877	5.7640775
35 H	5.1402137	5.6315366	5.2006168	6.2925909

C C C O

1 CO	5.4190166	5.5793991	4.6580829	1.9501230 *
2 C	10.3236344	10.0143602	8.7033228	7.2750435
3 C	10.3949609	10.2739681	9.0527396	7.0642734
4 C	9.2817294	9.2977223	8.1682174	5.8320599
5 C	7.9457930	7.9071359	6.7624692	4.6211154
6 C	7.7832220	7.4873730	6.2032554	4.8918230
7 C	9.1237089	8.7117743	7.3679161	6.3401822
8 C	9.4605453	8.8404144	7.4397533	7.1142203
9 C	8.6206020	7.8517433	6.4393424	6.7530569
10 C	7.2025311	6.4752708	5.0672426	5.4281094
11 C	6.7084149	6.2423494	4.8993577	4.3477437
12 N	5.3109444	4.9792811	3.7276551	2.9854966 *
13 C	4.3279164	3.7768335	2.4484914 *	3.0652955
14 C	2.8750922 *	2.4959817 *	1.4389208 *	2.4985306 *
15 C	2.4378666 *	2.8238720 *	2.4409959 *	1.4550413 *
16 C	1.4193187 *	2.4667316 *	2.8385399 *	2.4482187 *
17 C	0.0000000	1.4228842 *	2.4530402 *	3.7429926
18 C	1.4228842 *	0.0000000	1.4181587 *	4.2661070
19 C	2.4530402 *	1.4181587 *	0.0000000	3.7774357
20 O	3.7429926	4.2661070	3.7774357	0.0000000
21 N	7.0210549	7.2187033	6.2596277	3.5107680
22 H	11.2870957	10.9041490	9.5603206	8.3247900
23 H	11.4144708	11.3410121	10.1383986	8.0018890
24 H	9.5662147	9.7356153	8.7063883	5.9910546
25 H	10.5519006	9.8969795	8.4894838	8.2068178
26 H	9.1393504	8.2362160	6.8375804	7.6137337
27 H	6.6489529	5.7666883	4.3659626	5.4496722
28 H	4.8180224	3.9601723	2.5422352 *	4.1546883
29 H	2.1977105 *	3.4666885	3.9338773	2.6510017 *
30 H	1.1087041 *	2.2008967 *	3.4613498	4.6199163
31 H	2.2093237 *	1.1160147 *	2.2009398 *	5.3750256
32 H	3.4520624	2.1866264 *	1.0996541 *	4.6639291
33 H	3.8867703	4.6913419	4.4634454	0.9947384 *
34 H	6.9514260	7.1846066	6.2811935	3.6849865
35 H	7.5872846	7.9289735	7.0666159	3.9236078

N H H H

1 CO	1.9568681 *	6.4068024	6.1358409	4.3383780
2 C	4.3478957	1.0914000 *	2.1944439 *	3.4306693
3 C	3.7746518	2.1704158 *	1.1096402 *	2.1832983 *
4 C	2.4250875 *	3.4298781	2.1929423 *	1.1025759 *
5 C	1.5112570 *	3.9404044	3.4689774	2.1648180 *
6 C	2.6602375 *	3.5188966	4.0414344	3.5023328
7 C	3.9261330	2.1942388 *	3.4941228	3.9376560
8 C	5.1953727	2.6751440 *	4.6838656	5.3981637
9 C	5.5375780	4.0794812	5.9621889	6.2998757
10 C	4.7297652	4.8756696	6.2795648	6.0354228
11 C	3.3133217	4.6675553	5.5026615	4.8239955
12 N	3.0691887	5.9852964	6.4339531	5.2090652
13 C	4.2250629	7.1283725	7.7296856	6.4905606
14 C	4.8432200	8.4780528	8.8486677	7.3118482
15 C	4.6126800	9.0226115	9.0072430	7.1521200
16 C	5.8155523	10.4226643	10.3181148	8.3427723
17 C	7.0210549	11.2870957	11.4144708	9.5662147
18 C	7.2187033	10.9041490	11.3410121	9.7356153
19 C	6.2596277	9.5603206	10.1383986	8.7063883
20 O	3.5107680	8.3247900	8.0018890	5.9910546
21 N	0.0000000	5.4382013	4.6158405	2.5464683 *
22 H	5.4382013	0.0000000	2.5306654 *	4.3398850
23 H	4.6158405	2.5306654 *	0.0000000	2.5099213 *
24 H	2.5464683 *	4.3398850	2.5099213 *	0.0000000
25 H	6.1266651	2.3938976 *	4.7855710	5.9714676
26 H	6.6284985	4.7889934	6.8875555	7.3844076
27 H	5.4306093	5.9530983	7.3710136	6.9949798
28 H	5.0921996	7.2203529	8.1492943	7.1874859
29 H	5.9825869	10.9178598	10.5710591	8.4342823
30 H	7.9771508	12.3763855	12.4373997	10.5137962
31 H	8.2925402	11.7501309	12.3214486	10.7939026
32 H	6.7473843	9.4292736	10.2742413	9.0794765
33 H	3.9975235	9.0455439	8.5106262	6.3508432
34 H	1.0493353 *	5.9032055	5.0166265	2.9101493 *
35 H	1.0477889 *	5.7989691	4.5562830	2.1982017 *

H H H H

1 CO	6.4592746	6.2649645	4.5084287	3.8531192
2 C	2.6809514 *	4.6952601	5.3964971	6.4630473
3 C	4.0828071	5.9646426	6.2867251	7.0426303
4 C	4.8902855	6.2947706	6.0417001	6.4254066
5 C	4.6973550	5.5367471	4.8539048	5.0586152
6 C	3.5386763	4.0719921	3.5291927	4.1216224
7 C	2.2167471 *	3.5252469	3.9510450	5.0593054

8 C	1.1089810 *	2.2054666 *	3.4145273	4.9576602
9 C	2.1759319 *	1.1078487 *	2.1716912 *	3.9273479
10 C	3.4346762	2.1984832 *	1.1028177 *	2.5818155 *
11 C	3.9434956	3.4856873	2.1946113 *	2.6915613 *
12 N	5.3960158	4.6713823	2.6918583 *	2.1009210 *
13 C	6.2295343	4.9889024	2.6066240 *	1.1082483 *
14 C	7.6796520	6.3860814	3.9326080	2.1596048 *
15 C	8.5534037	7.5457091	5.1629766	3.5179879
16 C	9.9493384	8.8415999	6.4030362	4.6487533
17 C	10.5519006	9.1393504	6.6489529	4.8180224
18 C	9.8969795	8.2362160	5.7666883	3.9601723
19 C	8.4894838	6.8375804	4.3659626	2.5422352 *
20 O	8.2068178	7.6137337	5.4496722	4.1546883
21 N	6.1266651	6.6284985	5.4306093	5.0921996
22 H	2.3938976 *	4.7889934	5.9530983	7.2203529
23 H	4.7855710	6.8875555	7.3710136	8.1492943
24 H	5.9714676	7.3844076	6.9949798	7.1874859
25 H	0.0000000	2.5408662 *	4.3332096	5.9834797
26 H	2.5408662 *	0.0000000	2.4930018 *	4.3757204
27 H	4.3332096	2.4930018 *	0.0000000	1.9431957 *
28 H	5.9834797	4.3757204	1.9431957 *	0.0000000
29 H	10.6481804	9.7170742	7.3251203	5.6274632
30 H	11.6585235	10.2183882	7.7262711	5.9002086
31 H	10.5842846	8.7394682	6.3349249	4.6243335
32 H	8.1140369	6.2287554	3.8488167	2.2126883 *
33 H	9.0735779	8.5668189	6.4208900	5.1210708
34 H	6.5901404	7.0410511	5.7870271	5.2396003
35 H	6.7815537	7.4852505	6.3708836	6.0569548

H H H H

1 CO	4.5972309	6.4025735	6.6488373	5.2214746
2 C	9.8720822	11.4031063	10.9028106	8.6593502
3 C	9.6542613	11.4339698	11.2414151	9.1711081
4 C	8.3820138	10.2855743	10.3165833	8.4299526
5 C	7.1964066	8.9729111	8.9168221	7.0288257
6 C	7.4372459	8.8664915	8.4029298	6.2566389
7 C	8.8836804	10.2193959	9.5587698	7.2621375
8 C	9.5408433	10.5674337	9.5619438	7.1215070
9 C	8.9877450	9.7195375	8.4770088	5.9870722
10 C	7.5825717	8.3035165	7.1553126	4.7098466
11 C	6.7104011	7.8120367	7.0915180	4.8505028
12 N	5.2612495	6.4066780	5.9156967	3.9335943
13 C	4.7661461	5.4359660	4.6482905	2.6057500 *
14 C	3.4762022	3.9833709	3.5023422	2.1844135 *
15 C	2.1727618 *	3.4390231	3.9378120	3.4356708

16 C	1.0956985 *	2.1866289 *	3.4792045	3.9380248
17 C	2.1977105 *	1.1087041 *	2.2093237 *	3.4520624
18 C	3.4666885	2.2008967 *	1.1160147 *	2.1866264 *
19 C	3.9338773	3.4613498	2.2009398 *	1.0996541 *
20 O	2.6510017 *	4.6199163	5.3750256	4.6639291
21 N	5.9825869	7.9771508	8.2925402	6.7473843
22 H	10.9178598	12.3763855	11.7501309	9.4292736
23 H	10.5710591	12.4373997	12.3214486	10.2742413
24 H	8.4342823	10.5137962	10.7939026	9.0794765
25 H	10.6481804	11.6585235	10.5842846	8.1140369
26 H	9.7170742	10.2183882	8.7394682	6.2287554
27 H	7.3251203	7.7262711	6.3349249	3.8488167
28 H	5.6274632	5.9002086	4.6243335	2.2126883 *
29 H	0.0000000	2.5306640 *	4.3943697	5.0333959
30 H	2.5306640 *	0.0000000	2.5477912 *	4.3740085
31 H	4.3943697	2.5477912 *	0.0000000	2.5282825 *
32 H	5.0333959	4.3740085	2.5282825 *	0.0000000
33 H	2.2734494 *	4.5794628	5.7765714	5.4318885
34 H	5.9007357	7.8792673	8.2521475	6.7955972
35 H	6.2960069	8.4777294	9.0251880	7.6282448

H H H

1 CO	2.6614638 *	2.5401725 *	2.5616019 *
2 C	7.9804144	4.8363352	4.7343526
3 C	7.6404450	4.2364835	3.8998211
4 C	6.3438667	2.9180419 *	2.4929552 *
5 C	5.2525595	2.1494961 *	2.1161854 *
6 C	5.6992506	3.2019012	3.4571480
7 C	7.1441278	4.4342653	4.5701397
8 C	7.9940836	5.6656160	5.9225020
9 C	7.6924287	5.9699820	6.3861140
10 C	6.3884310	5.1352539	5.6498830
11 C	5.2762405	3.7532218	4.2465390
12 N	3.9535908	3.4184325	3.9990677
13 C	4.0430813	4.4031868	5.1402137
14 C	3.3282764	4.9159521	5.6315366
15 C	2.0417977 *	4.6527877	5.2006168
16 C	2.4926560 *	5.7640775	6.2925909
17 C	3.8867703	6.9514260	7.5872846
18 C	4.6913419	7.1846066	7.9289735
19 C	4.4634454	6.2811935	7.0666159
20 O	0.9947384 *	3.6849865	3.9236078
21 N	3.9975235	1.0493353 *	1.0477889 *
22 H	9.0455439	5.9032055	5.7989691
23 H	8.5106262	5.0166265	4.5562830

24 H	6.3508432	2.9101493 *	2.1982017 *
25 H	9.0735779	6.5901404	6.7815537
26 H	8.5668189	7.0410511	7.4852505
27 H	6.4208900	5.7870271	6.3708836
28 H	5.1210708	5.2396003	6.0569548
29 H	2.2734494 *	5.9007357	6.2960069
30 H	4.5794628	7.8792673	8.4777294
31 H	5.7765714	8.2521475	9.0251880
32 H	5.4318885	6.7955972	7.6282448
33 H	0.0000000	4.1490449	4.1802827
34 H	4.1490449	0.0000000	1.6490356 *
35 H	4.1802827	1.6490356 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.77 , TOTAL = 1397.9 SECONDS (23.3 MIN)
WALL CLOCK TIME: STEP = 0.77 , TOTAL = 1292.6 SECONDS (21.5 MIN)

CPU UTILIZATION: STEP = 99.85%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.95 , TOTAL = 1398.9 SECONDS (23.3 MIN)
WALL CLOCK TIME: STEP = 0.95 , TOTAL = 1293.5 SECONDS (21.6 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.622837697	-284.622837697	0.574604932	0.007114125	198423188
11348190					
2 1	-284.625117389	-0.002279692	0.187038900	0.001279224	179224614
12977222					
3 2	-284.624939984	0.000177406	0.139095155	0.002282854	173385516
13481534					
4 3	-284.625311885	-0.000371901	0.037912267	0.000765784	168664598
13874023					
5 4	-284.625283344	0.000028541	0.012474159	0.001041333	160904066
14511845					

6 5	-284.625331640	-0.000048297	0.013361277	0.000131534	152511078
15171855					
7 6	-284.625329851	0.000001789	0.001933223	0.000249155	150300969
15386672					
8 7	-284.625333194	-0.000003343	0.003210446	0.000085872	161337595
14501644					
9 8	-284.625333211	-0.000000017	0.000544967	0.000100988	178039945
13135343					
10 9	-284.625333761	-0.000000550	0.001558093	0.000070449	169127832
13919394					

-----DISABLING FDIFF OPTION-----

11 10	-284.625334243	-0.000000482	0.001743810	0.000076213	198306175
11358753					
12 11	-284.625334665	-0.000000422	0.001419416	0.000071389	198306121
11358744					
13 12	-284.625334997	-0.000000332	0.001311277	0.000063389	198306205
11358762					
14 13	-284.625335275	-0.000000278	0.000938999	0.000050124	198306175
11358773					
15 14	-284.625335496	-0.000000220	0.000922234	0.000039423	198306153
11358778					
16 15	-284.625335636	-0.000000140	0.000412410	0.000033214	198305948
11358766					
17 16	-284.625335695	-0.000000059	0.000397743	0.000028722	198305766
11358774					
18 17	-284.625335724	-0.000000029	0.000261969	0.000022343	198305866
11358758					
19 18	-284.625335765	-0.000000041	0.000641216	0.000015847	198305990
11358741					
20 19	-284.625335816	-0.000000052	0.000561465	0.000017488	198306382
11358740					
21 20	-284.625335838	-0.000000021	0.000120933	0.000015247	198306265
11358759					
22 21	-284.625335844	-0.000000007	0.000183358	0.000012426	198306253
11358763					
23 22	-284.625335854	-0.000000009	0.000210966	0.000009295	198306206
11358755					
24 23	-284.625335863	-0.000000009	0.000195100	0.000005298	198305815
11358767					
25 24	-284.625335866	-0.000000003	0.000138962	0.000007288	198305764
11358770					
26 25	-284.625335868	-0.000000002	0.000022573	0.000002317	198305835
11358761					
27 26	-284.625335868	0.000000000	0.000029717	0.000001294	198305850
11358760					

28 27 -284.625335868 0.000000000 0.000016080 0.000000574 198305781
11358764

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 96.1 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 30.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 3.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6253358683 AFTER 28 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6090744180
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000591073

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 100.25 , TOTAL = 1499.1 SECONDS (25.0 MIN)
WALL CLOCK TIME: STEP = 92.22 , TOTAL = 1385.7 SECONDS (23.1
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 4.03 , TOTAL = 1503.1 SECONDS (25.1 MIN)
WALL CLOCK TIME: STEP = 3.99 , TOTAL = 1389.7 SECONDS (23.2
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.89 , TOTAL = 1506.0 SECONDS (25.1 MIN)

WALL CLOCK TIME: STEP = 2.74 , TOTAL = 1392.5 SECONDS (23.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 10 ENERGY= -284.6253359

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0018548	0.0062265	0.0001857
2 C	6.0	0.0109249	0.0073612	0.0016111
3 C	6.0	-0.0105395	-0.0047983	0.0000230
4 C	6.0	0.0041867	-0.0020297	-0.0005841
5 C	6.0	-0.0075418	-0.0000411	0.0002913
6 C	6.0	0.0020518	0.0015203	0.0002335
7 C	6.0	-0.0052435	-0.0113498	-0.0014853
8 C	6.0	-0.0027105	0.0038023	0.0010268
9 C	6.0	-0.0034345	0.0045699	0.0012012
10 C	6.0	-0.0006171	0.0069578	0.0017558
11 C	6.0	0.0067679	-0.0030357	-0.0010570
12 N	7.0	0.0032922	-0.0002260	-0.0001555
13 C	6.0	-0.0067652	-0.0031374	-0.0008132
14 C	6.0	-0.0013752	0.0005717	-0.0034026
15 C	6.0	0.0080572	0.0013031	-0.0020271
16 C	6.0	-0.0092992	-0.0045054	-0.0024268
17 C	6.0	0.0084105	-0.0007074	-0.0003647
18 C	6.0	0.0022204	-0.0071223	-0.0004448
19 C	6.0	0.0077313	0.0032090	-0.0008412
20 O	8.0	0.0000818	0.0034845	0.0008605
21 N	7.0	0.0073265	0.0050509	0.0018605
22 H	1.0	-0.0069878	-0.0062242	-0.0011746
23 H	1.0	0.0029663	-0.0019967	-0.0010768
24 H	1.0	-0.0019727	0.0029637	0.0009893
25 H	1.0	0.0008320	0.0029735	0.0004141
26 H	1.0	-0.0019008	0.0026761	0.0004396
27 H	1.0	-0.0002643	0.0001937	-0.0006095
28 H	1.0	-0.0003006	0.0016176	0.0018103
29 H	1.0	0.0034784	0.0075459	-0.0019379
30 H	1.0	-0.0020139	-0.0008100	0.0025371
31 H	1.0	-0.0062480	0.0048274	0.0018219
32 H	1.0	0.0004813	-0.0042490	0.0025673
33 H	1.0	-0.0008327	-0.0026651	0.0017596
34 H	1.0	-0.0005922	-0.0069882	-0.0026027
35 H	1.0	-0.0020248	-0.0069686	-0.0003848

MAXIMUM GRADIENT = 0.0113498 RMS GRADIENT = 0.0040909
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0020412022
PREDICTED ENERGY CHANGE WAS -0.0025179952 RATIO= 0.811
GDIIS STEP HAS LENGTH = 0.139520
RADIUS OF STEP TAKEN= 0.13952 CURRENT TRUST RADIUS= 0.25042

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 1506.1 SECONDS (25.1 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1392.5 SECONDS (23.2
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 11

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1359065024	-1.6123763979	1.0335358343
C	6.0	4.9719859286	0.6456690813	0.4319079574
C	6.0	5.1781347733	-0.7102831605	0.1832123923
C	6.0	4.0381377265	-1.5605863928	0.0557925051
C	6.0	2.7288750868	-1.0810372396	0.1677887740
C	6.0	2.4457999495	0.3415729686	0.4576790205
C	6.0	3.6418339054	1.2076717527	0.5763035509
C	6.0	3.5162245295	2.6266129429	0.8336438369
C	6.0	2.2660698013	3.2382810675	0.9923265807
C	6.0	1.0909650384	2.4276398886	0.9147310786
C	6.0	1.1539966513	1.0386273214	0.6480518503
N	7.0	-0.0687797786	0.2557133911	0.6479814523
C	6.0	-1.2810013323	0.7875745746	0.5201438600
C	6.0	-2.5667442979	0.0934617242	0.5333550897
C	6.0	-2.8166077954	-1.3169499035	0.6195957040
C	6.0	-4.0983957349	-1.8804329839	0.5369817951
C	6.0	-5.2299098779	-1.0174523003	0.5017974338
C	6.0	-5.0475394384	0.3980790035	0.4999080440
C	6.0	-3.7401489185	0.9261371876	0.4788492349
O	8.0	-1.7052568439	-2.2193597357	0.9088610619
N	7.0	1.6843409792	-2.1663229569	-0.0397612758
H	1.0	5.8343116332	1.3329498028	0.5202138632
H	1.0	6.1815254193	-1.1270273705	0.0728542694
H	1.0	4.1972960376	-2.6332056178	-0.1547657103
H	1.0	4.4304656243	3.2340438655	0.9099603140
H	1.0	2.1653036490	4.3258003548	1.1969406879

H	1.0	0.1207960612	2.9116247068	1.0942703264
H	1.0	-1.3796719637	1.8899541951	0.3681505919
H	1.0	-4.2330120728	-2.9759788123	0.5278689617
H	1.0	-6.2455048536	-1.4491787476	0.5238571901
H	1.0	-5.9296479652	1.0728453070	0.5399350500
H	1.0	-3.5936016217	2.0256182306	0.4708802657
H	1.0	-2.0294784448	-3.1482988988	1.0788468105
H	1.0	1.4324290573	-2.2818590504	-1.0406395736
H	1.0	2.0868995857	-3.0784227980	0.2518281724

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3710697	5.1923875	4.0231919
2 C	5.3710697	0.0000000	1.3938986 *	2.4250976 *
3 C	5.1923875	1.3938986 *	0.0000000	1.4278812 *
4 C	4.0231919	2.4250976 *	1.4278812 *	0.0000000
5 C	2.7848385 *	2.8430301 *	2.4772100 *	1.3988135 *
6 C	3.0797949	2.5445538 *	2.9406439 *	2.5130186 *
7 C	4.5225280	1.4512069 *	2.4886326 *	2.8445108 *
8 C	5.4254527	2.4909379 *	3.7841620	4.2906974
9 C	5.2979403	3.7891540	4.9725192	5.2006201
10 C	4.1530691	4.2977740	5.2044824	5.0328472
11 C	2.8658203 *	3.8442394	4.4123068	3.9274614
12 N	1.9184129 *	5.0604419	5.3553032	4.5295037
13 C	2.8338955 *	6.2552196	6.6390918	5.8329000
14 C	3.2348703	7.5596083	7.7943414	6.8255701
15 C	2.9959913 *	8.0342574	8.0295942	6.8822067
16 C	4.2717368	9.4161593	9.3567314	8.1570228
17 C	5.4248194	10.3368049	10.4174490	9.2946555
18 C	5.5852306	10.0228146	10.2904410	9.3050061
19 C	4.6664263	8.7167746	9.0719930	8.1770725
20 O	1.9426413 *	7.2815826	7.0841343	5.8436538
21 N	1.9637904 *	4.3518250	3.7916176	2.4323664 *
22 H	6.4350810	1.1062361 *	2.1723119 *	3.4372198
23 H	6.1406824	2.1758580 *	1.0920840 *	2.1868643 *
24 H	4.3530493	3.4198464	2.1849267 *	1.1046167 *
25 H	6.4765962	2.6872779 *	4.0798146	4.8858984
26 H	6.2775072	4.6910667	5.9554121	6.2816619
27 H	4.5244340	5.3951202	6.2868846	6.0352857
28 H	3.8737624	6.4727018	7.0569303	6.4308988
29 H	4.6046238	9.8922965	9.6861680	8.4046482
30 H	6.4038127	11.4117896	11.4525782	10.2948920
31 H	6.6516921	10.9105349	11.2556491	10.3211486

32 H	5.2403070	8.6761206	9.1930011	8.4425474
33 H	2.6551842 *	7.9895698	7.6613165	6.3547964
34 H	2.5360168 *	4.8236169	4.2424021	2.9175530 *
35 H	2.5625637 *	4.7143411	3.8946795	2.4798362 *

C C C C

1 CO	2.7848385 *	3.0797949	4.5225280	5.4254527
2 C	2.8430301 *	2.5445538 *	1.4512069 *	2.4909379 *
3 C	2.4772100 *	2.9406439 *	2.4886326 *	3.7841620
4 C	1.3988135 *	2.5130186 *	2.8445108 *	4.2906974
5 C	0.0000000	1.4791848 *	2.4977123 *	3.8483700
6 C	1.4791848 *	0.0000000	1.4814507 *	2.5511891 *
7 C	2.4977123 *	1.4814507 *	0.0000000	1.4475482 *
8 C	3.8483700	2.5511891 *	1.4475482 *	0.0000000
9 C	4.4216017	2.9511131 *	2.4878055 *	1.4007873 *
10 C	3.9435374	2.5290610 *	2.8477688 *	2.4347585 *
11 C	2.6840031 *	1.4801629 *	2.4946058 *	2.8524136 *
12 N	3.1375723	2.5232317 *	3.8314509	4.3020799
13 C	4.4379019	3.7539136	4.9410467	5.1472051
14 C	5.4366048	5.0192515	6.3079118	6.5961760
15 C	5.5688567	5.5199502	6.9344832	7.4633953
16 C	6.8838190	6.9115915	8.3336122	8.8534690
17 C	7.9660444	7.7952176	9.1468337	9.4807279
18 C	7.9227969	7.4936714	8.7273413	8.8552694
19 C	6.7803967	6.2135438	7.3879922	7.4613975
20 O	4.6375093	4.8982868	6.3597578	7.1241123
21 N	1.5205175 *	2.6677347 *	3.9490701	5.2048889
22 H	3.9490851	3.5311117	2.1967702 *	2.6730751 *
23 H	3.4542614	4.0324337	3.4863038	4.6660953
24 H	2.1609091 *	3.5060141	3.9490935	5.3950443
25 H	4.6974625	3.5369258	2.1998752 *	1.1002878 *
26 H	5.5326901	4.0619274	3.5054326	2.2009565 *
27 H	4.8581677	3.5236426	3.9458146	3.4173224
28 H	5.0741594	4.1279214	5.0719186	4.9728415
29 H	7.2241494	7.4577213	8.9173133	9.5672985
30 H	8.9889826	8.8741169	10.2382163	10.5829772
31 H	8.9301581	8.4077139	9.5725005	9.5773152
32 H	7.0510201	6.2698129	7.2822852	7.1443978
33 H	5.2674022	5.7090430	7.1687386	8.0102779
34 H	2.1408046 *	3.1865773	4.4354030	5.6522773
35 H	2.0997010 *	3.4449318	4.5709640	5.9100687

C C C N

1 CO	5.2979403	4.1530691	2.8658203 *	1.9184129 *
------	-----------	-----------	-------------	-------------

2 C	3.7891540	4.2977740	3.8442394	5.0604419
3 C	4.9725192	5.2044824	4.4123068	5.3553032
4 C	5.2006201	5.0328472	3.9274614	4.5295037
5 C	4.4216017	3.9435374	2.6840031 *	3.1375723
6 C	2.9511131 *	2.5290610 *	1.4801629 *	2.5232317 *
7 C	2.4878055 *	2.8477688 *	2.4946058 *	3.8314509
8 C	1.4007873 *	2.4347585 *	2.8524136 *	4.3020799
9 C	0.0000000	1.4296963 *	2.4887162 *	3.8033940
10 C	1.4296963 *	0.0000000	1.4157848 *	2.4765759 *
11 C	2.4887162 *	1.4157848 *	0.0000000	1.4519423 *
12 N	3.8033940	2.4765759 *	1.4519423 *	0.0000000
13 C	4.3371226	2.9106250 *	2.4512452 *	1.3299248 *
14 C	5.7841711	4.3557632	3.8406258	2.5058515 *
15 C	6.8353982	5.4201645	4.6168445	3.1661703
16 C	8.1801586	6.7551204	6.0100645	4.5621538
17 C	8.6337475	7.2105918	6.7084362	5.3178553
18 C	7.8611770	6.4786135	6.2362888	4.9829952
19 C	6.4563404	5.0778111	4.8983614	3.7359102
20 O	6.7501293	5.4234211	4.3425605	2.9786074 *
21 N	5.5329340	4.7294445	3.3205509	3.0680095
22 H	4.0725333	4.8839868	4.6913022	6.0019373
23 H	5.9356668	6.2656381	5.5042673	6.4272123
24 H	6.2864785	6.0336782	4.8361704	5.2143704
25 H	2.1659666 *	3.4354875	3.9526825	5.4020639
26 H	1.1111791 *	2.1992860 *	3.4827471	4.6752639
27 H	2.1723941 *	1.0989556 *	2.1851164 *	2.6998107 *
28 H	3.9368787	2.5868713 *	2.6874856 *	2.1136430 *
29 H	9.0039331	7.5956231	6.7194769	5.2724844
30 H	9.7282396	8.3070028	7.8075109	6.4088998
31 H	8.4890258	7.1599544	7.0845523	5.9185433
32 H	6.0065137	4.7226888	4.8523428	3.9482017
33 H	7.6972478	6.3918069	5.2773525	3.9518709
34 H	5.9413681	5.1107194	3.7356168	3.3976967
35 H	6.3624828	5.6345410	4.2399767	3.9900320

C C C C

1 CO	2.8338955 *	3.2348703	2.9959913 *	4.2717368
2 C	6.2552196	7.5596083	8.0342574	9.4161593
3 C	6.6390918	7.7943414	8.0295942	9.3567314
4 C	5.8329000	6.8255701	6.8822067	8.1570228
5 C	4.4379019	5.4366048	5.5688567	6.8838190
6 C	3.7539136	5.0192515	5.5199502	6.9115915
7 C	4.9410467	6.3079118	6.9344832	8.3336122
8 C	5.1472051	6.5961760	7.4633953	8.8534690
9 C	4.3371226	5.7841711	6.8353982	8.1801586

10	C	2.9106250 *	4.3557632	5.4201645	6.7551204
11	C	2.4512452 *	3.8406258	4.6168445	6.0100645
12	N	1.3299248 *	2.5058515 *	3.1661703	4.5621538
13	C	0.0000000	1.4611989 *	2.6071059 *	3.8802396
14	C	1.4611989 *	0.0000000	1.4349670 *	2.4984454 *
15	C	2.6071059 *	1.4349670 *	0.0000000	1.4026113 *
16	C	3.8802396	2.4984454 *	1.4026113 *	0.0000000
17	C	4.3419278	2.8857541 *	2.4346668 *	1.4234809 *
18	C	3.7866774	2.4996510 *	2.8165059 *	2.4685755 *
19	C	2.4633943 *	1.4398603 *	2.4298513 *	2.8299393 *
20	O	3.0614944	2.4964592 *	1.4605201 *	2.4454610 *
21	N	4.2228260	4.8483827	4.6276048	5.8184542
22	H	7.1361833	8.4920106	9.0482182	10.4395779
23	H	7.7171934	8.8449917	9.0167288	10.3179365
24	H	6.4937649	7.3253305	7.1782318	8.3584498
25	H	6.2255942	7.6789345	8.5624721	9.9518070
26	H	4.9853900	6.3832056	7.5493973	8.8423305
27	H	2.6088783 *	3.9344049	5.1705416	6.4090535
28	H	1.1171744 *	2.1595876 *	3.5231014	4.6514280
29	H	4.7831748	3.4925555	2.1833442 *	1.1038230 *
30	H	5.4451239	3.9891238	3.4327810	2.1900297 *
31	H	4.6574335	3.5026214	3.9253645	3.4749599
32	H	2.6236042 *	2.1889650 *	3.4349086	3.9390891
33	H	4.0451782	3.3309500	2.0455619 *	2.4862664 *
34	H	4.3840817	4.9104985	4.6628044	5.7654189
35	H	5.1342658	5.6388394	5.2232580	6.3066925

C C C O

1	CO	5.4248194	5.5852306	4.6664263	1.9426413 *
2	C	10.3368049	10.0228146	8.7167746	7.2815826
3	C	10.4174490	10.2904410	9.0719930	7.0841343
4	C	9.2946555	9.3050061	8.1770725	5.8436538
5	C	7.9660444	7.9227969	6.7803967	4.6375093
6	C	7.7952176	7.4936714	6.2135438	4.8982868
7	C	9.1468337	8.7273413	7.3879922	6.3597578
8	C	9.4807279	8.8552694	7.4613975	7.1241123
9	C	8.6337475	7.8611770	6.4563404	6.7501293
10	C	7.2105918	6.4786135	5.0778111	5.4234211
11	C	6.7084362	6.2362888	4.8983614	4.3425605
12	N	5.3178553	4.9829952	3.7359102	2.9786074 *
13	C	4.3419278	3.7866774	2.4633943 *	3.0614944
14	C	2.8857541 *	2.4996510 *	1.4398603 *	2.4964592 *
15	C	2.4346668 *	2.8165059 *	2.4298513 *	1.4605201 *
16	C	1.4234809 *	2.4685755 *	2.8299393 *	2.4454610 *
17	C	0.0000000	1.4272321 *	2.4489701 *	3.7461262

18 C	1.4272321 *	0.0000000	1.4101627 *	4.2648659
19 C	2.4489701 *	1.4101627 *	0.0000000	3.7709212
20 O	3.7461262	4.2648659	3.7709212	0.0000000
21 N	7.0299399	7.2239611	6.2655692	3.5202373
22 H	11.3111329	10.9219540	9.5831885	8.3435629
23 H	11.4200199	11.3402038	10.1400167	8.0058374
24 H	9.5871761	9.7511162	8.7220079	6.0118800
25 H	10.5624179	9.9016877	8.5012488	8.2089404
26 H	9.1500140	8.2424484	6.8518417	7.6094250
27 H	6.6647374	5.7777911	4.3849515	5.4493896
28 H	4.8265107	3.9618561	2.5520676 *	4.1575034
29 H	2.1977969 *	3.4710953	3.9334242	2.6659283 *
30 H	1.1037697 *	2.2018301 *	3.4526743	4.6211750
31 H	2.2046387 *	1.1113178 *	2.1952587 *	5.3684449
32 H	3.4552480	2.1825814 *	1.1092331 *	4.6666381
33 H	3.8879628	4.6926174	4.4595314	0.9984702 *
34 H	6.9544659	7.1795088	6.2734081	3.6945273
35 H	7.6056416	7.9402663	7.0740747	3.9433656

N H H H

1 CO	1.9637904 *	6.4350810	6.1406824	4.3530493
2 C	4.3518250	1.1062361 *	2.1758580 *	3.4198464
3 C	3.7916176	2.1723119 *	1.0920840 *	2.1849267 *
4 C	2.4323664 *	3.4372198	2.1868643 *	1.1046167 *
5 C	1.5205175 *	3.9490851	3.4542614	2.1609091 *
6 C	2.6677347 *	3.5311117	4.0324337	3.5060141
7 C	3.9490701	2.1967702 *	3.4863038	3.9490935
8 C	5.2048889	2.6730751 *	4.6660953	5.3950443
9 C	5.5329340	4.0725333	5.9356668	6.2864785
10 C	4.7294445	4.8839868	6.2656381	6.0336782
11 C	3.3205509	4.6913022	5.5042673	4.8361704
12 N	3.0680095	6.0019373	6.4272123	5.2143704
13 C	4.2228260	7.1361833	7.7171934	6.4937649
14 C	4.8483827	8.4920106	8.8449917	7.3253305
15 C	4.6276048	9.0482182	9.0167288	7.1782318
16 C	5.8184542	10.4395779	10.3179365	8.3584498
17 C	7.0299399	11.3111329	11.4200199	9.5871761
18 C	7.2239611	10.9219540	11.3402038	9.7511162
19 C	6.2655692	9.5831885	10.1400167	8.7220079
20 O	3.5202373	8.3435629	8.0058374	6.0118800
21 N	0.0000000	5.4571731	4.6170863	2.5585442 *
22 H	5.4571731	0.0000000	2.5243169 *	4.3434786
23 H	4.6170863	2.5243169 *	0.0000000	2.5015095 *
24 H	2.5585442 *	4.3434786	2.5015095 *	0.0000000
25 H	6.1324655	2.3951711 *	4.7734578	5.9676315

26 H	6.6263430	4.7829628	6.8649062	7.3745418
27 H	5.4328862	5.9553350	7.3543485	6.9945040
28 H	5.0997992	7.2370530	8.1462312	7.1996520
29 H	5.9994011	10.9507046	10.5871739	8.4648437
30 H	7.9821311	12.3960566	12.4393837	10.5315972
31 H	8.2946420	11.7668513	12.3182030	10.8061287
32 H	6.7594233	9.4534529	10.2786530	9.0991296
33 H	4.0010018	9.0682333	8.5157586	6.3686609
34 H	1.0385401 *	5.9059019	5.0127259	2.9245010 *
35 H	1.0387512 *	5.7944228	4.5393762	2.1948371 *

H H H H

1 CO	6.4765962	6.2775072	4.5244340	3.8737624
2 C	2.6872779 *	4.6910667	5.3951202	6.4727018
3 C	4.0798146	5.9554121	6.2868846	7.0569303
4 C	4.8858984	6.2816619	6.0352857	6.4308988
5 C	4.6974625	5.5326901	4.8581677	5.0741594
6 C	3.5369258	4.0619274	3.5236426	4.1279214
7 C	2.1998752 *	3.5054326	3.9458146	5.0719186
8 C	1.1002878 *	2.2009565 *	3.4173224	4.9728415
9 C	2.1659666 *	1.1111791 *	2.1723941 *	3.9368787
10 C	3.4354875	2.1992860 *	1.0989556 *	2.5868713 *
11 C	3.9526825	3.4827471	2.1851164 *	2.6874856 *
12 N	5.4020639	4.6752639	2.6998107 *	2.1136430 *
13 C	6.2255942	4.9853900	2.6088783 *	1.1171744 *
14 C	7.6789345	6.3832056	3.9344049	2.1595876 *
15 C	8.5624721	7.5493973	5.1705416	3.5231014
16 C	9.9518070	8.8423305	6.4090535	4.6514280
17 C	10.5624179	9.1500140	6.6647374	4.8265107
18 C	9.9016877	8.2424484	5.7777911	3.9618561
19 C	8.5012488	6.8518417	4.3849515	2.5520676 *
20 O	8.2089404	7.6094250	5.4493896	4.1575034
21 N	6.1324655	6.6263430	5.4328862	5.0997992
22 H	2.3951711 *	4.7829628	5.9553350	7.2370530
23 H	4.7734578	6.8649062	7.3543485	8.1462312
24 H	5.9676315	7.3745418	6.9945040	7.1996520
25 H	0.0000000	2.5308593 *	4.3256417	5.9881411
26 H	2.5308593 *	0.0000000	2.4880605 *	4.3803073
27 H	4.3256417	2.4880605 *	0.0000000	1.9551125 *
28 H	5.9881411	4.3803073	1.9551125 *	0.0000000
29 H	10.6661249	9.7314994	7.3444081	5.6430811
30 H	11.6643901	10.2247310	7.7376847	5.9034213
31 H	10.5896011	8.7488065	6.3479343	4.6259549
32 H	8.1264223	6.2436361	3.8691566	2.2204600 *
33 H	9.0826042	8.5715986	6.4301316	5.1294573

34 H	6.5740587	7.0146300	5.7663242	5.2246175
35 H	6.7655506	7.4647107	6.3604985	6.0593250

H H H H

1 CO	4.6046238	6.4038127	6.6516921	5.2403070
2 C	9.8922965	11.4117896	10.9105349	8.6761206
3 C	9.6861680	11.4525782	11.2556491	9.1930011
4 C	8.4046482	10.2948920	10.3211486	8.4425474
5 C	7.2241494	8.9889826	8.9301581	7.0510201
6 C	7.4577213	8.8741169	8.4077139	6.2698129
7 C	8.9173133	10.2382163	9.5725005	7.2822852
8 C	9.5672985	10.5829772	9.5773152	7.1443978
9 C	9.0039331	9.7282396	8.4890258	6.0065137
10 C	7.5956231	8.3070028	7.1599544	4.7226888
11 C	6.7194769	7.8075109	7.0845523	4.8523428
12 N	5.2724844	6.4088998	5.9185433	3.9482017
13 C	4.7831748	5.4451239	4.6574335	2.6236042 *
14 C	3.4925555	3.9891238	3.5026214	2.1889650 *
15 C	2.1833442 *	3.4327810	3.9253645	3.4349086
16 C	1.1038230 *	2.1900297 *	3.4749599	3.9390891
17 C	2.1977969 *	1.1037697 *	2.2046387 *	3.4552480
18 C	3.4710953	2.2018301 *	1.1113178 *	2.1825814 *
19 C	3.9334242	3.4526743	2.1952587 *	1.1092331 *
20 O	2.6659283 *	4.6211750	5.3684449	4.6666381
21 N	5.9994011	7.9821311	8.2946420	6.7594233
22 H	10.9507046	12.3960566	11.7668513	9.4534529
23 H	10.5871739	12.4393837	12.3182030	10.2786530
24 H	8.4648437	10.5315972	10.8061287	9.0991296
25 H	10.6661249	11.6643901	10.5896011	8.1264223
26 H	9.7314994	10.2247310	8.7488065	6.2436361
27 H	7.3444081	7.7376847	6.3479343	3.8691566
28 H	5.6430811	5.9034213	4.6259549	2.2204600 *
29 H	0.0000000	2.5261159 *	4.3899540	5.0426250
30 H	2.5261159 *	0.0000000	2.5417768 *	4.3714541
31 H	4.3899540	2.5417768 *	0.0000000	2.5238180 *
32 H	5.0426250	4.3714541	2.5238180 *	0.0000000
33 H	2.2779006 *	4.5792905	5.7723311	5.4392576
34 H	5.9193956	7.8798271	8.2433267	6.7897008
35 H	6.3267667	8.4945512	9.0322238	7.6398503

H H H

1 CO	2.6551842 *	2.5360168 *	2.5625637 *
2 C	7.9895698	4.8236169	4.7143411
3 C	7.6613165	4.2424021	3.8946795

4 C	6.3547964	2.9175530 *	2.4798362 *
5 C	5.2674022	2.1408046 *	2.0997010 *
6 C	5.7090430	3.1865773	3.4449318
7 C	7.1687386	4.4354030	4.5709640
8 C	8.0102779	5.6522773	5.9100687
9 C	7.6972478	5.9413681	6.3624828
10 C	6.3918069	5.1107194	5.6345410
11 C	5.2773525	3.7356168	4.2399767
12 N	3.9518709	3.3976967	3.9900320
13 C	4.0451782	4.3840817	5.1342658
14 C	3.3309500	4.9104985	5.6388394
15 C	2.0455619 *	4.6628044	5.2232580
16 C	2.4862664 *	5.7654189	6.3066925
17 C	3.8879628	6.9544659	7.6056416
18 C	4.6926174	7.1795088	7.9402663
19 C	4.4595314	6.2734081	7.0740747
20 O	0.9984702 *	3.6945273	3.9433656
21 N	4.0010018	1.0385401 *	1.0387512 *
22 H	9.0682333	5.9059019	5.7944228
23 H	8.5157586	5.0127259	4.5393762
24 H	6.3686609	2.9245010 *	2.1948371 *
25 H	9.0826042	6.5740587	6.7655506
26 H	8.5715986	7.0146300	7.4647107
27 H	6.4301316	5.7663242	6.3604985
28 H	5.1294573	5.2246175	6.0593250
29 H	2.2779006 *	5.9193956	6.3267667
30 H	4.5792905	7.8798271	8.4945512
31 H	5.7723311	8.2433267	9.0322238
32 H	5.4392576	6.7897008	7.6398503
33 H	0.0000000	4.1506318	4.1992155
34 H	4.1506318	0.0000000	1.6532750 *
35 H	4.1992155	1.6532750 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.63 , TOTAL = 1506.7 SECONDS (25.1 MIN)
WALL CLOCK TIME: STEP = 0.63 , TOTAL = 1393.1 SECONDS (23.2 MIN)

CPU UTILIZATION: STEP = 99.44% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.16 , TOTAL = 1507.8 SECONDS (25.1 MIN)

WALL CLOCK TIME: STEP = 1.16, TOTAL = 1394.3 SECONDS (23.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.624805668	-284.624805668	0.288244233	0.006133653	197898359
11386919						
2	1	-284.626454304	-0.001648636	0.164094816	0.002052844	176353928
13205904						
3	2	-284.626371690	0.000082614	0.121807642	0.003091017	170974482
13686078						
4	3	-284.626726290	-0.000354600	0.018980137	0.000742513	168378561
13882993						
5	4	-284.626694194	0.000032096	0.016908035	0.000924061	157417307
14788886						
6	5	-284.626746834	-0.000052640	0.011132035	0.000111555	153964325
15047093						
7	6	-284.626746146	0.000000688	0.000866481	0.000136338	144454371
15875250						
8	7	-284.626748046	-0.000001900	0.001548574	0.000076875	155296051
14951061						
9	8	-284.626748268	-0.000000222	0.001561115	0.000057309	172132025
13673776						

-----DISABLING FDIFF OPTION-----

10	9	-284.626748706	-0.000000438	0.002025993	0.000070334	197914816
11385744						
11	10	-284.626749020	-0.000000314	0.000954412	0.000073198	197915276
11385725						
12	11	-284.626749186	-0.000000166	0.001646044	0.000073080	197915681
11385683						
13	12	-284.626749376	-0.000000190	0.003124978	0.000057285	197914932
11385721						
14	13	-284.626749619	-0.000000243	0.002684844	0.000031238	197913771
11385815						
15	14	-284.626749697	-0.000000078	0.001711396	0.000047214	197914809
11385737						
16	15	-284.626749757	-0.000000061	0.000433982	0.000032154	197915356
11385696						
17	16	-284.626749780	-0.000000023	0.000641657	0.000025917	197915306
11385708						

18 17	-284.626749815	-0.000000035	0.000752049	0.000017947	197915125
11385722					
19 18	-284.626749860	-0.000000045	0.000887349	0.000013255	197915137
11385725					
20 19	-284.626749876	-0.000000016	0.000428553	0.000013441	197915308
11385700					
21 20	-284.626749887	-0.000000011	0.001024004	0.000012686	197915216
11385714					
22 21	-284.626749902	-0.000000016	0.000491849	0.000010190	197914970
11385739					
23 22	-284.626749910	-0.000000008	0.000573885	0.000007361	197914975
11385732					
24 23	-284.626749914	-0.000000004	0.000075465	0.000008131	197915268
11385711					
25 24	-284.626749917	-0.000000003	0.000073459	0.000005453	197915137
11385716					
26 25	-284.626749919	-0.000000001	0.000063330	0.000002091	197915106
11385719					
27 26	-284.626749919	-0.000000001	0.000085871	0.000001793	197915109
11385719					
28 27	-284.626749920	0.000000000	0.000039293	0.000000680	197915096
11385720					
29 28	-284.626749920	0.000000000	0.000017692	0.000000539	197915090
11385721					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 99.2 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 31.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 3.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6267499195 AFTER 29 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6097127394
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000637078

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 103.57 , TOTAL = 1611.4 SECONDS (26.9 MIN)
WALL CLOCK TIME: STEP = 94.95 , TOTAL = 1489.2 SECONDS (24.8 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.77 , TOTAL = 1615.2 SECONDS (26.9 MIN)
WALL CLOCK TIME: STEP = 3.73 , TOTAL = 1493.0 SECONDS (24.9 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.86 , TOTAL = 1618.0 SECONDS (27.0 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 1495.7 SECONDS (24.9 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 11 ENERGY= -284.6267499

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0006440	0.0036179	0.0014736
2 C	6.0	0.0015416	-0.0103735	-0.0013216
3 C	6.0	0.0065079	-0.0007726	-0.0003130
4 C	6.0	-0.0059167	0.0015654	0.0003384
5 C	6.0	0.0033312	-0.0070906	-0.0011199
6 C	6.0	-0.0001008	-0.0032210	-0.0004396
7 C	6.0	0.0010923	0.0076245	0.0018129
8 C	6.0	0.0005354	0.0022979	0.0006429
9 C	6.0	0.0038787	-0.0002985	-0.0000455
10 C	6.0	-0.0043472	0.0024801	0.0012206
11 C	6.0	-0.0054639	0.0056889	0.0006105
12 N	7.0	0.0018449	-0.0003262	-0.0012104
13 C	6.0	0.0025923	-0.0077779	0.0008457

14 C	6.0	0.0019504	0.0033704	-0.0021939
15 C	6.0	-0.0024143	-0.0000654	-0.0030913
16 C	6.0	0.0015392	0.0012609	-0.0013637
17 C	6.0	0.0015519	-0.0044890	-0.0006189
18 C	6.0	0.0065798	0.0022474	-0.0010264
19 C	6.0	-0.0011874	-0.0095350	-0.0007451
20 O	8.0	0.0039333	0.0072773	0.0012944
21 N	7.0	0.0032990	-0.0060654	-0.0064474
22 H	1.0	0.0003563	0.0003771	-0.0001961
23 H	1.0	-0.0079408	0.0025561	0.0003852
24 H	1.0	-0.0012797	0.0019556	0.0008496
25 H	1.0	-0.0039009	-0.0003436	0.0000346
26 H	1.0	-0.0019541	0.0046742	0.0008102
27 H	1.0	0.0018978	-0.0014728	-0.0010910
28 H	1.0	-0.0022997	0.0069333	0.0004779
29 H	1.0	0.0010800	0.0021000	-0.0022400
30 H	1.0	0.0008143	0.0007464	0.0023811
31 H	1.0	-0.0043534	0.0023342	0.0022631
32 H	1.0	0.0010754	0.0018652	0.0021554
33 H	1.0	-0.0020103	-0.0055200	0.0016483
34 H	1.0	0.0009118	-0.0038055	0.0041826
35 H	1.0	-0.0025003	0.0001843	0.0000367

MAXIMUM GRADIENT = 0.0103735 RMS GRADIENT = 0.0033860
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0014140512
 PREDICTED ENERGY CHANGE WAS -0.0016851596 RATIO= 0.839
 GDIIS STEP HAS LENGTH = 0.118824
 RADIUS OF STEP TAKEN= 0.11882 CURRENT TRUST RADIUS= 0.19731

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.01 , TOTAL = 1618.1 SECONDS (27.0 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1495.7 SECONDS (24.9 MIN)
 CPU UTILIZATION: STEP = 55.40% , TOTAL = 100.00%

INSERCH= 12

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1316163284	-1.6268852017	1.0325665323
C	6.0	4.9723905708	0.6554228026	0.4317429429
C	6.0	5.1749895014	-0.7062270185	0.1824523163
C	6.0	4.0469725133	-1.5572289489	0.0550629646

C	6.0	2.7294487736	-1.0742051803	0.1678980527
C	6.0	2.4481727326	0.3444939723	0.4574815076
C	6.0	3.6438765824	1.2066568509	0.5744482831
C	6.0	3.5230933580	2.6203846169	0.8315202693
C	6.0	2.2685046045	3.2265674909	0.9895489635
C	6.0	1.0975968755	2.4201832642	0.9124568764
C	6.0	1.1534786483	1.0280867044	0.6467370598
N	7.0	-0.0710619561	0.2509311662	0.6514435093
C	6.0	-1.2800067572	0.7935376609	0.5231414215
C	6.0	-2.5680339529	0.0925591561	0.5449428479
C	6.0	-2.8194357243	-1.3144751693	0.6315527214
C	6.0	-4.1031961288	-1.8811076937	0.5444634097
C	6.0	-5.2353710163	-1.0104264833	0.5013793504
C	6.0	-5.0573849811	0.3953874581	0.4988692185
C	6.0	-3.7440322651	0.9305369155	0.4803530908
O	8.0	-1.7131217740	-2.2243655119	0.9123926875
N	7.0	1.6767244244	-2.1607080377	-0.0341332296
H	1.0	5.8396791767	1.3346304585	0.5212340279
H	1.0	6.1856167659	-1.1216140792	0.0760740430
H	1.0	4.2067164742	-2.6307969886	-0.1553227588
H	1.0	4.4330603414	3.2329368076	0.9100842527
H	1.0	2.1733702135	4.3105712445	1.1941172919
H	1.0	0.1270350427	2.9126903538	1.0965191967
H	1.0	-1.3796483164	1.8831686633	0.3598406016
H	1.0	-4.2457902616	-2.9791235599	0.5340885275
H	1.0	-6.2491943452	-1.4484219640	0.5156067273
H	1.0	-5.9235439068	1.0647531344	0.5360883216
H	1.0	-3.6034780815	2.0237082345	0.4616276332
H	1.0	-2.0319255676	-3.1415785567	1.0682770424
H	1.0	1.4307049054	-2.2618241641	-1.0420687569
H	1.0	2.0981742017	-3.0671133978	0.2504000540

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3854446	5.1967219	4.0361342
2 C	5.3854446	0.0000000	1.3990291 *	2.4277797 *
3 C	5.1967219	1.3990291 *	0.0000000	1.4187511 *
4 C	4.0361342	2.4277797 *	1.4187511 *	0.0000000
5 C	2.7931774 *	2.8446467 *	2.4731133 *	1.4078041 *
6 C	3.0957216	2.5434258 *	2.9351636 *	2.5168734 *
7 C	4.5359459	1.4453972 *	2.4813489 *	2.8410055 *
8 C	5.4389187	2.4741381 *	3.7704635	4.2813304
9 C	5.3032203	3.7726558	4.9564031	5.1885374

10 C	4.1624882	4.2847977	5.1896511	5.0253108
11 C	2.8708784 *	3.8430703	4.4040838	3.9250786
12 N	1.9267920 *	5.0644146	5.3532383	4.5368845
13 C	2.8479186 *	6.2545905	6.6356868	5.8413962
14 C	3.2376500	7.5622504	7.7925523	6.8352098
15 C	2.9945150 *	8.0394638	8.0300991	6.8948410
16 C	4.2704227	9.4240632	9.3592802	8.1712703
17 C	5.4283270	10.3430315	10.4196861	9.3091403
18 C	5.5946541	10.0333704	10.2963664	9.3219633
19 C	4.6761095	8.7208989	9.0728546	8.1896035
20 O	1.9428029 *	7.2952231	7.0910954	5.8616356
21 N	1.9519668 *	4.3599368	3.7947705	2.4474924 *
22 H	6.4508928	1.1052245 *	2.1729438 *	3.4342340
23 H	6.1498860	2.1808893 *	1.0978298 *	2.1826592 *
24 H	4.3618071	3.4249297	2.1807371 *	1.1055897 *
25 H	6.4911703	2.6764278 *	4.0739316	4.8811692
26 H	6.2807839	4.6664590	5.9330809	6.2640969
27 H	4.5400283	5.3865253	6.2780511	6.0357866
28 H	3.8803298	6.4700022	7.0498024	6.4325297
29 H	4.6085483	9.9093521	9.6974635	8.4274055
30 H	6.4042050	11.4174062	11.4531141	10.3070360
31 H	6.6450262	10.9041197	11.2445041	10.3207254
32 H	5.2539256	8.6843895	9.1973898	8.4568197
33 H	2.6413036 *	7.9926741	7.6586714	6.3631571
34 H	2.5288120 *	4.8193348	4.2354458	2.9231847 *
35 H	2.5599593 *	4.7065147	3.8788134	2.4729987 *

C C C C

1 CO	2.7931774 *	3.0957216	4.5359459	5.4389187
2 C	2.8446467 *	2.5434258 *	1.4453972 *	2.4741381 *
3 C	2.4731133 *	2.9351636 *	2.4813489 *	3.7704635
4 C	1.4078041 *	2.5168734 *	2.8410055 *	4.2813304
5 C	0.0000000	1.4750193 *	2.4907414 *	3.8366991
6 C	1.4750193 *	0.0000000	1.4787541 *	2.5446095 *
7 C	2.4907414 *	1.4787541 *	0.0000000	1.4419781 *
8 C	3.8366991	2.5446095 *	1.4419781 *	0.0000000
9 C	4.4027520	2.9362773 *	2.4787085 *	1.4022923 *
10 C	3.9278568	2.5178451 *	2.8408514 *	2.4350902 *
11 C	2.6706928 *	1.4762620 *	2.4978380 *	2.8608795 *
12 N	3.1357077	2.5284222 *	3.8366793	4.3086761
13 C	4.4373860	3.7556988	4.9414499	5.1480324
14 C	5.4375385	5.0232908	6.3110947	6.6010499
15 C	5.5734033	5.5254120	6.9378508	7.4666447
16 C	6.8904230	6.9196317	8.3398036	8.8603683
17 C	7.9720532	7.8022164	9.1521492	9.4869637

18 C	7.9312057	7.5058444	8.7393262	8.8705061
19 C	6.7839941	6.2199174	7.3936658	7.4692716
20 O	4.6490401	4.9114514	6.3705221	7.1341498
21 N	1.5262810 *	2.6669936 *	3.9470502	5.1978150
22 H	3.9497935	3.5336597	2.2001723 *	2.6675853 *
23 H	3.4577126	4.0327946	3.4827669	4.6542759
24 H	2.1702004 *	3.5100372	3.9465690	5.3866602
25 H	4.6909066	3.5337983	2.2002893 *	1.0997420 *
26 H	5.5098245	4.0432558	3.4900807	2.1931621 *
27 H	4.8507969	3.5201821	3.9435115	3.4189003
28 H	5.0663183	4.1266533	5.0734138	4.9802455
29 H	7.2399426	7.4740513	8.9313621	9.5811539
30 H	8.9931625	8.8804347	10.2433275	10.5902122
31 H	8.9210419	8.4030109	9.5685497	9.5784250
32 H	7.0561538	6.2803069	7.2941381	7.1610658
33 H	5.2683395	5.7093829	7.1669902	8.0071536
34 H	2.1356952 *	3.1743954	4.4205901	5.6324407
35 H	2.0921275 *	3.4357600	4.5562392	5.8920055

C C C N

1 CO	5.3032203	4.1624882	2.8708784 *	1.9267920 *
2 C	3.7726558	4.2847977	3.8430703	5.0644146
3 C	4.9564031	5.1896511	4.4040838	5.3532383
4 C	5.1885374	5.0253108	3.9250786	4.5368845
5 C	4.4027520	3.9278568	2.6706928 *	3.1357077
6 C	2.9362773 *	2.5178451 *	1.4762620 *	2.5284222 *
7 C	2.4787085 *	2.8408514 *	2.4978380 *	3.8366793
8 C	1.4022923 *	2.4350902 *	2.8608795 *	4.3086761
9 C	0.0000000	1.4238060 *	2.4887990 *	3.8003024
10 C	1.4238060 *	0.0000000	1.4183309 *	2.4778107 *
11 C	2.4887990 *	1.4183309 *	0.0000000	1.4503422 *
12 N	3.8003024	2.4778107 *	1.4503422 *	0.0000000
13 C	4.3277134	2.9069815 *	2.4478849 *	1.3313267 *
14 C	5.7802931	4.3577230	3.8386495	2.5042550 *
15 C	6.8290824	5.4193842	4.6121443	3.1629813
16 C	8.1783261	6.7590510	6.0088686	4.5623613
17 C	8.6312558	7.2141909	6.7077615	5.3182357
18 C	7.8692443	6.4926616	6.2447578	4.9907478
19 C	6.4561317	5.0840075	4.9013072	3.7392308
20 O	6.7507016	5.4288095	4.3435488	2.9818700 *
21 N	5.5155115	4.7133838	3.3023904	3.0562684
22 H	4.0684189	4.8804533	4.6978927	6.0106755
23 H	5.9232497	6.2555424	5.5017528	6.4312486
24 H	6.2750391	6.0265396	4.8324933	5.2205955
25 H	2.1660233 *	3.4330585	3.9606025	5.4079913

26 H	1.1072321 *	2.1932140 *	3.4805903	4.6704013
27 H	2.1669918 *	1.1038263 *	2.1926289 *	2.7059743 *
28 H	3.9383084	2.5943233 *	2.6889044 *	2.1122570 *
29 H	9.0085561	7.6057520	6.7247698	5.2797142
30 H	9.7278643	8.3125771	7.8070390	6.4090227
31 H	8.4846171	7.1606747	7.0779825	5.9099203
32 H	6.0171216	4.7392558	4.8635548	3.9568589
33 H	7.6846068	6.3836812	5.2640863	3.9405404
34 H	5.9120066	5.0845182	3.7084273	3.3818969
35 H	6.3392249	5.6169297	4.2213975	3.9844499

C C C C

1 CO	2.8479186 *	3.2376500	2.9945150 *	4.2704227
2 C	6.2545905	7.5622504	8.0394638	9.4240632
3 C	6.6356868	7.7925523	8.0300991	9.3592802
4 C	5.8413962	6.8352098	6.8948410	8.1712703
5 C	4.4373860	5.4375385	5.5734033	6.8904230
6 C	3.7556988	5.0232908	5.5254120	6.9196317
7 C	4.9414499	6.3110947	6.9378508	8.3398036
8 C	5.1480324	6.6010499	7.4666447	8.8603683
9 C	4.3277134	5.7802931	6.8290824	8.1783261
10 C	2.9069815 *	4.3577230	5.4193842	6.7590510
11 C	2.4478849 *	3.8386495	4.6121443	6.0088686
12 N	1.3313267 *	2.5042550 *	3.1629813	4.5623613
13 C	0.0000000	1.4665811 *	2.6125299 *	3.8890334
14 C	1.4665811 *	0.0000000	1.4319391 *	2.5004168 *
15 C	2.6125299 *	1.4319391 *	0.0000000	1.4059508 *
16 C	3.8890334	2.5004168 *	1.4059508 *	0.0000000
17 C	4.3473747	2.8867217 *	2.4384696 *	1.4289024 *
18 C	3.7983811	2.5081261 *	2.8195127 *	2.4688024 *
19 C	2.4682020 *	1.4454586 *	2.4326569 *	2.8352168 *
20 O	3.0735720	2.4968048 *	1.4596925 *	2.4424687 *
21 N	4.2166790	4.8405078	4.6232785	5.8155337
22 H	7.1402180	8.4989966	9.0559484	10.4499895
23 H	7.7203115	8.8498845	9.0242297	10.3274339
24 H	6.5031157	7.3351404	7.1915708	8.3729554
25 H	6.2241087	7.6818371	8.5647671	9.9576505
26 H	4.9744896	6.3791823	7.5422634	8.8404877
27 H	2.6075538 *	3.9396413	5.1736653	6.4171739
28 H	1.1062962 *	2.1570363 *	3.5173486	4.6499005
29 H	4.7988503	3.5000313	2.1943201 *	1.1072848 *
30 H	5.4515379	3.9907926	3.4343310	2.1893739 *
31 H	4.6514689	3.4935207	3.9122025	3.4629225
32 H	2.6297571 *	2.1928116 *	3.4332296	3.9375332
33 H	4.0432282	3.3197798	2.0369603 *	2.4805905 *

34 H	4.3741372	4.9042470	4.6649946	5.7694098
35 H	5.1372289	5.6430297	5.2344919	6.3206073

C C C O

1 CO	5.4283270	5.5946541	4.6761095	1.9428029 *
2 C	10.3430315	10.0333704	8.7208989	7.2952231
3 C	10.4196861	10.2963664	9.0728546	7.0910954
4 C	9.3091403	9.3219633	8.1896035	5.8616356
5 C	7.9720532	7.9312057	6.7839941	4.6490401
6 C	7.8022164	7.5058444	6.2199174	4.9114514
7 C	9.1521492	8.7393262	7.3936658	6.3705221
8 C	9.4869637	8.8705061	7.4692716	7.1341498
9 C	8.6312558	7.8692443	6.4561317	6.7507016
10 C	7.2141909	6.4926616	5.0840075	5.4288095
11 C	6.7077615	6.2447578	4.9013072	4.3435488
12 N	5.3182357	4.9907478	3.7392308	2.9818700 *
13 C	4.3473747	3.7983811	2.4682020 *	3.0735720
14 C	2.8867217 *	2.5081261 *	1.4454586 *	2.4968048 *
15 C	2.4384696 *	2.8195127 *	2.4326569 *	1.4596925 *
16 C	1.4289024 *	2.4688024 *	2.8352168 *	2.4424687 *
17 C	0.0000000	1.4170385 *	2.4478301 *	3.7481755
18 C	1.4170385 *	0.0000000	1.4183170 *	4.2682788
19 C	2.4478301 *	1.4183170 *	0.0000000	3.7768591
20 O	3.7481755	4.2682788	3.7768591	0.0000000
21 N	7.0275874	7.2225996	6.2613972	3.5200882
22 H	11.3206194	10.9374899	9.5923140	8.3584843
23 H	11.4294448	11.3527590	10.1475463	8.0190748
24 H	9.6025973	9.7677702	8.7350780	6.0290702
25 H	10.5665385	9.9140979	8.5059131	8.2193496
26 H	9.1478057	8.2520212	6.8519883	7.6085207
27 H	6.6708647	5.7941531	4.3924657	5.4598006
28 H	4.8228128	3.9697064	2.5519291 *	4.1579268
29 H	2.2036579 *	3.4709150	3.9420925	2.6696785 *
30 H	1.1044819 *	2.1955234 *	3.4549277	4.6190347
31 H	2.1865857 *	1.0952931 *	2.1843515 *	5.3560770
32 H	3.4453778	2.1832684 *	1.1023292 *	4.6714844
33 H	3.8891188	4.6891106	4.4563537	0.9834712 *
34 H	6.9559181	7.1784799	6.2679217	3.7020223
35 H	7.6206192	7.9531551	7.0827581	3.9590953

N H H H

1 CO	1.9519668 *	6.4508928	6.1498860	4.3618071
2 C	4.3599368	1.1052245 *	2.1808893 *	3.4249297
3 C	3.7947705	2.1729438 *	1.0978298 *	2.1807371 *

4 C	2.4474924 *	3.4342340	2.1826592 *	1.1055897 *
5 C	1.5262810 *	3.9497935	3.4577126	2.1702004 *
6 C	2.6669936 *	3.5336597	4.0327946	3.5100372
7 C	3.9470502	2.2001723 *	3.4827669	3.9465690
8 C	5.1978150	2.6675853 *	4.6542759	5.3866602
9 C	5.5155115	4.0684189	5.9232497	6.2750391
10 C	4.7133838	4.8804533	6.2555424	6.0265396
11 C	3.3023904	4.6978927	5.5017528	4.8324933
12 N	3.0562684	6.0106755	6.4312486	5.2205955
13 C	4.2166790	7.1402180	7.7203115	6.5031157
14 C	4.8405078	8.4989966	8.8498845	7.3351404
15 C	4.6232785	9.0559484	9.0242297	7.1915708
16 C	5.8155337	10.4499895	10.3274339	8.3729554
17 C	7.0275874	11.3206194	11.4294448	9.6025973
18 C	7.2225996	10.9374899	11.3527590	9.7677702
19 C	6.2613972	9.5923140	10.1475463	8.7350780
20 O	3.5200882	8.3584843	8.0190748	6.0290702
21 N	0.0000000	5.4640659	4.6283876	2.5761464 *
22 H	5.4640659	0.0000000	2.5201146 *	4.3415333
23 H	4.6283876	2.5201146 *	0.0000000	2.4994447 *
24 H	2.5761464 *	4.3415333	2.4994447 *	0.0000000
25 H	6.1302805	2.3944411 *	4.7675088	5.9640337
26 H	6.6055062	4.7697816	6.8452013	7.3578583
27 H	5.4239546	5.9544546	7.3500567	6.9957959
28 H	5.0842471	7.2419356	8.1450892	7.2006077
29 H	6.0057356	10.9692904	10.6053935	8.4877258
30 H	7.9768260	12.4050907	12.4468679	10.5439190
31 H	8.2760396	11.7663279	12.3135530	10.8054299
32 H	6.7554169	9.4684529	10.2892216	9.1128583
33 H	3.9914283	9.0718170	8.5201365	6.3779894
34 H	1.0424414 *	5.9006318	5.0159256	2.9374648 *
35 H	1.0393025 *	5.7833865	4.5301814	2.1911033 *

H H H H

1 CO	6.4911703	6.2807839	4.5400283	3.8803298
2 C	2.6764278 *	4.6664590	5.3865253	6.4700022
3 C	4.0739316	5.9330809	6.2780511	7.0498024
4 C	4.8811692	6.2640969	6.0357866	6.4325297
5 C	4.6909066	5.5098245	4.8507969	5.0663183
6 C	3.5337983	4.0432558	3.5201821	4.1266533
7 C	2.2002893 *	3.4900807	3.9435115	5.0734138
8 C	1.0997420 *	2.1931621 *	3.4189003	4.9802455
9 C	2.1660233 *	1.1072321 *	2.1669918 *	3.9383084
10 C	3.4330585	2.1932140 *	1.1038263 *	2.5943233 *
11 C	3.9606025	3.4805903	2.1926289 *	2.6889044 *

12 N	5.4079913	4.6704013	2.7059743 *	2.1122570 *
13 C	6.2241087	4.9744896	2.6075538 *	1.1062962 *
14 C	7.6818371	6.3791823	3.9396413	2.1570363 *
15 C	8.5647671	7.5422634	5.1736653	3.5173486
16 C	9.9576505	8.8404877	6.4171739	4.6499005
17 C	10.5665385	9.1478057	6.6708647	4.8228128
18 C	9.9140979	8.2520212	5.7941531	3.9697064
19 C	8.5059131	6.8519883	4.3924657	2.5519291 *
20 O	8.2193496	7.6085207	5.4598006	4.1579268
21 N	6.1302805	6.6055062	5.4239546	5.0842471
22 H	2.3944411 *	4.7697816	5.9544546	7.2419356
23 H	4.7675088	6.8452013	7.3500567	8.1450892
24 H	5.9640337	7.3578583	6.9957959	7.2006077
25 H	0.0000000	2.5195575 *	4.3219405	5.9926809
26 H	2.5195575 *	0.0000000	2.4801379 *	4.3831771
27 H	4.3219405	2.4801379 *	0.0000000	1.9679190 *
28 H	5.9926809	4.3831771	1.9679190 *	0.0000000
29 H	10.6795840	9.7355488	7.3587635	5.6468591
30 H	11.6696743	10.2257505	7.7468097	5.9022231
31 H	10.5877356	8.7480487	6.3512566	4.6203738
32 H	8.1393671	6.2560578	3.8871718	2.2305898 *
33 H	9.0805019	8.5577383	6.4277586	5.1161932
34 H	6.5587680	6.9820098	5.7488011	5.2004231
35 H	6.7511117	7.4381777	6.3529017	6.0508280

H H H H

1 CO	4.6085483	6.4042050	6.6450262	5.2539256
2 C	9.9093521	11.4174062	10.9041197	8.6843895
3 C	9.6974635	11.4531141	11.2445041	9.1973898
4 C	8.4274055	10.3070360	10.3207254	8.4568197
5 C	7.2399426	8.9931625	8.9210419	7.0561538
6 C	7.4740513	8.8804347	8.4030109	6.2803069
7 C	8.9313621	10.2433275	9.5685497	7.2941381
8 C	9.5811539	10.5902122	9.5784250	7.1610658
9 C	9.0085561	9.7278643	8.4846171	6.0171216
10 C	7.6057520	8.3125771	7.1606747	4.7392558
11 C	6.7247698	7.8070390	7.0779825	4.8635548
12 N	5.2797142	6.4090227	5.9099203	3.9568589
13 C	4.7988503	5.4515379	4.6514689	2.6297571 *
14 C	3.5000313	3.9907926	3.4935207	2.1928116 *
15 C	2.1943201 *	3.4343310	3.9122025	3.4332296
16 C	1.1072848 *	2.1893739 *	3.4629225	3.9375332
17 C	2.2036579 *	1.1044819 *	2.1865857 *	3.4453778
18 C	3.4709150	2.1955234 *	1.0952931 *	2.1832684 *
19 C	3.9420925	3.4549277	2.1843515 *	1.1023292 *

20 O	2.6696785 *	4.6190347	5.3560770	4.6714844
21 N	6.0057356	7.9768260	8.2760396	6.7554169
22 H	10.9692904	12.4050907	11.7663279	9.4684529
23 H	10.6053935	12.4468679	12.3135530	10.2892216
24 H	8.4877258	10.5439190	10.8054299	9.1128583
25 H	10.6795840	11.6696743	10.5877356	8.1393671
26 H	9.7355488	10.2257505	8.7480487	6.2560578
27 H	7.3587635	7.7468097	6.3512566	3.8871718
28 H	5.6468591	5.9022231	4.6203738	2.2305898 *
29 H	0.0000000	2.5213125 *	4.3781046	5.0444169
30 H	2.5213125 *	0.0000000	2.5342685 *	4.3655946
31 H	4.3781046	2.5342685 *	0.0000000	2.5115423 *
32 H	5.0444169	4.3655946	2.5115423 *	0.0000000
33 H	2.2831877 *	4.5779449	5.7550973	5.4330460
34 H	5.9347610	7.8783773	8.2244557	6.7801098
35 H	6.3509138	8.5070005	9.0278403	7.6465627

H H H

1 CO	2.6413036 *	2.5288120 *	2.5599593 *
2 C	7.9926741	4.8193348	4.7065147
3 C	7.6586714	4.2354458	3.8788134
4 C	6.3631571	2.9231847 *	2.4729987 *
5 C	5.2683395	2.1356952 *	2.0921275 *
6 C	5.7093829	3.1743954	3.4357600
7 C	7.1669902	4.4205901	4.5562392
8 C	8.0071536	5.6324407	5.8920055
9 C	7.6846068	5.9120066	6.3392249
10 C	6.3836812	5.0845182	5.6169297
11 C	5.2640863	3.7084273	4.2213975
12 N	3.9405404	3.3818969	3.9844499
13 C	4.0432282	4.3741372	5.1372289
14 C	3.3197798	4.9042470	5.6430297
15 C	2.0369603 *	4.6649946	5.2344919
16 C	2.4805905 *	5.7694098	6.3206073
17 C	3.8891188	6.9559181	7.6206192
18 C	4.6891106	7.1784799	7.9531551
19 C	4.4563537	6.2679217	7.0827581
20 O	0.9834712 *	3.7020223	3.9590953
21 N	3.9914283	1.0424414 *	1.0393025 *
22 H	9.0718170	5.9006318	5.7833865
23 H	8.5201365	5.0159256	4.5301814
24 H	6.3779894	2.9374648 *	2.1911033 *
25 H	9.0805019	6.5587680	6.7511117
26 H	8.5577383	6.9820098	7.4381777
27 H	6.4277586	5.7488011	6.3529017

28 H	5.1161932	5.2004231	6.0508280
29 H	2.2831877 *	5.9347610	6.3509138
30 H	4.5779449	7.8783773	8.5070005
31 H	5.7550973	8.2244557	9.0278403
32 H	5.4330460	6.7801098	7.6465627
33 H	0.0000000	4.1493779	4.2109609
34 H	4.1493779	0.0000000	1.6626730 *
35 H	4.2109609	1.6626730 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.61 , TOTAL = 1618.7 SECONDS (27.0 MIN)
WALL CLOCK TIME: STEP = 0.61 , TOTAL = 1496.3 SECONDS (24.9 MIN)

CPU UTILIZATION: STEP = 99.48%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.92 , TOTAL = 1619.6 SECONDS (27.0 MIN)
WALL CLOCK TIME: STEP = 0.91 , TOTAL = 1497.2 SECONDS (25.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.626890727	-284.626890727	0.100765953	0.005050646	197765891
11392489					
2 1	-284.627812788	-0.000922060	0.017801563	0.000893091	172414532
13493166					
3 2	-284.627765312	0.000047476	0.017077925	0.001007550	162911668
14304543					
4 3	-284.627902928	-0.000137616	0.004203917	0.000327947	160633594
14479562					
5 4	-284.627894175	0.000008753	0.002874783	0.000558335	149458035
15437594					
6 5	-284.627907257	-0.000013082	0.000758932	0.000085764	145862700
15721802					
7 6	-284.627906973	0.000000284	0.000490473	0.000120508	134983358
16580466					

8 7	-284.627907789	-0.000000817	0.000412900	0.000069642	151658240
15291305					
9 8	-284.627907910	-0.000000121	0.000572455	0.000053711	146672677
15713307					
10 9	-284.627908179	-0.000000269	0.001152238	0.000056006	164088315
14474745					
-----DISABLING FDIFF OPTION-----					
11 10	-284.627908317	-0.000000139	0.000763511	0.000060706	197757443
11393387					
12 11	-284.627908504	-0.000000187	0.000444721	0.000058390	197757466
11393373					
13 12	-284.627908648	-0.000000145	0.001406230	0.000048662	197757818
11393359					
14 13	-284.627908897	-0.000000248	0.000911813	0.000035671	197757484
11393358					
15 14	-284.627908981	-0.000000084	0.000586527	0.000037643	197757683
11393352					
16 15	-284.627909037	-0.000000056	0.000284544	0.000034519	197757623
11393371					
17 16	-284.627909092	-0.000000055	0.000428533	0.000023933	197757374
11393374					
18 17	-284.627909134	-0.000000042	0.000143897	0.000012857	197757285
11393371					
19 18	-284.627909146	-0.000000011	0.000067471	0.000008177	197757289
11393373					
20 19	-284.627909152	-0.000000006	0.000049173	0.000006524	197757278
11393368					
21 20	-284.627909155	-0.000000003	0.000050719	0.000006109	197757281
11393367					
22 21	-284.627909158	-0.000000003	0.000087931	0.000005027	197757254
11393372					
23 22	-284.627909160	-0.000000003	0.000061397	0.000003668	197757248
11393376					
24 23	-284.627909161	-0.000000001	0.000043455	0.000004354	197757256
11393374					
25 24	-284.627909163	-0.000000001	0.000046858	0.000003829	197757255
11393375					
26 25	-284.627909163	-0.000000001	0.000023225	0.000001938	197757224
11393376					
27 26	-284.627909164	0.000000000	0.000013165	0.000001153	197757221
11393377					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 91.7 SECONDS (3.4 SEC/ITER)

OF THE ABOVE TIME, DFT PART= 29.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.8, LAST ITERATION= 3.0
TIME TO SOLVE SCF EQUATIONS= 3.9 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6279091637 AFTER 27 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6190202252
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000765790

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 96.62 , TOTAL = 1716.2 SECONDS (28.6 MIN)
WALL CLOCK TIME: STEP = 88.43 , TOTAL = 1585.6 SECONDS (26.4
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.90 , TOTAL = 1720.1 SECONDS (28.7 MIN)
WALL CLOCK TIME: STEP = 3.87 , TOTAL = 1589.5 SECONDS (26.5
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.86 , TOTAL = 1723.0 SECONDS (28.7 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 1592.2 SECONDS (26.5
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 12 ENERGY= -284.6279092

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0019464	0.0007080	0.0002561
2 C	6.0	-0.0000390	-0.0015829	0.0000400
3 C	6.0	-0.0037155	-0.0054195	-0.0009453
4 C	6.0	0.0064058	0.0031957	0.0004929
5 C	6.0	-0.0014088	-0.0034813	-0.0013846
6 C	6.0	0.0009529	0.0014760	0.0003755
7 C	6.0	-0.0001091	0.0054298	0.0015604
8 C	6.0	0.0046795	-0.0011986	-0.0001055
9 C	6.0	-0.0014803	-0.0012450	0.0001306
10 C	6.0	0.0027566	0.0038386	0.0007239
11 C	6.0	-0.0057582	0.0001518	-0.0003808
12 N	7.0	0.0016379	-0.0004419	-0.0011383
13 C	6.0	0.0041522	0.0041469	-0.0003110
14 C	6.0	0.0032562	-0.0045155	-0.0007155
15 C	6.0	0.0017266	0.0046465	-0.0026134
16 C	6.0	0.0022632	-0.0019533	-0.0011455
17 C	6.0	0.0006197	0.0061386	-0.0009053
18 C	6.0	-0.0091036	-0.0011629	-0.0007900
19 C	6.0	0.0015188	0.0012081	-0.0011726
20 O	8.0	-0.0022246	-0.0048806	0.0029337
21 N	7.0	-0.0029908	-0.0071260	-0.0017092
22 H	1.0	0.0006426	-0.0006138	-0.0002584
23 H	1.0	-0.0042676	0.0010681	0.0001584
24 H	1.0	-0.0010868	0.0013590	0.0006356
25 H	1.0	-0.0042701	-0.0001698	0.0001051
26 H	1.0	-0.0009589	0.0021140	0.0003026
27 H	1.0	-0.0006159	0.0003864	-0.0004336
28 H	1.0	-0.0023322	0.0001285	0.0010034
29 H	1.0	0.0001741	-0.0003460	-0.0022671
30 H	1.0	0.0006153	0.0001789	0.0021621
31 H	1.0	0.0046763	-0.0040829	0.0022088
32 H	1.0	-0.0000077	-0.0026049	0.0017881
33 H	1.0	0.0025512	0.0063772	-0.0005913
34 H	1.0	0.0007432	-0.0024331	0.0009948
35 H	1.0	-0.0009497	0.0007057	0.0009954

MAXIMUM GRADIENT = 0.0091036 RMS GRADIENT = 0.0026787

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0011592441

PREDICTED ENERGY CHANGE WAS -0.0012309303 RATIO= 0.942

GDIIS STEP HAS LENGTH = 0.175298

RADIUS OF STEP TAKEN= 0.17530 CURRENT TRUST RADIUS= 0.23765

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 1723.0 SECONDS (28.7 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1592.2 SECONDS (26.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 13

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1281881017	-1.6432901168	1.0380410878
C	6.0	4.9786543150	0.6653213626	0.4310907754
C	6.0	5.1839861249	-0.6939603608	0.1831096696
C	6.0	4.0505974808	-1.5582417133	0.0528080615
C	6.0	2.7369833051	-1.0651213146	0.1674687934
C	6.0	2.4530236653	0.3460226711	0.4557036886
C	6.0	3.6530497406	1.2018190280	0.5704952339
C	6.0	3.5262299314	2.6187975671	0.8300152400
C	6.0	2.2774527849	3.2204393147	0.9871886551
C	6.0	1.1037631641	2.4085388132	0.9098058432
C	6.0	1.1628808046	1.0197659322	0.6462312962
N	7.0	-0.0746317438	0.2470776629	0.6583620588
C	6.0	-1.2849428650	0.7883127050	0.5265211991
C	6.0	-2.5791226191	0.0974755871	0.5577500934
C	6.0	-2.8295233480	-1.3181019271	0.6518442510
C	6.0	-4.1190454429	-1.8796670069	0.5535439134
C	6.0	-5.2486624715	-1.0127619664	0.4999467454
C	6.0	-5.0601984924	0.3931628293	0.4970853856
C	6.0	-3.7555825602	0.9316357981	0.4811479031
O	8.0	-1.7221258459	-2.2170984071	0.9309586569
N	7.0	1.6783024228	-2.1471741913	-0.0282870477
H	1.0	5.8522238043	1.3361036648	0.5219784496
H	1.0	6.1998491864	-1.1179420132	0.0794666368
H	1.0	4.2244334818	-2.6289331826	-0.1562124086
H	1.0	4.4452037023	3.2377877649	0.9111223839
H	1.0	2.1848314292	4.2981818355	1.1916117654
H	1.0	0.1358365882	2.9143075645	1.1002834235
H	1.0	-1.3783925994	1.8754772636	0.3458335678
H	1.0	-4.2669339541	-2.9807464458	0.5432204827
H	1.0	-6.2616757797	-1.4475853231	0.5037317554
H	1.0	-5.9339096751	1.0625125301	0.5308956501
H	1.0	-3.6202152772	2.0245410775	0.4482186425
H	1.0	-2.0482664467	-3.1541351616	1.0479696386

H 1.0 1.4269138216 -2.2404879076 -1.0445575230
H 1.0 2.1168222658 -3.0609289340 0.2384930316

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1	CO	0.0000000	5.4060242	5.2147127
2	C	5.4060242	0.0000000	1.3968903 *
3	C	5.2147127	1.3968903 *	0.0000000
4	C	4.0451468	2.4389793 *	1.4312689 *
5	C	2.8103359 *	2.8441198 *	2.4750410 *
6	C	3.1146978	2.5458530 *	2.9349665 *
7	C	4.5538879	1.4368336 *	2.4673494 *
8	C	5.4548469	2.4667279 *	3.7604531
9	C	5.3176864	3.7595694	4.9413565
10	C	4.1695933	4.2758340	5.1770462
11	C	2.8837426 *	3.8382345	4.3955236
12	N	1.9387580 *	5.0756556	5.3632527
13	C	2.8585458 *	6.2655314	6.6454576
14	C	3.2543012	7.5801374	7.8123354
15	C	3.0004920	8.0591773	8.0514346
16	C	4.2813087	9.4477564	9.3856016
17	C	5.4403707	10.3643000	10.4423262
18	C	5.5999222	10.0427581	10.3064900
19	C	4.6929786	8.7384394	9.0910548
20	O	1.9402021 *	7.3115434	7.1115125
21	N	1.9477703 *	4.3604451	3.8008338
22	H	6.4736151	1.1051394 *	2.1639163 *
23	H	6.1692726	2.1897454 *	1.1056582 *
24	H	4.3791506	3.4301439	2.1863212 *
25	H	6.5174883	2.6706897 *	4.0662569
26	H	6.2892332	4.6455908	5.9104559
27	H	4.5580291	5.3813234	6.2725289
28	H	3.8898150	6.4717688	7.0493477
29	H	4.6206855	9.9391793	9.7303114
30	H	6.4151498	11.4374242	11.4749259
31	H	6.6578971	10.9202461	11.2611615
32	H	5.2774429	8.7056493	9.2181612
33	H	2.6494727 *	8.0216210	7.6880375
34	H	2.5259752 *	4.8203865	4.2443499
35	H	2.5697554 *	4.7023524	3.8746744

C C C C

1 CO	2.8103359 *	3.1146978	4.5538879	5.4548469
2 C	2.8441198 *	2.5458530 *	1.4368336 *	2.4667279 *
3 C	2.4750410 *	2.9349665 *	2.4673494 *	3.7604531
4 C	1.4077986 *	2.5180925 *	2.8361910 *	4.2809660
5 C	0.0000000	1.4680054 *	2.4780288 *	3.8253283
6 C	1.4680054 *	0.0000000	1.4783866 *	2.5411388 *
7 C	2.4780288 *	1.4783866 *	0.0000000	1.4461197 *
8 C	3.8253283	2.5411388 *	1.4461197 *	0.0000000
9 C	4.3873841	2.9284078 *	2.4780493 *	1.3950343 *
10 C	3.9095763	2.5061296 *	2.8408038 *	2.4328832 *
11 C	2.6558929 *	1.4678894 *	2.4979633 *	2.8593877 *
12 N	3.1413407	2.5376963 *	3.8490078	4.3151738
13 C	4.4429750	3.7647084	4.9554709	5.1565654
14 C	5.4557248	5.0393140	6.3292740	6.6110909
15 C	5.5932652	5.5419387	6.9556001	7.4784037
16 C	6.9150321	6.9394063	8.3607002	8.8748440
17 C	7.9927355	7.8207559	9.1733214	9.5024158
18 C	7.9392244	7.5134840	8.7510004	8.8764320
19 C	6.7999151	6.2362153	7.4140957	7.4828481
20 O	4.6683640	4.9221266	6.3805519	7.1373187
21 N	1.5264220 *	2.6552722 *	3.9336907	5.1832428
22 H	3.9492128	3.5410753	2.2038042 *	2.6740303 *
23 H	3.4643866	4.0402288	3.4797396	4.6556187
24 H	2.1823806 *	3.5160626	3.9407164	5.3850544
25 H	4.6889300	3.5409734	2.2110413 *	1.1109636 *
26 H	5.4880562	4.0290259	3.4826590	2.1795489 *
27 H	4.8447871	3.5186540	3.9476678	3.4139622
28 H	5.0611513	4.1268697	5.0813089	4.9842030
29 H	7.2708779	7.4988587	8.9566031	9.6005493
30 H	9.0130581	8.8974897	10.2628253	10.6040100
31 H	8.9355073	8.4178181	9.5880533	9.5919621
32 H	7.0738114	6.3009294	7.3206699	7.1812665
33 H	5.2950803	5.7326692	7.1907806	8.0280300
34 H	2.1370017 *	3.1612849	4.4060814	5.6154970
35 H	2.0911461 *	3.4303835	4.5432632	5.8818043

C C C N

1 CO	5.3176864	4.1695933	2.8837426 *	1.9387580 *
2 C	3.7595694	4.2758340	3.8382345	5.0756556
3 C	4.9413565	5.1770462	4.3955236	5.3632527
4 C	5.1819785	5.0153390	3.9162715	4.5434997
5 C	4.3873841	3.9095763	2.6558929 *	3.1413407
6 C	2.9284078 *	2.5061296 *	1.4678894 *	2.5376963 *
7 C	2.4780493 *	2.8408038 *	2.4979633 *	3.8490078
8 C	1.3950343 *	2.4328832 *	2.8593877 *	4.3151738

9 C	0.0000000	1.4292368 *	2.4902783 *	3.8054314
10 C	1.4292368 *	0.0000000	1.4147991 *	2.4746218 *
11 C	2.4902783 *	1.4147991 *	0.0000000	1.4589831 *
12 N	3.8054314	2.4746218 *	1.4589831 *	0.0000000
13 C	4.3379854	2.9116930 *	2.4616543 *	1.3323552 *
14 C	5.7899607	4.3621788	3.8550017	2.5109715 *
15 C	6.8404691	5.4244943	4.6265482	3.1684787
16 C	8.1923331	6.7670792	6.0261138	4.5707015
17 C	8.6486883	7.2267970	6.7275892	5.3275590
18 C	7.8787575	6.4981922	6.2563242	4.9903133
19 C	6.4724195	5.0968844	4.9220221	3.7482561
20 O	6.7503043	5.4205734	4.3452990	2.9766944 *
21 N	5.4955843	4.6866443	3.2787413	3.0457687
22 H	4.0676934	4.8834829	4.7016429	6.0276193
23 H	5.9186743	6.2526493	5.5010970	6.4472870
24 H	6.2700286	6.0208888	4.8301166	5.2361180
25 H	2.1691545 *	3.4428012	3.9703188	5.4256011
26 H	1.1008617 *	2.1951934 *	3.4770438	4.6691513
27 H	2.1663395 *	1.1085872 *	2.2023331 *	2.7117719 *
28 H	3.9478430	2.6006377 *	2.6982497 *	2.1093012 *
29 H	9.0266722	7.6172940	6.7451908	5.2922116
30 H	9.7437622	8.3237179	7.8250986	6.4167988
31 H	8.5024305	7.1752490	7.0978563	5.9171209
32 H	6.0417837	4.7619838	4.8915018	3.9717375
33 H	7.7039432	6.3951327	5.2815065	3.9516170
34 H	5.8883899	5.0534554	3.6820830	3.3678712
35 H	6.3278697	5.6028588	4.2105018	3.9901965

C C C C

1 CO	2.8585458 *	3.2543012	3.0004920	4.2813087
2 C	6.2655314	7.5801374	8.0591773	9.4477564
3 C	6.6454576	7.8123354	8.0514346	9.3856016
4 C	5.8479665	6.8519745	6.9103237	8.1912829
5 C	4.4429750	5.4557248	5.5932652	6.9150321
6 C	3.7647084	5.0393140	5.5419387	6.9394063
7 C	4.9554709	6.3292740	6.9556001	8.3607002
8 C	5.1565654	6.6110909	7.4784037	8.8748440
9 C	4.3379854	5.7899607	6.8404691	8.1923331
10 C	2.9116930 *	4.3621788	5.4244943	6.7670792
11 C	2.4616543 *	3.8550017	4.6265482	6.0261138
12 N	1.3323552 *	2.5109715 *	3.1684787	4.5707015
13 C	0.0000000	1.4673556 *	2.6150368 *	3.8924264
14 C	1.4673556 *	0.0000000	1.4406297 *	2.5060872 *
15 C	2.6150368 *	1.4406297 *	0.0000000	1.4099239 *
16 C	3.8924264	2.5060872 *	1.4099239 *	0.0000000

17 C	4.3538086	2.8917835 *	2.4430594 *	1.4249322 *
18 C	3.7959933	2.4993696 *	2.8157217 *	2.4606325 *
19 C	2.4752092 *	1.4442123 *	2.4388610 *	2.8356251 *
20 O	3.0638529	2.4961933 *	1.4534197 *	2.4498011 *
21 N	4.2078163	4.8484596	4.6336198	5.8326092
22 H	7.1581592	8.5219177	9.0793395	10.4770410
23 H	7.7366515	8.8756037	9.0497099	10.3578261
24 H	6.5189664	7.3641987	7.2200790	8.4070681
25 H	6.2435908	7.7024407	8.5874915	9.9831142
26 H	4.9800462	6.3830222	7.5483605	8.8493961
27 H	2.6206243 *	3.9496694	5.1872678	6.4331281
28 H	1.1060324 *	2.1559107 *	3.5211321	4.6535395
29 H	4.8060750	3.5106081	2.2005307 *	1.1110146 *
30 H	5.4559719	3.9939115	3.4377861	2.1863304 *
31 H	4.6570481	3.4909331	3.9139709	3.4569735
32 H	2.6434616 *	2.1930464 *	3.4409184	3.9373552
33 H	4.0493785	3.3309302	2.0342801 *	2.4813004 *
34 H	4.3584502	4.9073201	4.6739525	5.7828872
35 H	5.1450585	5.6682751	5.2606692	6.3545797

C C C O

1 CO	5.4403707	5.5999222	4.6929786	1.9402021 *
2 C	10.3643000	10.0427581	8.7384394	7.3115434
3 C	10.4423262	10.3064900	9.0910548	7.1115125
4 C	9.3259700	9.3280204	8.2048408	5.8761871
5 C	7.9927355	7.9392244	6.7999151	4.6683640
6 C	7.8207559	7.5134840	6.2362153	4.9221266
7 C	9.1733214	8.7510004	7.4140957	6.3805519
8 C	9.5024158	8.8764320	7.4828481	7.1373187
9 C	8.6486883	7.8787575	6.4724195	6.7503043
10 C	7.2267970	6.4981922	5.0968844	5.4205734
11 C	6.7275892	6.2563242	4.9220221	4.3452990
12 N	5.3275590	4.9903133	3.7482561	2.9766944 *
13 C	4.3538086	3.7959933	2.4752092 *	3.0638529
14 C	2.8917835 *	2.4993696 *	1.4442123 *	2.4961933 *
15 C	2.4430594 *	2.8157217 *	2.4388610 *	1.4534197 *
16 C	1.4249322 *	2.4606325 *	2.8356251 *	2.4498011 *
17 C	0.0000000	1.4185032 *	2.4515962 *	3.7513542
18 C	1.4185032 *	0.0000000	1.4114637 *	4.2596289
19 C	2.4515962 *	1.4114637 *	0.0000000	3.7751560
20 O	3.7513542	4.2596289	3.7751560	0.0000000
21 N	7.0390883	7.2205764	6.2662350	3.5338300
22 H	11.3466881	10.9531145	9.6164029	8.3763526
23 H	11.4567136	11.3686638	10.1721550	8.0430636
24 H	9.6323466	9.7859212	8.7615373	6.0591350

25 H	10.5927938	9.9305583	8.5297192	8.2335977
26 H	9.1619515	8.2596609	6.8649042	7.6013901
27 H	6.6914206	5.8067891	4.4110610	5.4600387
28 H	4.8316318	3.9718796	2.5612846 *	4.1484575
29 H	2.1996878 *	3.4662171	3.9461460	2.6850601 *
30 H	1.1023981 *	2.1981687 *	3.4556774	4.6240877
31 H	2.1857003 *	1.1011555 *	2.1828222 *	5.3530385
32 H	3.4466978	2.1765419 *	1.1017489 *	4.6719682
33 H	3.8895171	4.6859931	4.4642737	0.9990481 *
34 H	6.9610433	7.1690589	6.2648555	3.7174806
35 H	7.6494256	7.9691434	7.1052511	3.9911253

N H H H

1 CO	1.9477703 *	6.4736151	6.1692726	4.3791506
2 C	4.3604451	1.1051394 *	2.1897454 *	3.4301439
3 C	3.8008338	2.1639163 *	1.1056582 *	2.1863212 *
4 C	2.4456496 *	3.4413970	2.1940505 *	1.1046668 *
5 C	1.5264220 *	3.9492128	3.4643866	2.1823806 *
6 C	2.6552722 *	3.5410753	4.0402288	3.5160626
7 C	3.9336907	2.2038042 *	3.4797396	3.9407164
8 C	5.1832428	2.6740303 *	4.6556187	5.3850544
9 C	5.4955843	4.0676934	5.9186743	6.2700286
10 C	4.6866443	4.8834829	6.2526493	6.0208888
11 C	3.2787413	4.7016429	5.5010970	4.8301166
12 N	3.0457687	6.0276193	6.4472870	5.2361180
13 C	4.2078163	7.1581592	7.7366515	6.5189664
14 C	4.8484596	8.5219177	8.8756037	7.3641987
15 C	4.6336198	9.0793395	9.0497099	7.2200790
16 C	5.8326092	10.4770410	10.3578261	8.4070681
17 C	7.0390883	11.3466881	11.4567136	9.6323466
18 C	7.2205764	10.9531145	11.3686638	9.7859212
19 C	6.2662350	9.6164029	10.1721550	8.7615373
20 O	3.5338300	8.3763526	8.0430636	6.0591350
21 N	0.0000000	5.4642142	4.6384604	2.5944633 *
22 H	5.4642142	0.0000000	2.5177371 *	4.3394886
23 H	4.6384604	2.5177371 *	0.0000000	2.4981806 *
24 H	2.5944633 *	4.3394886	2.4981806 *	0.0000000
25 H	6.1266670	2.3974030 *	4.7689426	5.9671063
26 H	6.5793114	4.7615210	6.8331275	7.3458511
27 H	5.4103114	5.9583762	7.3534585	7.0016373
28 H	5.0660710	7.2528453	8.1523775	7.2064848
29 H	6.0305306	11.0014999	10.6413654	8.5273853
30 H	7.9884744	12.4296348	12.4731019	10.5730599
31 H	8.2801297	11.7893119	12.3363801	10.8300889
32 H	6.7605145	9.4977097	10.3172111	9.1410434

33 H	4.0074449	9.1025632	8.5507597	6.4087952
34 H	1.0510515 *	5.9016447	5.0303530	2.9607707 *
35 H	1.0480549 *	5.7764595	4.5245548	2.1873358 *

	H	H	H	H
--	---	---	---	---

1 CO	6.5174883	6.2892332	4.5580291	3.8898150
2 C	2.6706897 *	4.6455908	5.3813234	6.4717688
3 C	4.0662569	5.9104559	6.2725289	7.0493477
4 C	4.8881813	6.2510522	6.0354167	6.4304139
5 C	4.6889300	5.4880562	4.8447871	5.0611513
6 C	3.5409734	4.0290259	3.5186540	4.1268697
7 C	2.2110413 *	3.4826590	3.9476678	5.0813089
8 C	1.1109636 *	2.1795489 *	3.4139622	4.9842030
9 C	2.1691545 *	1.1008617 *	2.1663395 *	3.9478430
10 C	3.4428012	2.1951934 *	1.1085872 *	2.6006377 *
11 C	3.9703188	3.4770438	2.2023331 *	2.6982497 *
12 N	5.4256011	4.6691513	2.7117719 *	2.1093012 *
13 C	6.2435908	4.9800462	2.6206243 *	1.1060324 *
14 C	7.7024407	6.3830222	3.9496694	2.1559107 *
15 C	8.5874915	7.5483605	5.1872678	3.5211321
16 C	9.9831142	8.8493961	6.4331281	4.6535395
17 C	10.5927938	9.1619515	6.6914206	4.8316318
18 C	9.9305583	8.2596609	5.8067891	3.9718796
19 C	8.5297192	6.8649042	4.4110610	2.5612846 *
20 O	8.2335977	7.6013901	5.4600387	4.1484575
21 N	6.1266670	6.5793114	5.4103114	5.0660710
22 H	2.3974030 *	4.7615210	5.9583762	7.2528453
23 H	4.7689426	6.8331275	7.3534585	8.1523775
24 H	5.9671063	7.3458511	7.0016373	7.2064848
25 H	0.0000000	2.5124475 *	4.3256290	6.0074716
26 H	2.5124475 *	0.0000000	2.4742330 *	4.3910595
27 H	4.3256290	2.4742330 *	0.0000000	1.9852589 *
28 H	6.0074716	4.3910595	1.9852589 *	0.0000000
29 H	10.7101289	9.7482555	7.3787783	5.6538077
30 H	11.6942702	10.2386768	7.7659609	5.9088181
31 H	10.6114273	8.7647053	6.3714337	4.6311873
32 H	8.1692858	6.2785861	3.9146901	2.2491046 *
33 H	9.1126594	8.5718597	6.4497318	5.1223752
34 H	6.5533398	6.9519130	5.7305444	5.1714699
35 H	6.7488979	7.4208875	6.3537735	6.0494756

	H	H	H	H
--	---	---	---	---

1 CO	4.6206855	6.4151498	6.6578971	5.2774429
2 C	9.9391793	11.4374242	10.9202461	8.7056493

3 C	9.7303114	11.4749259	11.2611615	9.2181612
4 C	8.4525353	10.3227204	10.3337943	8.4754971
5 C	7.2708779	9.0130581	8.9355073	7.0738114
6 C	7.4988587	8.8974897	8.4178181	6.3009294
7 C	8.9566031	10.2628253	9.5880533	7.3206699
8 C	9.6005493	10.6040100	9.5919621	7.1812665
9 C	9.0266722	9.7437622	8.5024305	6.0417837
10 C	7.6172940	8.3237179	7.1752490	4.7619838
11 C	6.7451908	7.8250986	7.0978563	4.8915018
12 N	5.2922116	6.4167988	5.9171209	3.9717375
13 C	4.8060750	5.4559719	4.6570481	2.6434616 *
14 C	3.5106081	3.9939115	3.4909331	2.1930464 *
15 C	2.2005307 *	3.4377861	3.9139709	3.4409184
16 C	1.1110146 *	2.1863304 *	3.4569735	3.9373552
17 C	2.1996878 *	1.1023981 *	2.1857003 *	3.4466978
18 C	3.4662171	2.1981687 *	1.1011555 *	2.1765419 *
19 C	3.9461460	3.4556774	2.1828222 *	1.1017489 *
20 O	2.6850601 *	4.6240877	5.3530385	4.6719682
21 N	6.0305306	7.9884744	8.2801297	6.7605145
22 H	11.0014999	12.4296348	11.7893119	9.4977097
23 H	10.6413654	12.4731019	12.3363801	10.3172111
24 H	8.5273853	10.5730599	10.8300889	9.1410434
25 H	10.7101289	11.6942702	10.6114273	8.1692858
26 H	9.7482555	10.2386768	8.7647053	6.2785861
27 H	7.3787783	7.7659609	6.3714337	3.9146901
28 H	5.6538077	5.9088181	4.6311873	2.2491046 *
29 H	0.0000000	2.5161751 *	4.3734315	5.0477890
30 H	2.5161751 *	0.0000000	2.5315528 *	4.3630330
31 H	4.3734315	2.5315528 *	0.0000000	2.5070932 *
32 H	5.0477890	4.3630330	2.5070932 *	0.0000000
33 H	2.2819555 *	4.5783540	5.7572308	5.4451274
34 H	5.9572581	7.8829122	8.2203155	6.7743904
35 H	6.3915281	8.5365367	9.0500030	7.6693931

H H H

1 CO	2.6494727 *	2.5259752 *	2.5697554 *
2 C	8.0216210	4.8203865	4.7023524
3 C	7.6880375	4.2443499	3.8746744
4 C	6.3822695	2.9246174 *	2.4560200 *
5 C	5.2950803	2.1370017 *	2.0911461 *
6 C	5.7326692	3.1612849	3.4303835
7 C	7.1907806	4.4060814	4.5432632
8 C	8.0280300	5.6154970	5.8818043
9 C	7.7039432	5.8883899	6.3278697
10 C	6.3951327	5.0534554	5.6028588

11	C	5.2815065	3.6820830	4.2105018
12	N	3.9516170	3.3678712	3.9901965
13	C	4.0493785	4.3584502	5.1450585
14	C	3.3309302	4.9073201	5.6682751
15	C	2.0342801 *	4.6739525	5.2606692
16	C	2.4813004 *	5.7828872	6.3545797
17	C	3.8895171	6.9610433	7.6494256
18	C	4.6859931	7.1690589	7.9691434
19	C	4.4642737	6.2648555	7.1052511
20	O	0.9990481 *	3.7174806	3.9911253
21	N	4.0074449	1.0510515 *	1.0480549 *
22	H	9.1025632	5.9016447	5.7764595
23	H	8.5507597	5.0303530	4.5245548
24	H	6.4087952	2.9607707 *	2.1873358 *
25	H	9.1126594	6.5533398	6.7488979
26	H	8.5718597	6.9519130	7.4208875
27	H	6.4497318	5.7305444	6.3537735
28	H	5.1223752	5.1714699	6.0494756
29	H	2.2819555 *	5.9572581	6.3915281
30	H	4.5783540	7.8829122	8.5365367
31	H	5.7572308	8.2203155	9.0500030
32	H	5.4451274	6.7743904	7.6693931
33	H	0.0000000	4.1581605	4.2440433
34	H	4.1581605	0.0000000	1.6719198 *
35	H	4.2440433	1.6719198 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.61 , TOTAL = 1723.6 SECONDS (28.7 MIN)
WALL CLOCK TIME: STEP = 0.61 , TOTAL = 1592.8 SECONDS (26.5 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.19 , TOTAL = 1724.8 SECONDS (28.7 MIN)
WALL CLOCK TIME: STEP = 1.19 , TOTAL = 1594.0 SECONDS (26.6 MIN)

CPU UTILIZATION: STEP = 99.88%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.626964015	-284.626964015	0.091980549	0.005139286	197274896
11430471						
2	1	-284.628388307	-0.001424292	0.131145663	0.001447689	174511127
13340403						
3	2	-284.628279164	0.000109142	0.042815980	0.001989418	168988100
13823455						
4	3	-284.628556044	-0.000276880	0.009262473	0.000376367	164771035
14147110						
5	4	-284.628541866	0.000014178	0.005751821	0.000721608	152093008
15216398						
6	5	-284.628563516	-0.000021649	0.003456179	0.000126609	147644328
15564863						
7	6	-284.628563233	0.000000282	0.000893800	0.000108536	139707662
16214316						
8	7	-284.628564755	-0.000001522	0.001043947	0.000107970	153656989
15099125						
9	8	-284.628565295	-0.000000540	0.001883767	0.000108358	171725535
13700665						

-----DISABLING FDIFF OPTION-----

10	9	-284.628566536	-0.000001241	0.003202055	0.000112377	197271000
11430223						
11	10	-284.628567833	-0.000001297	0.002864102	0.000112057	197271046
11430225						
12	11	-284.628568837	-0.000001004	0.000975396	0.000126722	197270173
11430231						
13	12	-284.628569438	-0.000000601	0.001521666	0.000087340	197269597
11430231						
14	13	-284.628570067	-0.000000630	0.001319595	0.000060587	197269291
11430247						
15	14	-284.628570247	-0.000000179	0.000594203	0.000038118	197269496
11430237						
16	15	-284.628570358	-0.000000111	0.000167484	0.000038796	197269325
11430231						
17	16	-284.628570399	-0.000000041	0.000330823	0.000034707	197269396
11430221						
18	17	-284.628570463	-0.000000064	0.000606570	0.000024991	197269277
11430225						
19	18	-284.628570524	-0.000000061	0.000253794	0.000023350	197268959
11430249						
20	19	-284.628570551	-0.000000027	0.000127435	0.000020259	197269109
11430236						
21	20	-284.628570570	-0.000000019	0.000190310	0.000013451	197269056
11430229						

22 21	-284.628570585	-0.000000016	0.000125944	0.000007629	197268975
11430240					
23 22	-284.628570590	-0.000000005	0.000066511	0.000005385	197269031
11430242					
24 23	-284.628570592	-0.000000002	0.000055862	0.000004510	197268998
11430244					
25 24	-284.628570594	-0.000000002	0.000037230	0.000003360	197269025
11430237					
26 25	-284.628570595	-0.000000001	0.000041242	0.000002141	197269078
11430239					
27 26	-284.628570595	0.000000000	0.000018720	0.000001141	197269060
11430242					
28 27	-284.628570595	0.000000000	0.000007003	0.000000426	197269066
11430241					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 96.3 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 30.2 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 3.2 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6285705954 AFTER 28 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6036523022
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000932377

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 100.75 , TOTAL = 1825.5 SECONDS (30.4 MIN)
WALL CLOCK TIME: STEP = 92.56 , TOTAL = 1686.6 SECONDS (28.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.91 , TOTAL = 1829.4 SECONDS (30.5 MIN)
WALL CLOCK TIME: STEP = 3.88 , TOTAL = 1690.5 SECONDS (28.2 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.87 , TOTAL = 1832.3 SECONDS (30.5 MIN)
WALL CLOCK TIME: STEP = 2.72 , TOTAL = 1693.2 SECONDS (28.2 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 13 ENERGY= -284.6285706

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0023194	-0.0033883	-0.0002405
2 C	6.0	-0.0046441	0.0026118	0.0007556
3 C	6.0	-0.0018326	0.0060172	0.0010590
4 C	6.0	-0.0020771	-0.0062796	-0.0011055
5 C	6.0	-0.0007605	0.0018543	-0.0008293
6 C	6.0	-0.0045846	0.0035750	0.0007174
7 C	6.0	0.0057656	-0.0037283	-0.0003078
8 C	6.0	-0.0069801	-0.0010189	0.0004055
9 C	6.0	0.0048693	0.0026087	0.0005515
10 C	6.0	0.0021271	-0.0035174	-0.0010148
11 C	6.0	0.0038092	-0.0017320	-0.0008350
12 N	7.0	-0.0011910	0.0034532	-0.0015119
13 C	6.0	0.0021569	0.0023093	-0.0001175
14 C	6.0	0.0022211	0.0035571	-0.0007351
15 C	6.0	0.0047504	-0.0046001	-0.0004212
16 C	6.0	-0.0023831	0.0032678	-0.0019077
17 C	6.0	-0.0015922	0.0023955	-0.0010818
18 C	6.0	0.0021290	-0.0020178	-0.0009937
19 C	6.0	-0.0032687	-0.0001618	-0.0011495
20 O	8.0	0.0032877	0.0111242	0.0016288
21 N	7.0	-0.0056944	0.0005319	0.0043418
22 H	1.0	0.0017949	-0.0018658	-0.0004088
23 H	1.0	0.0004164	-0.0014668	-0.0002725

24 H	1.0	0.0001751	0.0019395	0.0006902
25 H	1.0	0.0019874	0.0039740	0.0006975
26 H	1.0	0.0001720	-0.0020411	-0.0004738
27 H	1.0	-0.0025058	0.0031368	0.0004181
28 H	1.0	-0.0020932	-0.0004908	0.0007143
29 H	1.0	-0.0006816	-0.0023670	-0.0023250
30 H	1.0	0.0018168	0.0004380	0.0019807
31 H	1.0	0.0012363	-0.0020704	0.0026667
32 H	1.0	-0.0003221	-0.0029381	0.0013539
33 H	1.0	-0.0026278	-0.0057495	0.0002866
34 H	1.0	-0.0004438	-0.0027643	-0.0048871
35 H	1.0	0.0026479	-0.0045965	0.0023507

MAXIMUM GRADIENT = 0.0111242 RMS GRADIENT = 0.0028778
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0006614317
 PREDICTED ENERGY CHANGE WAS -0.0010937854 RATIO= 0.605
 GDIIS STEP HAS LENGTH = 0.084956
 RADIUS OF STEP TAKEN= 0.08496 CURRENT TRUST RADIUS= 0.17530

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 1832.3 SECONDS (30.5 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1693.2 SECONDS (28.2
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 14

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1215397930	-1.6487628716	1.0387273578
C	6.0	4.9839477330	0.6655855551	0.4296385028
C	6.0	5.1889323796	-0.6935196196	0.1822716466
C	6.0	4.0502255662	-1.5533917213	0.0531142981
C	6.0	2.7397458501	-1.0637402717	0.1693851048
C	6.0	2.4573481963	0.3424282722	0.4545820290
C	6.0	3.6504922904	1.2024084321	0.5688335732
C	6.0	3.5317403092	2.6172983752	0.8285662263
C	6.0	2.2757833880	3.2130085223	0.9849897273
C	6.0	1.1022358814	2.4040222272	0.9089044692
C	6.0	1.1621359763	1.0173339600	0.6468844427
N	7.0	-0.0755322660	0.2421542982	0.6623735012
C	6.0	-1.2896126170	0.7833206665	0.5286985143
C	6.0	-2.5862724839	0.0967590664	0.5646778394

C	6.0	-2.8359515734	-1.3143007671	0.6595666728
C	6.0	-4.1224053958	-1.8833890998	0.5604530240
C	6.0	-5.2496054015	-1.0175911891	0.5017583068
C	6.0	-5.0588097617	0.3932875965	0.4981459791
C	6.0	-3.7540634226	0.9336197333	0.4843415804
O	8.0	-1.7288174702	-2.2274331119	0.9295750531
N	7.0	1.6856100802	-2.1390723726	-0.0302779066
H	1.0	5.8528236506	1.3408707711	0.5233539209
H	1.0	6.2039033362	-1.1139472621	0.0813740781
H	1.0	4.2295225448	-2.6305461536	-0.1576420538
H	1.0	4.4493353767	3.2336092530	0.9103381053
H	1.0	2.1890528513	4.2929399028	1.1908123068
H	1.0	0.1400326782	2.9118598934	1.1015213467
H	1.0	-1.3744235832	1.8758332947	0.3399010253
H	1.0	-4.2724246791	-2.9794979648	0.5505866970
H	1.0	-6.2658121820	-1.4478229671	0.4958118536
H	1.0	-5.9377223671	1.0658266792	0.5243666542
H	1.0	-3.6243323287	2.0291291118	0.4407394438
H	1.0	-2.0482536289	-3.1505383453	1.0422373902
H	1.0	1.4257106333	-2.2256937079	-1.0407031526
H	1.0	2.1199176463	-3.0509431855	0.2349794425

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4194288	5.2272817	4.0515553
2 C	5.4194288	0.0000000	1.3965586 *	2.4366920 *
3 C	5.2272817	1.3965586 *	0.0000000	1.4327299 *
4 C	4.0515553	2.4366920 *	1.4327299 *	0.0000000
5 C	2.8201082 *	2.8451260 *	2.4770434 *	1.4037929 *
6 C	3.1244310	2.5473041 *	2.9340915 *	2.5084992 *
7 C	4.5610836	1.4441806 *	2.4719974 *	2.8319936 *
8 C	5.4656119	2.4652044 *	3.7583904	4.2737347
9 C	5.3179389	3.7592463	4.9388010	5.1706487
10 C	4.1717725	4.2801337	5.1791746	5.0084074
11 C	2.8886768 *	3.8441082	4.3997698	3.9118097
12 N	1.9380525 *	5.0824991	5.3684794	4.5406013
13 C	2.8577108 *	6.2754469	6.6537669	5.8481003
14 C	3.2563503	7.5927619	7.8246141	6.8576819
15 C	3.0003971	8.0699221	8.0629983	6.9169635
16 C	4.2772499	9.4572751	9.3946699	8.1950099
17 C	5.4346954	10.3713015	10.4484528	9.3260506
18 C	5.5944812	10.0466819	10.3100507	9.3253492
19 C	4.6900260	8.7422922	9.0948338	8.2023234

20	O	1.9418021 *	7.3267121	7.1250695	5.8838638
21	N	1.9569087 *	4.3539247	3.7957960	2.4374951 *
22	H	6.4846846	1.1044175 *	2.1669871 *	3.4419821
23	H	6.1804287	2.1854786 *	1.1032252 *	2.1982352 *
24	H	4.3898429	3.4319878	2.1881683 *	1.1121274 *
25	H	6.5256307	2.6667636 *	4.0619485	4.8794979
26	H	6.2929780	4.6420386	5.9060317	6.2400252
27	H	4.5610925	5.3815135	6.2717756	6.0272081
28	H	3.8921771	6.4731475	7.0501108	6.4240680
29	H	4.6169320	9.9489543	9.7405662	8.4585912
30	H	6.4135325	11.4467451	11.4838345	10.3260719
31	H	6.6594460	10.9294119	11.2700832	10.3364156
32	H	5.2835629	8.7156101	9.2278522	8.4784166
33	H	2.6388151 *	8.0243339	7.6911211	6.3812765
34	H	2.5214563 *	4.8148158	4.2432373	2.9217298 *
35	H	2.5701429 *	4.6960778	3.8702811	2.4498620 *

C C C C

1	CO	2.8201082 *	3.1244310	4.5610836	5.4656119
2	C	2.8451260 *	2.5473041 *	1.4441806 *	2.4652044 *
3	C	2.4770434 *	2.9340915 *	2.4719974 *	3.7583904
4	C	1.4037929 *	2.5084992 *	2.8319936 *	4.2737347
5	C	0.0000000	1.4623254 *	2.4747622 *	3.8225411
6	C	1.4623254 *	0.0000000	1.4751990 *	2.5434655 *
7	C	2.4747622 *	1.4751990 *	0.0000000	1.4434253 *
8	C	3.8225411	2.5434655 *	1.4434253 *	0.0000000
9	C	4.3784760	2.9248127 *	2.4709357 *	1.3988448 *
10	C	3.9055991	2.5085669 *	2.8378045 *	2.4401706 *
11	C	2.6547558 *	1.4731098 *	2.4964498 *	2.8649466 *
12	N	3.1423222	2.5433670 *	3.8489085	4.3221921
13	C	4.4470743	3.7735387	4.9580119	5.1670919
14	C	5.4652984	5.0508003	6.3340124	6.6221474
15	C	5.6028083	5.5502966	6.9581615	7.4855549
16	C	6.9219851	6.9468431	8.3630231	8.8833563
17	C	7.9963951	7.8261748	9.1730386	9.5095351
18	C	7.9403075	7.5164563	8.7470918	8.8799185
19	C	6.8013384	6.2395535	7.4099144	7.4857331
20	O	4.6797573	4.9349558	6.3899077	7.1522789
21	N	1.5190150 *	2.6435798 *	3.9223960	5.1738644
22	H	3.9495192	3.5398970	2.2071483 *	2.6664302 *
23	H	3.4656390	4.0369530	3.4818140	4.6498328
24	H	2.1866097 *	3.5148253	3.9439300	5.3851072
25	H	4.6839002	3.5404313	2.2091972 *	1.1083801 *
26	H	5.4809305	4.0274756	3.4747730	2.1775689 *
27	H	4.8407420	3.5200086	3.9407242	3.4153992

28 H	5.0593042	4.1287962	5.0750065	4.9858809
29 H	7.2791468	7.5056148	8.9588664	9.6076216
30 H	9.0196535	8.9050675	10.2646068	10.6126327
31 H	8.9420088	8.4264693	9.5892905	9.6005378
32 H	7.0810285	6.3112589	7.3227692	7.1906695
33 H	5.2954260	5.7311955	7.1866516	8.0280713
34 H	2.1309946 *	3.1456962	4.3922826	5.6021515
35 H	2.0826582 *	3.4171705	4.5326722	5.8715033

C C C N

1 CO	5.3179389	4.1717725	2.8886768 *	1.9380525 *
2 C	3.7592463	4.2801337	3.8441082	5.0824991
3 C	4.9388010	5.1791746	4.3997698	5.3684794
4 C	5.1706487	5.0084074	3.9118097	4.5406013
5 C	4.3784760	3.9055991	2.6547558 *	3.1423222
6 C	2.9248127 *	2.5085669 *	1.4731098 *	2.5433670 *
7 C	2.4709357 *	2.8378045 *	2.4964498 *	3.8489085
8 C	1.3988448 *	2.4401706 *	2.8649466 *	4.3221921
9 C	0.0000000	1.4273968 *	2.4850579 *	3.8024652
10 C	1.4273968 *	0.0000000	1.4124967 *	2.4741844 *
11 C	2.4850579 *	1.4124967 *	0.0000000	1.4604678 *
12 N	3.8024652	2.4741844 *	1.4604678 *	0.0000000
13 C	4.3386211	2.9141327 *	2.4657253 *	1.3359346 *
14 C	5.7902729	4.3642925	3.8606712	2.5168434 *
15 C	6.8361000	5.4219384	4.6283243	3.1689864
16 C	8.1908681	6.7675838	6.0289338	4.5722538
17 C	8.6465579	7.2262780	6.7284775	5.3276438
18 C	7.8729981	6.4938632	6.2539366	4.9882729
19 C	6.4657029	5.0917561	4.9195980	3.7471871
20 O	6.7556128	5.4282289	4.3550016	2.9838919 *
21 N	5.4794017	4.6756922	3.2703937	3.0416490
22 H	4.0636467	4.8833415	4.7034548	6.0309127
23 H	5.9134756	6.2520338	5.5028701	6.4504173
24 H	6.2665649	6.0219866	4.8335445	5.2400697
25 H	2.1749311 *	3.4483752	3.9732813	5.4299831
26 H	1.1027860 *	2.1974197 *	3.4756309	4.6708091
27 H	2.1600234 *	1.1049142 *	2.2001405 *	2.7141568 *
28 H	3.9405822	2.5954943 *	2.6954395 *	2.1118746 *
29 H	9.0230190	7.6156193	6.7467317	5.2920172
30 H	9.7427665	8.3243912	7.8277861	6.4189821
31 H	8.5020139	7.1763256	7.1010809	5.9213812
32 H	6.0422797	4.7644696	4.8965809	3.9794953
33 H	7.6938483	6.3872142	5.2757999	3.9428783
34 H	5.8656233	5.0338728	3.6653311	3.3532781
35 H	6.3106181	5.5898568	4.1997488	3.9808488

	C	C	C	C
1 CO	2.8577108 *	3.2563503	3.0003971	4.2772499
2 C	6.2754469	7.5927619	8.0699221	9.4572751
3 C	6.6537669	7.8246141	8.0629983	9.3946699
4 C	5.8481003	6.8576819	6.9169635	8.1950099
5 C	4.4470743	5.4652984	5.6028083	6.9219851
6 C	3.7735387	5.0508003	5.5502966	6.9468431
7 C	4.9580119	6.3340124	6.9581615	8.3630231
8 C	5.1670919	6.6221474	7.4855549	8.8833563
9 C	4.3386211	5.7902729	6.8361000	8.1908681
10 C	2.9141327 *	4.3642925	5.4219384	6.7675838
11 C	2.4657253 *	3.8606712	4.6283243	6.0289338
12 N	1.3359346 *	2.5168434 *	3.1689864	4.5722538
13 C	0.0000000	1.4676471 *	2.6092731 *	3.8906380
14 C	1.4676471 *	0.0000000	1.4361175 *	2.5061343 *
15 C	2.6092731 *	1.4361175 *	0.0000000	1.4101945 *
16 C	3.8906380	2.5061343 *	1.4101945 *	0.0000000
17 C	4.3503508	2.8877461 *	2.4369376 *	1.4225438 *
18 C	3.7894467	2.4911436 *	2.8076704 *	2.4625174 *
19 C	2.4694281 *	1.4389320 *	2.4344978 *	2.8420077 *
20 O	3.0689153	2.5040464 *	1.4602949 *	2.4461972 *
21 N	4.2077055	4.8581782	4.6476503	5.8435760
22 H	7.1641668	8.5304083	9.0864352	10.4834356
23 H	7.7429004	8.8863144	9.0605422	10.3660122
24 H	6.5258258	7.3766525	7.2333434	8.4159732
25 H	6.2518067	7.7109719	8.5919601	9.9890356
26 H	4.9856730	6.3877782	7.5481150	8.8531858
27 H	2.6272973 *	3.9554688	5.1877009	6.4385982
28 H	1.1119448 *	2.1643030 *	3.5235218	4.6617379
29 H	4.8017133	3.5080857	2.2018659 *	1.1063714 *
30 H	5.4535902	3.9911763	3.4363626	2.1881702 *
31 H	4.6566890	3.4889731	3.9120669	3.4633151
32 H	2.6477711 *	2.1970396 *	3.4420855	3.9459101
33 H	4.0391218	3.3260288	2.0343730 *	2.4778799 *
34 H	4.3462823	4.9058173	4.6779610	5.7846750
35 H	5.1393333	5.6714157	5.2684761	6.3589081

	C	C	C	O
1 CO	5.4346954	5.5944812	4.6900260	1.9418021 *
2 C	10.3713015	10.0466819	8.7422922	7.3267121
3 C	10.4484528	10.3100507	9.0948338	7.1250695
4 C	9.3260506	9.3253492	8.2023234	5.8838638
5 C	7.9963951	7.9403075	6.8013384	4.6797573

6 C	7.8261748	7.5164563	6.2395535	4.9349558
7 C	9.1730386	8.7470918	7.4099144	6.3899077
8 C	9.5095351	8.8799185	7.4857331	7.1522789
9 C	8.6465579	7.8729981	6.4657029	6.7556128
10 C	7.2262780	6.4938632	5.0917561	5.4282289
11 C	6.7284775	6.2539366	4.9195980	4.3550016
12 N	5.3276438	4.9882729	3.7471871	2.9838919 *
13 C	4.3503508	3.7894467	2.4694281 *	3.0689153
14 C	2.8877461 *	2.4911436 *	1.4389320 *	2.5040464 *
15 C	2.4369376 *	2.8076704 *	2.4344978 *	1.4602949 *
16 C	1.4225438 *	2.4625174 *	2.8420077 *	2.4461972 *
17 C	0.0000000	1.4237257 *	2.4584900 *	3.7473580
18 C	1.4237257 *	0.0000000	1.4122721 *	4.2594785
19 C	2.4584900 *	1.4122721 *	0.0000000	3.7804906
20 O	3.7473580	4.2594785	3.7804906	0.0000000
21 N	7.0454238	7.2235225	6.2686775	3.5478784
22 H	11.3501868	10.9527299	9.6155943	8.3892247
23 H	11.4616260	11.3707591	10.1742821	8.0552688
24 H	9.6379614	9.7901351	8.7665881	6.0701200
25 H	10.5975985	9.9318756	8.5303679	8.2457823
26 H	9.1657063	8.2594544	6.8632910	7.6113873
27 H	6.6969023	5.8082038	4.4111596	5.4712429
28 H	4.8389190	3.9746301	2.5634577 *	4.1605415
29 H	2.1923377 *	3.4636446	3.9478573	2.6793976 *
30 H	1.1035447 *	2.2014878 *	3.4612545	4.6238797
31 H	2.1942302 *	1.1070157 *	2.1880236 *	5.3595368
32 H	3.4536561	2.1764647 *	1.1040254 *	4.6851103
33 H	3.8846151	4.6816862	4.4610965	0.9832881 *
34 H	6.9569062	7.1607349	6.2559637	3.7192804
35 H	7.6495465	7.9665620	7.1022938	3.9966729

N H H H

1 CO	1.9569087 *	6.4846846	6.1804287	4.3898429
2 C	4.3539247	1.1044175 *	2.1854786 *	3.4319878
3 C	3.7957960	2.1669871 *	1.1032252 *	2.1881683 *
4 C	2.4374951 *	3.4419821	2.1982352 *	1.1121274 *
5 C	1.5190150 *	3.9495192	3.4656390	2.1866097 *
6 C	2.6435798 *	3.5398970	4.0369530	3.5148253
7 C	3.9223960	2.2071483 *	3.4818140	3.9439300
8 C	5.1738644	2.6664302 *	4.6498328	5.3851072
9 C	5.4794017	4.0636467	5.9134756	6.2665649
10 C	4.6756922	4.8833415	6.2520338	6.0219866
11 C	3.2703937	4.7034548	5.5028701	4.8335445
12 N	3.0416490	6.0309127	6.4504173	5.2400697
13 C	4.2077055	7.1641668	7.7429004	6.5258258

14 C	4.8581782	8.5304083	8.8863144	7.3766525
15 C	4.6476503	9.0864352	9.0605422	7.2333434
16 C	5.8435760	10.4834356	10.3660122	8.4159732
17 C	7.0454238	11.3501868	11.4616260	9.6379614
18 C	7.2235225	10.9527299	11.3707591	9.7901351
19 C	6.2686775	9.6155943	10.1742821	8.7665881
20 O	3.5478784	8.3892247	8.0552688	6.0701200
21 N	0.0000000	5.4573053	4.6344710	2.5940815 *
22 H	5.4573053	0.0000000	2.5188757 *	4.3440781
23 H	4.6344710	2.5188757 *	0.0000000	2.5010759 *
24 H	2.5940815 *	4.3440781	2.5010759 *	0.0000000
25 H	6.1146254	2.3878851 *	4.7609808	5.9646641
26 H	6.5662240	4.7522026	6.8252697	7.3427859
27 H	5.4020085	5.9530047	7.3497178	7.0019772
28 H	5.0616505	7.2493408	8.1508688	7.2082742
29 H	6.0449894	11.0084959	10.6514735	8.5385281
30 H	7.9987319	12.4353892	12.4810671	10.5819605
31 H	8.2881968	11.7937537	12.3436920	10.8397960
32 H	6.7669232	9.5024739	10.3248384	9.1517031
33 H	4.0143606	9.1032422	8.5538913	6.4125327
34 H	1.0469050 *	5.8962689	5.0325106	2.9673327 *
35 H	1.0442667 *	5.7711157	4.5226637	2.1866225 *

H H H H

1 CO	6.5256307	6.2929780	4.5610925	3.8921771
2 C	2.6667636 *	4.6420386	5.3815135	6.4731475
3 C	4.0619485	5.9060317	6.2717756	7.0501108
4 C	4.8794979	6.2400252	6.0272081	6.4240680
5 C	4.6839002	5.4809305	4.8407420	5.0593042
6 C	3.5404313	4.0274756	3.5200086	4.1287962
7 C	2.2091972 *	3.4747730	3.9407242	5.0750065
8 C	1.1083801 *	2.1775689 *	3.4153992	4.9858809
9 C	2.1749311 *	1.1027860 *	2.1600234 *	3.9405822
10 C	3.4483752	2.1974197 *	1.1049142 *	2.5954943 *
11 C	3.9732813	3.4756309	2.2001405 *	2.6954395 *
12 N	5.4299831	4.6708091	2.7141568 *	2.1118746 *
13 C	6.2518067	4.9856730	2.6272973 *	1.1119448 *
14 C	7.7109719	6.3877782	3.9554688	2.1643030 *
15 C	8.5919601	7.5481150	5.1877009	3.5235218
16 C	9.9890356	8.8531858	6.4385982	4.6617379
17 C	10.5975985	9.1657063	6.6969023	4.8389190
18 C	9.9318756	8.2594544	5.8082038	3.9746301
19 C	8.5303679	6.8632910	4.4111596	2.5634577 *
20 O	8.2457823	7.6113873	5.4712429	4.1605415
21 N	6.1146254	6.5662240	5.4020085	5.0616505

22 H	2.3878851 *	4.7522026	5.9530047	7.2493408
23 H	4.7609808	6.8252697	7.3497178	8.1508688
24 H	5.9646641	7.3427859	7.0019772	7.2082742
25 H	0.0000000	2.5119165 *	4.3255246	6.0070893
26 H	2.5119165 *	0.0000000	2.4726178 *	4.3891706
27 H	4.3255246	2.4726178 *	0.0000000	1.9867044 *
28 H	6.0070893	4.3891706	1.9867044 *	0.0000000
29 H	10.7145332	9.7493042	7.3811521	5.6583602
30 H	11.7005140	10.2432479	7.7722948	5.9157993
31 H	10.6178728	8.7694290	6.3780916	4.6383008
32 H	8.1765155	6.2835417	3.9225362	2.2573784 *
33 H	9.1100714	8.5663416	6.4455243	5.1197398
34 H	6.5385669	6.9321668	5.7128409	5.1545459
35 H	6.7363117	7.4061471	6.3423860	6.0410724

H H H H

1 CO	4.6169320	6.4135325	6.6594460	5.2835629
2 C	9.9489543	11.4467451	10.9294119	8.7156101
3 C	9.7405662	11.4838345	11.2700832	9.2278522
4 C	8.4585912	10.3260719	10.3364156	8.4784166
5 C	7.2791468	9.0196535	8.9420088	7.0810285
6 C	7.5056148	8.9050675	8.4264693	6.3112589
7 C	8.9588664	10.2646068	9.5892905	7.3227692
8 C	9.6076216	10.6126327	9.6005378	7.1906695
9 C	9.0230190	9.7427665	8.5020139	6.0422797
10 C	7.6156193	8.3243912	7.1763256	4.7644696
11 C	6.7467317	7.8277861	7.1010809	4.8965809
12 N	5.2920172	6.4189821	5.9213812	3.9794953
13 C	4.8017133	5.4535902	4.6566890	2.6477711 *
14 C	3.5080857	3.9911763	3.4889731	2.1970396 *
15 C	2.2018659 *	3.4363626	3.9120669	3.4420855
16 C	1.1063714 *	2.1881702 *	3.4633151	3.9459101
17 C	2.1923377 *	1.1035447 *	2.1942302 *	3.4536561
18 C	3.4636446	2.2014878 *	1.1070157 *	2.1764647 *
19 C	3.9478573	3.4612545	2.1880236 *	1.1040254 *
20 O	2.6793976 *	4.6238797	5.3595368	4.6851103
21 N	6.0449894	7.9987319	8.2881968	6.7669232
22 H	11.0084959	12.4353892	11.7937537	9.5024739
23 H	10.6514735	12.4810671	12.3436920	10.3248384
24 H	8.5385281	10.5819605	10.8397960	9.1517031
25 H	10.7145332	11.7005140	10.6178728	8.1765155
26 H	9.7493042	10.2432479	8.7694290	6.2835417
27 H	7.3811521	7.7722948	6.3780916	3.9225362
28 H	5.6583602	5.9157993	4.6383008	2.2573784 *
29 H	0.0000000	2.5144825 *	4.3747635	5.0515775

30 H	2.5144825 *	0.0000000	2.5351317 *	4.3668804
31 H	4.3747635	2.5351317 *	0.0000000	2.5073330 *
32 H	5.0515775	4.3668804	2.5073330 *	0.0000000
33 H	2.2842750 *	4.5810065	5.7596780	5.4474562
34 H	5.9639895	7.8819721	8.2160633	6.7676527
35 H	6.4005275	8.5415744	9.0530162	7.6711068

H H H

1 CO	2.6388151 *	2.5214563 *	2.5701429 *
2 C	8.0243339	4.8148158	4.6960778
3 C	7.6911211	4.2432373	3.8702811
4 C	6.3812765	2.9217298 *	2.4498620 *
5 C	5.2954260	2.1309946 *	2.0826582 *
6 C	5.7311955	3.1456962	3.4171705
7 C	7.1866516	4.3922826	4.5326722
8 C	8.0280713	5.6021515	5.8715033
9 C	7.6938483	5.8656233	6.3106181
10 C	6.3872142	5.0338728	5.5898568
11 C	5.2757999	3.6653311	4.1997488
12 N	3.9428783	3.3532781	3.9808488
13 C	4.0391218	4.3462823	5.1393333
14 C	3.3260288	4.9058173	5.6714157
15 C	2.0343730 *	4.6779610	5.2684761
16 C	2.4778799 *	5.7846750	6.3589081
17 C	3.8846151	6.9569062	7.6495465
18 C	4.6816862	7.1607349	7.9665620
19 C	4.4610965	6.2559637	7.1022938
20 O	0.9832881 *	3.7192804	3.9966729
21 N	4.0143606	1.0469050 *	1.0442667 *
22 H	9.1032422	5.8962689	5.7711157
23 H	8.5538913	5.0325106	4.5226637
24 H	6.4125327	2.9673327 *	2.1866225 *
25 H	9.1100714	6.5385669	6.7363117
26 H	8.5663416	6.9321668	7.4061471
27 H	6.4455243	5.7128409	6.3423860
28 H	5.1197398	5.1545459	6.0410724
29 H	2.2842750 *	5.9639895	6.4005275
30 H	4.5810065	7.8819721	8.5415744
31 H	5.7596780	8.2160633	9.0530162
32 H	5.4474562	6.7676527	7.6711068
33 H	0.0000000	4.1548052	4.2467913
34 H	4.1548052	0.0000000	1.6704269 *
35 H	4.2467913	1.6704269 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.79 , TOTAL = 1833.1 SECONDS (30.6 MIN)
WALL CLOCK TIME: STEP = 0.79 , TOTAL = 1694.0 SECONDS (28.2 MIN)
CPU UTILIZATION: STEP = 99.61% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.04 , TOTAL = 1834.2 SECONDS (30.6 MIN)
WALL CLOCK TIME: STEP = 1.03 , TOTAL = 1695.0 SECONDS (28.3 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

		NONZERO BLOCKS				
ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD	
-----START SECOND ORDER SCF-----						
1	0	-284.628604820	-284.628604820	0.189569036	0.005392804	197158121
11437390						
2	1	-284.629187337	-0.000582517	0.086590080	0.001185277	171137194
13615758						
3	2	-284.629154313	0.000033023	0.070614397	0.001419787	164613718
14162252						
4	3	-284.629271213	-0.000116899	0.010099253	0.000234434	162326017
14365445						
5	4	-284.629265222	0.000005991	0.003496279	0.000475700	149772879
15406162						
6	5	-284.629274913	-0.000009691	0.001801995	0.000119462	144750167
15806517						
7	6	-284.629274365	0.000000548	0.000623311	0.000198507	135601805
16535142						
8	7	-284.629275367	-0.000001002	0.000370969	0.000074609	151619381
15279845						
9	8	-284.629275442	-0.000000075	0.000486639	0.000060068	145958438
15744757						
10	9	-284.629275666	-0.000000223	0.001882722	0.000046948	162314744
14559223						
-----DISABLING FDIFF OPTION-----						
11	10	-284.629275993	-0.000000327	0.001041646	0.000043174	197146166
11438604						

12 11	-284.629276163	-0.000000170	0.000269631	0.000050002	197146197
11438605					
13 12	-284.629276291	-0.000000129	0.000523358	0.000041268	197146206
11438605					
14 13	-284.629276439	-0.000000148	0.000941318	0.000024231	197146117
11438611					
15 14	-284.629276578	-0.000000139	0.001558402	0.000034228	197146318
11438604					
16 15	-284.629276668	-0.000000090	0.000198215	0.000046004	197146266
11438605					
17 16	-284.629276712	-0.000000044	0.000236371	0.000036249	197146274
11438604					
18 17	-284.629276735	-0.000000023	0.000232228	0.000020048	197146080
11438613					
19 18	-284.629276756	-0.000000021	0.000226934	0.000007690	197146381
11438608					
20 19	-284.629276760	-0.000000004	0.000083602	0.000002629	197146257
11438612					
21 20	-284.629276762	-0.000000001	0.000042619	0.000001889	197146383
11438608					
22 21	-284.629276762	0.000000000	0.000016863	0.000001559	197146380
11438607					
23 22	-284.629276762	0.000000000	0.000012222	0.000001258	197146374
11438609					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 78.0 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 24.8 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 3.2 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6292767620 AFTER 23 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6077032658
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000963215

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 82.04 , TOTAL = 1916.2 SECONDS (31.9 MIN)
WALL CLOCK TIME: STEP = 75.19 , TOTAL = 1770.2 SECONDS (29.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.67 , TOTAL = 1919.9 SECONDS (32.0 MIN)
WALL CLOCK TIME: STEP = 3.64 , TOTAL = 1773.9 SECONDS (29.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.99 , TOTAL = 1922.9 SECONDS (32.0 MIN)
WALL CLOCK TIME: STEP = 2.82 , TOTAL = 1776.7 SECONDS (29.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 14 ENERGY= -284.6292768

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0008419	-0.0027680	0.0005131
2 C	6.0	0.0004696	0.0014748	0.0002973
3 C	6.0	0.0005679	0.0040621	0.0004687
4 C	6.0	-0.0078713	0.0002652	0.0000834
5 C	6.0	-0.0005553	0.0020050	0.0000511
6 C	6.0	0.0005472	-0.0015237	-0.0006517
7 C	6.0	-0.0023417	-0.0006438	0.0003357
8 C	6.0	0.0001619	-0.0007945	0.0002652
9 C	6.0	-0.0001196	-0.0005511	0.0001391
10 C	6.0	0.0000069	-0.0036414	-0.0009789
11 C	6.0	0.0023237	0.0022241	-0.0000875
12 N	7.0	0.0017775	0.0022888	-0.0011314
13 C	6.0	-0.0021641	-0.0011354	0.0002998

14 C	6.0	-0.0036617	0.0025891	-0.0006399
15 C	6.0	0.0039826	0.0031910	-0.0008064
16 C	6.0	-0.0026642	-0.0004054	-0.0018326
17 C	6.0	0.0001313	-0.0026997	-0.0009450
18 C	6.0	0.0057054	-0.0013565	-0.0008172
19 C	6.0	0.0021820	-0.0020688	-0.0005556
20 O	8.0	-0.0014046	-0.0054080	0.0032742
21 N	7.0	-0.0010922	-0.0006180	0.0006561
22 H	1.0	0.0011634	-0.0018229	-0.0002805
23 H	1.0	-0.0007461	-0.0001890	0.0000862
24 H	1.0	0.0014856	-0.0026129	-0.0002040
25 H	1.0	0.0010519	0.0028384	0.0005686
26 H	1.0	0.0009322	-0.0008460	-0.0002482
27 H	1.0	-0.0002125	0.0023362	0.0000965
28 H	1.0	-0.0015460	0.0033916	-0.0000520
29 H	1.0	-0.0009268	0.0005677	-0.0022438
30 H	1.0	0.0009878	0.0002860	0.0016610
31 H	1.0	-0.0018680	0.0004692	0.0026643
32 H	1.0	-0.0008730	-0.0011414	0.0008675
33 H	1.0	0.0025287	0.0065842	-0.0011225
34 H	1.0	-0.0003811	-0.0022026	-0.0019922
35 H	1.0	0.0015807	-0.0021445	0.0022617

MAXIMUM GRADIENT = 0.0078713 RMS GRADIENT = 0.0020474
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0007061666
 PREDICTED ENERGY CHANGE WAS -0.0007109643 RATIO= 0.993
 GDIIS STEP HAS LENGTH = 0.086177
 RADIUS OF STEP TAKEN= 0.08618 CURRENT TRUST RADIUS= 0.16991

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 1922.9 SECONDS (32.0 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1776.7 SECONDS (29.6
 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

INSERCH= 15

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1175533630	-1.6508864685	1.0419819347
C	6.0	4.9884458428	0.6645991804	0.4283271959
C	6.0	5.1945144082	-0.6972417775	0.1812774154
C	6.0	4.0617211203	-1.5517035469	0.0527904774

C	6.0	2.7443983980	-1.0653620719	0.1696061774
C	6.0	2.4601985231	0.3436394808	0.4544535092
C	6.0	3.6551746898	1.2050605207	0.5673044791
C	6.0	3.5354784727	2.6184215855	0.8275095392
C	6.0	2.2761552692	3.2109073275	0.9837184097
C	6.0	1.1037893998	2.4053351181	0.9094126659
C	6.0	1.1595201619	1.0139760647	0.6475802245
N	7.0	-0.0782637765	0.2368966856	0.6671166997
C	6.0	-1.2904369346	0.7802623879	0.5294181847
C	6.0	-2.5888950356	0.0935259099	0.5701824402
C	6.0	-2.8470963837	-1.3159509946	0.6677098135
C	6.0	-4.1244840994	-1.8855119427	0.5671571158
C	6.0	-5.2544134375	-1.0181921810	0.5032380132
C	6.0	-5.0676226685	0.3947844113	0.4993357871
C	6.0	-3.7582798909	0.9383557768	0.4862133188
O	8.0	-1.7340476030	-2.2268054815	0.9332614294
N	7.0	1.6931657173	-2.1333978104	-0.0324535121
H	1.0	5.8561010854	1.3463520778	0.5244545029
H	1.0	6.2110787109	-1.1122705401	0.0824587096
H	1.0	4.2341304430	-2.6295126077	-0.1585114813
H	1.0	4.4538261179	3.2301205505	0.9095818905
H	1.0	2.1919467426	4.2926630951	1.1908488800
H	1.0	0.1426973307	2.9081952731	1.1028209133
H	1.0	-1.3704734625	1.8712012720	0.3342887303
H	1.0	-4.2786177669	-2.9806875745	0.5581958821
H	1.0	-6.2732990661	-1.4484223783	0.4881166905
H	1.0	-5.9421197655	1.0677325967	0.5173356944
H	1.0	-3.6286279212	2.0334745838	0.4338741452
H	1.0	-2.0551015904	-3.1599501021	1.0350073379
H	1.0	1.4246242978	-2.2141010092	-1.0371877024
H	1.0	2.1232563081	-3.0444024116	0.2264614882

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4280420	5.2369632	4.0675295
2 C	5.4280420	0.0000000	1.3993244 *	2.4314285 *
3 C	5.2369632	1.3993244 *	0.0000000	1.4247226 *
4 C	4.0675295	2.4314285 *	1.4247226 *	0.0000000
5 C	2.8291683 *	2.8452507 *	2.4776435 *	1.4090824 *
6 C	3.1323010	2.5486726 *	2.9384592 *	2.5136692 *
7 C	4.5712708	1.4453460 *	2.4773651 *	2.8336818 *
8 C	5.4731345	2.4673635 *	3.7634611	4.2739987
9 C	5.3197740	3.7614711	4.9431125	5.1708157

10	C	4.1765021	4.2839422	5.1855757	5.0141117
11	C	2.8883801 *	3.8510788	4.4075938	3.9190888
12	N	1.9345784 *	5.0903336	5.3768805	4.5514791
13	C	2.8558086 *	6.2807616	6.6602413	5.8575451
14	C	3.2542944	7.6001541	7.8331362	6.8706018
15	C	3.0068937	8.0855182	8.0800323	6.9401343
16	C	4.2749725	9.4640284	9.4023732	8.2091386
17	C	5.4358600	10.3804414	10.4588126	9.3422642
18	C	5.6004718	10.0599382	10.3249765	9.3452200
19	C	4.6941599	8.7512002	9.1060799	8.2183129
20	O	1.9421455 *	7.3353321	7.1351256	5.9010107
21	N	1.9671764 *	4.3474104	3.7904706	2.4404281 *
22	H	6.4947828	1.1076340 *	2.1752571 *	3.4410744
23	H	6.1920791	2.1844272 *	1.1024595 *	2.1940191 *
24	H	4.3983065	3.4299481	2.1843682 *	1.1117760 *
25	H	6.5303155	2.6644557 *	4.0624157	4.8737747
26	H	6.2969080	4.6437802	5.9104820	6.2408216
27	H	4.5595570	5.3823734	6.2744940	6.0292627
28	H	3.8884644	6.4730662	7.0511969	6.4268388
29	H	4.6183049	9.9590888	9.7517396	8.4769501
30	H	6.4180023	11.4584176	11.4964851	10.3447000
31	H	6.6622655	10.9383593	11.2806334	10.3515255
32	H	5.2894410	8.7251253	9.2395053	8.4935384
33	H	2.6453263 *	8.0378354	7.7039418	6.4005255
34	H	2.5196411 *	4.8099348	4.2423567	2.9293519 *
35	H	2.5748407 *	4.6911356	3.8657252	2.4527449 *

C C C C

1	CO	2.8291683 *	3.1323010	4.5712708	5.4731345
2	C	2.8452507 *	2.5486726 *	1.4453460 *	2.4673635 *
3	C	2.4776435 *	2.9384592 *	2.4773651 *	3.7634611
4	C	1.4090824 *	2.5136692 *	2.8336818 *	4.2739987
5	C	0.0000000	1.4653303 *	2.4784060 *	3.8247754
6	C	1.4653303 *	0.0000000	1.4774131 *	2.5436256 *
7	C	2.4784060 *	1.4774131 *	0.0000000	1.4420899 *
8	C	3.8247754	2.5436256 *	1.4420899 *	0.0000000
9	C	4.3781857	2.9215096 *	2.4695175 *	1.4004769 *
10	C	3.9095589	2.5094666 *	2.8402929 *	2.4423812 *
11	C	2.6578084 *	1.4759449 *	2.5042462 *	2.8725943 *
12	N	3.1481449	2.5495903 *	3.8582206	4.3308798
13	C	4.4514818	3.7767083	4.9639665	5.1727311
14	C	5.4724310	5.0566091	6.3422334	6.6294243
15	C	5.6192273	5.5648089	6.9746046	7.4994723
16	C	6.9290865	6.9526875	8.3710650	8.8897822
17	C	8.0059057	7.8340413	9.1830125	9.5179993

18	C	7.9541450	7.5281287	8.7606142	8.8918845
19	C	6.8117509	6.2469328	7.4186937	7.4925306
20	O	4.6892002	4.9424837	6.3996364	7.1592817
21	N	1.5121569 *	2.6383956 *	3.9184809	5.1685046
22	H	3.9528441	3.5415374	2.2058732 *	2.6636990 *
23	H	3.4680928	4.0406876	3.4839265	4.6510215
24	H	2.1848409 *	3.5159912	3.9453707	5.3852730
25	H	4.6819737	3.5374377	2.2036030 *	1.1064691 *
26	H	5.4823875	4.0260433	3.4732022	2.1771949 *
27	H	4.8403405	3.5168364	3.9401704	3.4162449
28	H	5.0579339	4.1257645	5.0749561	4.9869800
29	H	7.2898717	7.5148891	8.9702638	9.6167902
30	H	9.0314479	8.9155257	10.2772483	10.6238658
31	H	8.9513466	8.4336954	9.5984070	9.6086270
32	H	7.0914096	6.3190010	7.3319748	7.1987174
33	H	5.3076754	5.7445729	7.2027300	8.0428366
34	H	2.1255014 *	3.1367888	4.3863898	5.5933957
35	H	2.0750062 *	3.4123801	4.5299981	5.8671293

C C C N

1	CO	5.3197740	4.1765021	2.8883801 *	1.9345784 *
2	C	3.7614711	4.2839422	3.8510788	5.0903336
3	C	4.9431125	5.1855757	4.4075938	5.3768805
4	C	5.1708157	5.0141117	3.9190888	4.5514791
5	C	4.3781857	3.9095589	2.6578084 *	3.1481449
6	C	2.9215096 *	2.5094666 *	1.4759449 *	2.5495903 *
7	C	2.4695175 *	2.8402929 *	2.5042462 *	3.8582206
8	C	1.4004769 *	2.4423812 *	2.8725943 *	4.3308798
9	C	0.0000000	1.4243980 *	2.4872414 *	3.8063454
10	C	1.4243980 *	0.0000000	1.4168776 *	2.4815484 *
11	C	2.4872414 *	1.4168776 *	0.0000000	1.4616235 *
12	N	3.8063454	2.4815484 *	1.4616235 *	0.0000000
13	C	4.3399313	2.9184888 *	2.4639144 *	1.3355040 *
14	C	5.7929089	4.3698349	3.8605486	2.5165891 *
15	C	6.8439766	5.4328528	4.6348615	3.1745504
16	C	8.1923865	6.7722486	6.0277856	4.5701761
17	C	8.6501797	7.2327215	6.7297167	5.3286611
18	C	7.8801173	6.5035993	6.2596072	4.9946753
19	C	6.4673340	5.0961597	4.9210278	3.7506385
20	O	6.7566999	5.4323673	4.3539652	2.9803157 *
21	N	5.4712046	4.6727479	3.2639218	3.0406672
22	H	4.0624502	4.8840664	4.7099370	6.0388683
23	H	5.9148760	6.2563413	5.5098576	6.4589400
24	H	6.2648911	6.0240509	4.8350824	5.2435396
25	H	2.1790171 *	3.4500749	3.9789940	5.4367285

26 H	1.1046219 *	2.1966565 *	3.4800624	4.6773275
27 H	2.1581156 *	1.1018045 *	2.1975530 *	2.7156027 *
28 H	3.9388415	2.5957741 *	2.6895826 *	2.1098654 *
29 H	9.0267362	7.6225259	6.7482347	5.2922288
30 H	9.7492638	8.3336889	7.8317071	6.4226788
31 H	8.5059247	7.1824606	7.1030376	5.9243168
32 H	6.0460848	4.7707642	4.9001438	3.9858725
33 H	7.7039108	6.4005286	5.2825706	3.9473788
34 H	5.8514854	5.0230845	3.6509183	3.3422621
35 H	6.3028340	5.5861771	4.1924413	3.9759013

C C C C

1 CO	2.8558086 *	3.2542944	3.0068937	4.2749725
2 C	6.2807616	7.6001541	8.0855182	9.4640284
3 C	6.6602413	7.8331362	8.0800323	9.4023732
4 C	5.8575451	6.8706018	6.9401343	8.2091386
5 C	4.4514818	5.4724310	5.6192273	6.9290865
6 C	3.7767083	5.0566091	5.5648089	6.9526875
7 C	4.9639665	6.3422334	6.9746046	8.3710650
8 C	5.1727311	6.6294243	7.4994723	8.8897822
9 C	4.3399313	5.7929089	6.8439766	8.1923865
10 C	2.9184888 *	4.3698349	5.4328528	6.7722486
11 C	2.4639144 *	3.8605486	4.6348615	6.0277856
12 N	1.3355040 *	2.5165891 *	3.1745504	4.5701761
13 C	0.0000000	1.4694428 *	2.6146556 *	3.8909639
14 C	1.4694428 *	0.0000000	1.4362467 *	2.5049219 *
15 C	2.6146556 *	1.4362467 *	0.0000000	1.4022232 *
16 C	3.8909639	2.5049219 *	1.4022232 *	0.0000000
17 C	4.3529569	2.8888384 *	2.4312315 *	1.4258575 *
18 C	3.7969238	2.4979725 *	2.8081493 *	2.4685748 *
19 C	2.4732790 *	1.4450776 *	2.4382566 *	2.8486640 *
20 O	3.0663230	2.4993056 *	1.4625495 *	2.4422736 *
21 N	4.2079687	4.8639905	4.6660934	5.8537193
22 H	7.1689252	8.5375420	9.1024187	10.4908936
23 H	7.7494639	8.8955808	9.0793469	10.3757744
24 H	6.5284499	7.3823851	7.2492661	8.4229786
25 H	6.2564277	7.7170810	8.6039955	9.9937159
26 H	4.9901348	6.3933112	7.5579218	8.8575469
27 H	2.6288330 *	3.9582400	5.1934189	6.4401399
28 H	1.1111386 *	2.1680237 *	3.5283884	4.6638714
29 H	4.8036234	3.5080044	2.1983163 *	1.1060050 *
30 H	5.4587230	3.9948933	3.4334629	2.1942426 *
31 H	4.6605727	3.4922754	3.9094411	3.4681313
32 H	2.6545822 *	2.2052268 *	3.4473355	3.9524794
33 H	4.0454427	3.3295801	2.0402196 *	2.4749587 *

34 H	4.3349768	4.9007263	4.6862508	5.7857149
35 H	5.1354791	5.6717818	5.2807812	6.3634394

	C	C	C	O
--	---	---	---	---

1 CO	5.4358600	5.6004718	4.6941599	1.9421455 *
2 C	10.3804414	10.0599382	8.7512002	7.3353321
3 C	10.4588126	10.3249765	9.1060799	7.1351256
4 C	9.3422642	9.3452200	8.2183129	5.9010107
5 C	8.0059057	7.9541450	6.8117509	4.6892002
6 C	7.8340413	7.5281287	6.2469328	4.9424837
7 C	9.1830125	8.7606142	7.4186937	6.3996364
8 C	9.5179993	8.8918845	7.4925306	7.1592817
9 C	8.6501797	7.8801173	6.4673340	6.7566999
10 C	7.2327215	6.5035993	5.0961597	5.4323673
11 C	6.7297167	6.2596072	4.9210278	4.3539652
12 N	5.3286611	4.9946753	3.7506385	2.9803157 *
13 C	4.3529569	3.7969238	2.4732790 *	3.0663230
14 C	2.8888384 *	2.4979725 *	1.4450776 *	2.4993056 *
15 C	2.4312315 *	2.8081493 *	2.4382566 *	1.4625495 *
16 C	1.4258575 *	2.4685748 *	2.8486640 *	2.4422736 *
17 C	0.0000000	1.4252750 *	2.4630845 *	3.7468176
18 C	1.4252750 *	0.0000000	1.4177519 *	4.2630679
19 C	2.4630845 *	1.4177519 *	0.0000000	3.7835980
20 O	3.7468176	4.2630679	3.7835980	0.0000000
21 N	7.0568764	7.2375939	6.2787694	3.5618986
22 H	11.3593597	10.9651198	9.6231099	8.3991032
23 H	11.4735965	11.3865757	10.1860786	8.0679047
24 H	9.6471100	9.8031498	8.7763305	6.0805666
25 H	10.6048664	9.9431092	8.5363992	8.2503566
26 H	9.1720375	8.2687966	6.8668105	7.6146736
27 H	6.7011061	5.8162585	4.4133996	5.4698405
28 H	4.8437721	3.9844648	2.5680540 *	4.1574769
29 H	2.1923927 *	3.4669590	3.9540908	2.6802705 *
30 H	1.1060988 *	2.2025423 *	3.4672806	4.6269685
31 H	2.1964109 *	1.1035979 *	2.1878902 *	5.3604894
32 H	3.4584187	2.1818104 *	1.1040083 *	4.6892226
33 H	3.8865797	4.6902414	4.4719238	0.9920619 *
34 H	6.9579203	7.1635507	6.2546967	3.7229074
35 H	7.6558568	7.9756634	7.1079042	4.0058488

	N	H	H	H
--	---	---	---	---

1 CO	1.9671764 *	6.4947828	6.1920791	4.3983065
2 C	4.3474104	1.1076340 *	2.1844272 *	3.4299481
3 C	3.7904706	2.1752571 *	1.1024595 *	2.1843682 *

4 C	2.4404281 *	3.4410744	2.1940191 *	1.1117760 *
5 C	1.5121569 *	3.9528441	3.4680928	2.1848409 *
6 C	2.6383956 *	3.5415374	4.0406876	3.5159912
7 C	3.9184809	2.2058732 *	3.4839265	3.9453707
8 C	5.1685046	2.6636990 *	4.6510215	5.3852730
9 C	5.4712046	4.0624502	5.9148760	6.2648911
10 C	4.6727479	4.8840664	6.2563413	6.0240509
11 C	3.2639218	4.7099370	5.5098576	4.8350824
12 N	3.0406672	6.0388683	6.4589400	5.2435396
13 C	4.2079687	7.1689252	7.7494639	6.5284499
14 C	4.8639905	8.5375420	8.8955808	7.3823851
15 C	4.6660934	9.1024187	9.0793469	7.2492661
16 C	5.8537193	10.4908936	10.3757744	8.4229786
17 C	7.0568764	11.3593597	11.4735965	9.6471100
18 C	7.2375939	10.9651198	11.3865757	9.8031498
19 C	6.2787694	9.6231099	10.1860786	8.7763305
20 O	3.5618986	8.3991032	8.0679047	6.0805666
21 N	0.0000000	5.4542494	4.6332973	2.5920112 *
22 H	5.4542494	0.0000000	2.5231319 *	4.3479571
23 H	4.6332973	2.5231319 *	0.0000000	2.5036802 *
24 H	2.5920112 *	4.3479571	2.5036802 *	0.0000000
25 H	6.1054079	2.3797651 *	4.7569349	5.9602341
26 H	6.5604504	4.7487743	6.8260719	7.3421934
27 H	5.3954111	5.9512053	7.3505467	6.9997852
28 H	5.0554128	7.2481038	8.1513469	7.2049193
29 H	6.0604426	11.0198429	10.6654133	8.5500804
30 H	8.0127864	12.4472661	12.4954890	10.5933553
31 H	8.2974146	11.8015124	12.3548276	10.8481547
32 H	6.7750848	9.5100172	10.3362968	9.1606408
33 H	4.0302345	9.1189117	8.5691352	6.4234174
34 H	1.0431291 *	5.8952132	5.0376368	2.9728713 *
35 H	1.0401655 *	5.7707586	4.5237332	2.1854353 *

H H H H

1 CO	6.5303155	6.2969080	4.5595570	3.8884644
2 C	2.6644557 *	4.6437802	5.3823734	6.4730662
3 C	4.0624157	5.9104820	6.2744940	7.0511969
4 C	4.8737747	6.2408216	6.0292627	6.4268388
5 C	4.6819737	5.4823875	4.8403405	5.0579339
6 C	3.5374377	4.0260433	3.5168364	4.1257645
7 C	2.2036030 *	3.4732022	3.9401704	5.0749561
8 C	1.1064691 *	2.1771949 *	3.4162449	4.9869800
9 C	2.1790171 *	1.1046219 *	2.1581156 *	3.9388415
10 C	3.4500749	2.1966565 *	1.1018045 *	2.5957741 *
11 C	3.9789940	3.4800624	2.1975530 *	2.6895826 *

12 N	5.4367285	4.6773275	2.7156027 *	2.1098654 *
13 C	6.2564277	4.9901348	2.6288330 *	1.1111386 *
14 C	7.7170810	6.3933112	3.9582400	2.1680237 *
15 C	8.6039955	7.5579218	5.1934189	3.5283884
16 C	9.9937159	8.8575469	6.4401399	4.6638714
17 C	10.6048664	9.1720375	6.7011061	4.8437721
18 C	9.9431092	8.2687966	5.8162585	3.9844648
19 C	8.5363992	6.8668105	4.4133996	2.5680540 *
20 O	8.2503566	7.6146736	5.4698405	4.1574769
21 N	6.1054079	6.5604504	5.3954111	5.0554128
22 H	2.3797651 *	4.7487743	5.9512053	7.2481038
23 H	4.7569349	6.8260719	7.3505467	8.1513469
24 H	5.9602341	7.3421934	6.9997852	7.2049193
25 H	0.0000000	2.5147974 *	4.3274483	6.0083350
26 H	2.5147974 *	0.0000000	2.4746562 *	4.3918117
27 H	4.3274483	2.4746562 *	0.0000000	1.9888902 *
28 H	6.0083350	4.3918117	1.9888902 *	0.0000000
29 H	10.7216224	9.7555156	7.3840087	5.6611185
30 H	11.7105769	10.2525256	7.7796522	5.9229438
31 H	10.6256985	8.7759236	6.3839717	4.6453222
32 H	8.1843951	6.2893587	3.9288065	2.2661667 *
33 H	9.1222187	8.5792278	6.4542472	5.1256420
34 H	6.5272907	6.9203258	5.6974462	5.1364593
35 H	6.7281385	7.4004927	6.3343539	6.0316610

H H H H

1 CO	4.6183049	6.4180023	6.6622655	5.2894410
2 C	9.9590888	11.4584176	10.9383593	8.7251253
3 C	9.7517396	11.4964851	11.2806334	9.2395053
4 C	8.4769501	10.3447000	10.3515255	8.4935384
5 C	7.2898717	9.0314479	8.9513466	7.0914096
6 C	7.5148891	8.9155257	8.4336954	6.3190010
7 C	8.9702638	10.2772483	9.5984070	7.3319748
8 C	9.6167902	10.6238658	9.6086270	7.1987174
9 C	9.0267362	9.7492638	8.5059247	6.0460848
10 C	7.6225259	8.3336889	7.1824606	4.7707642
11 C	6.7482347	7.8317071	7.1030376	4.9001438
12 N	5.2922288	6.4226788	5.9243168	3.9858725
13 C	4.8036234	5.4587230	4.6605727	2.6545822 *
14 C	3.5080044	3.9948933	3.4922754	2.2052268 *
15 C	2.1983163 *	3.4334629	3.9094411	3.4473355
16 C	1.1060050 *	2.1942426 *	3.4681313	3.9524794
17 C	2.1923927 *	1.1060988 *	2.1964109 *	3.4584187
18 C	3.4669590	2.2025423 *	1.1035979 *	2.1818104 *
19 C	3.9540908	3.4672806	2.1878902 *	1.1040083 *

20 O	2.6802705 *	4.6269685	5.3604894	4.6892226
21 N	6.0604426	8.0127864	8.2974146	6.7750848
22 H	11.0198429	12.4472661	11.8015124	9.5100172
23 H	10.6654133	12.4954890	12.3548276	10.3362968
24 H	8.5500804	10.5933553	10.8481547	9.1606408
25 H	10.7216224	11.7105769	10.6256985	8.1843951
26 H	9.7555156	10.2525256	8.7759236	6.2893587
27 H	7.3840087	7.7796522	6.3839717	3.9288065
28 H	5.6611185	5.9229438	4.6453222	2.2661667 *
29 H	0.0000000	2.5162474 *	4.3770554	5.0576442
30 H	2.5162474 *	0.0000000	2.5380247 *	4.3727376
31 H	4.3770554	2.5380247 *	0.0000000	2.5083596 *
32 H	5.0576442	4.3727376	2.5083596 *	0.0000000
33 H	2.2811200 *	4.5849325	5.7662982	5.4597625
34 H	5.9715889	7.8848488	8.2131537	6.7632300
35 H	6.4107799	8.5508922	9.0578449	7.6754171

H H H

1 CO	2.6453263 *	2.5196411 *	2.5748407 *
2 C	8.0378354	4.8099348	4.6911356
3 C	7.7039418	4.2423567	3.8657252
4 C	6.4005255	2.9293519 *	2.4527449 *
5 C	5.3076754	2.1255014 *	2.0750062 *
6 C	5.7445729	3.1367888	3.4123801
7 C	7.2027300	4.3863898	4.5299981
8 C	8.0428366	5.5933957	5.8671293
9 C	7.7039108	5.8514854	6.3028340
10 C	6.4005286	5.0230845	5.5861771
11 C	5.2825706	3.6509183	4.1924413
12 N	3.9473788	3.3422621	3.9759013
13 C	4.0454427	4.3349768	5.1354791
14 C	3.3295801	4.9007263	5.6717818
15 C	2.0402196 *	4.6862508	5.2807812
16 C	2.4749587 *	5.7857149	6.3634394
17 C	3.8865797	6.9579203	7.6558568
18 C	4.6902414	7.1635507	7.9756634
19 C	4.4719238	6.2546967	7.1079042
20 O	0.9920619 *	3.7229074	4.0058488
21 N	4.0302345	1.0431291 *	1.0401655 *
22 H	9.1189117	5.8952132	5.7707586
23 H	8.5691352	5.0376368	4.5237332
24 H	6.4234174	2.9728713 *	2.1854353 *
25 H	9.1222187	6.5272907	6.7281385
26 H	8.5792278	6.9203258	7.4004927
27 H	6.4542472	5.6974462	6.3343539

28 H	5.1256420	5.1364593	6.0316610
29 H	2.2811200 *	5.9715889	6.4107799
30 H	4.5849325	7.8848488	8.5508922
31 H	5.7662982	8.2131537	9.0578449
32 H	5.4597625	6.7632300	7.6754171
33 H	0.0000000	4.1589800	4.2574373
34 H	4.1589800	0.0000000	1.6656219 *
35 H	4.2574373	1.6656219 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 1923.7 SECONDS (32.1 MIN)
WALL CLOCK TIME: STEP = 0.79 , TOTAL = 1777.5 SECONDS (29.6 MIN)
CPU UTILIZATION: STEP = 99.30% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.26 , TOTAL = 1924.9 SECONDS (32.1 MIN)
WALL CLOCK TIME: STEP = 1.26 , TOTAL = 1778.7 SECONDS (29.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.629287336	-284.629287336	0.130225200	0.003337707	196779191
11462131					
2 1	-284.629696540	-0.000409205	0.015729813	0.000965562	168343382
13837361					
3 2	-284.629685149	0.000011391	0.042014756	0.000973715	160215923
14505951					
4 3	-284.629762947	-0.000077797	0.002426758	0.000297442	159399734
14571316					
5 4	-284.629757733	0.000005214	0.004635848	0.000594154	144504973
15824407					
6 5	-284.629765435	-0.000007702	0.000732516	0.000087691	142172030
16014252					
7 6	-284.629765011	0.000000424	0.000505551	0.000123237	133789386
16626394					

8 7	-284.629765789	-0.000000778	0.000325975	0.000047742	150569570
15326077					
9 8	-284.629765852	-0.000000064	0.000426825	0.000045514	143803598
15905661					
10 9	-284.629766031	-0.000000179	0.002920902	0.000045680	160825118
14696462					
-----DISABLING FDIFF OPTION-----					
11 10	-284.629766476	-0.000000445	0.000957582	0.000051397	196733514
11466849					
12 11	-284.629766663	-0.000000187	0.000407696	0.000051621	196733460
11466836					
13 12	-284.629766779	-0.000000116	0.000439308	0.000039044	196733388
11466835					
14 13	-284.629766889	-0.000000110	0.000772573	0.000025355	196733524
11466841					
15 14	-284.629766954	-0.000000065	0.000393584	0.000017075	196733804
11466828					
16 15	-284.629766977	-0.000000023	0.000076388	0.000016362	196733603
11466841					
17 16	-284.629766984	-0.000000007	0.000097049	0.000013441	196733588
11466839					
18 17	-284.629766991	-0.000000007	0.000156458	0.000009878	196733581
11466841					
19 18	-284.629766997	-0.000000006	0.000114998	0.000003947	196733566
11466846					
20 19	-284.629767000	-0.000000003	0.000053190	0.000003416	196733590
11466845					
21 20	-284.629767001	-0.000000001	0.000036352	0.000002865	196733527
11466848					
22 21	-284.629767002	-0.000000001	0.000035373	0.000002792	196733539
11466847					
23 22	-284.629767002	-0.000000001	0.000051688	0.000002814	196733537
11466846					
24 23	-284.629767003	-0.000000001	0.000037045	0.000001892	196733612
11466845					
25 24	-284.629767003	0.000000000	0.000017379	0.000001190	196733557
11466848					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 84.1 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 26.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.3
TIME TO SOLVE SCF EQUATIONS= 3.2 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6297670033 AFTER 25 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5995318337
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000924898

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 88.51 , TOTAL = 2013.4 SECONDS (33.6 MIN)
WALL CLOCK TIME: STEP = 81.42 , TOTAL = 1860.2 SECONDS (31.0
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.78 , TOTAL = 2017.2 SECONDS (33.6 MIN)
WALL CLOCK TIME: STEP = 3.79 , TOTAL = 1863.9 SECONDS (31.1
MIN)
CPU UTILIZATION: STEP = 99.85% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.74 , TOTAL = 2020.0 SECONDS (33.7 MIN)
WALL CLOCK TIME: STEP = 2.69 , TOTAL = 1866.6 SECONDS (31.1
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 15 ENERGY= -284.6297670

GRADIENT (HARTREE/BOHR)

ATOM ZNUC DE/DX DE/DY DE/DZ

1	CO	27.0	-0.0010093	-0.0016169	0.0012117
2	C	6.0	-0.0002555	0.0002803	0.0000505
3	C	6.0	-0.0029266	-0.0021425	-0.0006131
4	C	6.0	0.0010795	0.0032493	0.0003591
5	C	6.0	-0.0047624	-0.0018946	-0.0002206
6	C	6.0	0.0010556	0.0006561	-0.0003857
7	C	6.0	-0.0015644	0.0019427	0.0005367
8	C	6.0	0.0021017	0.0000454	0.0004010
9	C	6.0	-0.0030774	-0.0033699	-0.0003065
10	C	6.0	0.0007098	0.0023146	0.0000554
11	C	6.0	-0.0004869	-0.0001226	-0.0004843
12	N	7.0	-0.0002345	0.0004799	-0.0007303
13	C	6.0	-0.0004506	0.0006560	-0.0000623
14	C	6.0	0.0003780	-0.0025824	-0.0000455
15	C	6.0	-0.0041636	0.0013628	-0.0010847
16	C	6.0	0.0051019	-0.0005537	-0.0013570
17	C	6.0	0.0008775	-0.0030169	-0.0008326
18	C	6.0	-0.0007196	-0.0000735	-0.0003237
19	C	6.0	0.0024689	0.0032752	-0.0006094
20	O	8.0	0.0016818	0.0023833	0.0025049
21	N	7.0	0.0025735	-0.0018655	-0.0021896
22	H	1.0	0.0023290	0.0000843	0.0000962
23	H	1.0	-0.0010861	0.0002785	0.0002074
24	H	1.0	0.0009004	-0.0023296	-0.0001680
25	H	1.0	0.0005005	0.0014668	0.0003961
26	H	1.0	0.0011371	0.0003169	-0.0000055
27	H	1.0	0.0014368	0.0008346	-0.0003447
28	H	1.0	-0.0010418	0.0029983	-0.0000065
29	H	1.0	-0.0011767	0.0007614	-0.0022135
30	H	1.0	-0.0007097	-0.0000982	0.0013186
31	H	1.0	0.0002577	-0.0005150	0.0024183
32	H	1.0	-0.0010879	-0.0011038	0.0005527
33	H	1.0	-0.0002084	-0.0007028	-0.0004646
34	H	1.0	-0.0000477	-0.0020154	0.0008187
35	H	1.0	0.0004194	0.0006168	0.0015209

MAXIMUM GRADIENT = 0.0051019 RMS GRADIENT = 0.0015981
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0004902413
 PREDICTED ENERGY CHANGE WAS -0.0004074662 RATIO= 1.203
 GDIIS STEP HAS LENGTH = 0.099027
 RADIUS OF STEP TAKEN= 0.09903 CURRENT TRUST RADIUS= 0.12187

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 0.02 , TOTAL = 2020.0 SECONDS (33.7 MIN)

WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1866.7 SECONDS (31.1 MIN)

CPU UTILIZATION: STEP = 86.57%, TOTAL = 100.00%

INSERCH= 16

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1124572768	-1.6514901434	1.0403932714
C	6.0	4.9919108881	0.6647698677	0.4269496625
C	6.0	5.2024052216	-0.6974162905	0.1810756365
C	6.0	4.0697809279	-1.5540088218	0.0522785911
C	6.0	2.7545894895	-1.0624387799	0.1714216848
C	6.0	2.4606205097	0.3431772885	0.4551650275
C	6.0	3.6583477871	1.2035154388	0.5646997508
C	6.0	3.5361898079	2.6174982510	0.8253173938
C	6.0	2.2791754916	3.2104242333	0.9821993609
C	6.0	1.1031996899	2.4009897123	0.9092021745
C	6.0	1.1566554236	1.0092622968	0.6490059109
N	7.0	-0.0815536607	0.2306234684	0.6728141455
C	6.0	-1.2905535821	0.7766055526	0.5308889442
C	6.0	-2.5911700915	0.0950665698	0.5771416351
C	6.0	-2.8503550245	-1.3192610919	0.6772794584
C	6.0	-4.1321103784	-1.8866964421	0.5770990824
C	6.0	-5.2580399995	-1.0145100331	0.5070958732
C	6.0	-5.0718578303	0.3967374180	0.5018186135
C	6.0	-3.7641657238	0.9382325232	0.4904586764
O	8.0	-1.7412150467	-2.2338879787	0.9252228129
N	7.0	1.6950555301	-2.1226841215	-0.0302916968
H	1.0	5.8526433918	1.3524632328	0.5258449610
H	1.0	6.2186206376	-1.1100057394	0.0835121945
H	1.0	4.2357931645	-2.6255818231	-0.1595549337
H	1.0	4.4563456272	3.2213798125	0.9077033014
H	1.0	2.1933140379	4.2877560764	1.1902822857
H	1.0	0.1436508926	2.9026087572	1.1045275047
H	1.0	-1.3636982716	1.8624613013	0.3292036169
H	1.0	-4.2810631750	-2.9832318490	0.5704848147
H	1.0	-6.2769641274	-1.4489282227	0.4772747025
H	1.0	-5.9433894563	1.0705447776	0.5049812229
H	1.0	-3.6295626913	2.0404708544	0.4254389885
H	1.0	-2.0574043439	-3.1626506077	1.0315103049
H	1.0	1.4238675373	-2.1956049526	-1.0344467537
H	1.0	2.1244770702	-3.0350855351	0.2188887804

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4360317	5.2494051	4.0799857
2 C	5.4360317	0.0000000	1.4001118 *	2.4318061 *
3 C	5.2494051	1.4001118 *	0.0000000	1.4258952 *
4 C	4.0799857	2.4318061 *	1.4258952 *	0.0000000
5 C	2.8430539 *	2.8379837 *	2.4749013 *	1.4091007 *
6 C	3.1360901	2.5517933 *	2.9453936 *	2.5201250 *
7 C	4.5771914	1.4448572 *	2.4788752 *	2.8347474 *
8 C	5.4765376	2.4679888 *	3.7656314	4.2759537
9 C	5.3231819	3.7613284	4.9455322	5.1740548
10 C	4.1738920	4.2859190	5.1897759	5.0176624
11 C	2.8849848 *	3.8570933	4.4158580	3.9259066
12 N	1.9274611 *	5.0979383	5.3873264	4.5610915
13 C	2.8502075 *	6.2843194	6.6673551	5.8646413
14 C	3.2518708	7.6059343	7.8437691	6.8820927
15 C	3.0034121	8.0932181	8.0919625	6.9522668
16 C	4.2762505	9.4752461	9.4183015	8.2253960
17 C	5.4343712	10.3869099	10.4703272	9.3544728
18 C	5.6002162	10.0676158	10.3373367	9.3582614
19 C	4.6943900	8.7605761	9.1197840	8.2324959
20 O	1.9464204 *	7.3474811	7.1504100	5.9153987
21 N	1.9679958 *	4.3414542	3.7917762	2.4432622 *
22 H	6.4990947	1.1061478 *	2.1779995 *	3.4424473
23 H	6.2043580	2.1846269 *	1.1011096 *	2.1944535 *
24 H	4.4034792	3.4266771	2.1836186 *	1.1048539 *
25 H	6.5293058	2.6559760 *	4.0548188	4.8667772
26 H	6.2950041	4.6412121	5.9097438	6.2403844
27 H	4.5546573	5.3826257	6.2772557	6.0318459
28 H	3.8772001	6.4682136	7.0490163	6.4243017
29 H	4.6149076	9.9657698	9.7628257	8.4880983
30 H	6.4173857	11.4655046	11.5077550	10.3560029
31 H	6.6610374	10.9431045	11.2897892	10.3613128
32 H	5.2925852	8.7305419	9.2498323	8.5052587
33 H	2.6442361 *	8.0440964	7.7139779	6.4100720
34 H	2.5141239 *	4.8008704	4.2425713	2.9314630 *
35 H	2.5763209 *	4.6855518	3.8651997	2.4506232 *
	C	C	C	C
1 CO	2.8430539 *	3.1360901	4.5771914	5.4765376
2 C	2.8379837 *	2.5517933 *	1.4448572 *	2.4679888 *
3 C	2.4749013 *	2.9453936 *	2.4788752 *	3.7656314

4 C	1.4091007 *	2.5201250 *	2.8347474 *	4.2759537
5 C	0.0000000	1.4637912 *	2.4710312 *	3.8184310
6 C	1.4637912 *	0.0000000	1.4787597 *	2.5429113 *
7 C	2.4710312 *	1.4787597 *	0.0000000	1.4429801 *
8 C	3.8184310	2.5429113 *	1.4429801 *	0.0000000
9 C	4.3750128	2.9209232 *	2.4706487 *	1.3986630 *
10 C	3.9072683	2.5066577 *	2.8427818 *	2.4440445 *
11 C	2.6595912 *	1.4770134 *	2.5106387 *	2.8774455 *
12 N	3.1570734	2.5539556 *	3.8658855	4.3368763
13 C	4.4580807	3.7768904	4.9673957	5.1742657
14 C	5.4846671	5.0593503	6.3470692	6.6308968
15 C	5.6335826	5.5695150	6.9814245	7.5038620
16 C	6.9477054	6.9606972	8.3809786	8.8967528
17 C	8.0198008	7.8373294	9.1883038	9.5200434
18 C	7.9681638	7.5328132	8.7676299	8.8957807
19 C	6.8263196	6.2532632	7.4276237	7.4984835
20 O	4.7066727	4.9515292	6.4110060	7.1691653
21 N	1.5124221 *	2.6272096 *	3.9079579	5.1566628
22 H	3.9440215	3.5396996	2.1996882 *	2.6563047 *
23 H	3.4654729	4.0462862	3.4840951	4.6518809
24 H	2.1787441 *	3.5132107	3.9395398	5.3804560
25 H	4.6678888	3.5315378	2.1968679 *	1.1036970 *
26 H	5.4751888	4.0213868	3.4713423	2.1740000 *
27 H	4.8383147	3.5129346	3.9409931	3.4159284
28 H	5.0537342	4.1169776	5.0705635	4.9824806
29 H	7.3040472	7.5185501	8.9756968	9.6199044
30 H	9.0449920	8.9195020	10.2836532	10.6280265
31 H	8.9619037	8.4355752	9.6028436	9.6103123
32 H	7.1028144	6.3223430	7.3371334	7.2000606
33 H	5.3203315	5.7476562	7.2077140	8.0461750
34 H	2.1234418 *	3.1207716	4.3708341	5.5755350
35 H	2.0713836 *	3.4031571	4.5208498	5.8576780

C C C N

1 CO	5.3231819	4.1738920	2.8849848 *	1.9274611 *
2 C	3.7613284	4.2859190	3.8570933	5.0979383
3 C	4.9455322	5.1897759	4.4158580	5.3873264
4 C	5.1740548	5.0176624	3.9259066	4.5610915
5 C	4.3750128	3.9072683	2.6595912 *	3.1570734
6 C	2.9209232 *	2.5066577 *	1.4770134 *	2.5539556 *
7 C	2.4706487 *	2.8427818 *	2.5106387 *	3.8658855
8 C	1.3986630 *	2.4440445 *	2.8774455 *	4.3368763
9 C	0.0000000	1.4294866 *	2.4932274 *	3.8141806
10 C	1.4294866 *	0.0000000	1.4168503 *	2.4839504 *
11 C	2.4932274 *	1.4168503 *	0.0000000	1.4628763 *

12 N	3.8141806	2.4839504 *	1.4628763 *	0.0000000
13 C	4.3439752	2.9174988 *	2.4610796 *	1.3341364 *
14 C	5.7956700	4.3675982	3.8583824	2.5150951 *
15 C	6.8500444	5.4336589	4.6345392	3.1730779
16 C	8.2005690	6.7751765	6.0301568	4.5715659
17 C	8.6536357	7.2313691	6.7278608	5.3267092
18 C	7.8857650	6.5049461	6.2602898	4.9959953
19 C	6.4750782	5.0996324	4.9238870	3.7544102
20 O	6.7681107	5.4381102	4.3579781	2.9819461 *
21 N	5.4597050	4.6579574	3.2496782	3.0312959
22 H	4.0533876	4.8788919	4.7101230	6.0410942
23 H	5.9154866	6.2591041	5.5167538	6.4681342
24 H	6.2602654	6.0184554	4.8318683	5.2431127
25 H	2.1784718 *	3.4520472	3.9809978	5.4398829
26 H	1.1005974 *	2.1970987 *	3.4808279	4.6800771
27 H	2.1610599 *	1.1002307 *	2.1950943 *	2.7159895 *
28 H	3.9387735	2.5907522 *	2.6800009 *	2.1035346 *
29 H	9.0314792	7.6219983	6.7464775	5.2891604
30 H	9.7556158	8.3351813	7.8314042	6.4220122
31 H	8.5098411	7.1824715	7.1017699	5.9240826
32 H	6.0491289	4.7710628	4.9011485	3.9906278
33 H	7.7087249	6.3998805	5.2802791	3.9429631
34 H	5.8329722	5.0009281	3.6299572	3.3268028
35 H	6.2938833	5.5740877	4.1807211	3.9670487

C C C C

1 CO	2.8502075 *	3.2518708	3.0034121	4.2762505
2 C	6.2843194	7.6059343	8.0932181	9.4752461
3 C	6.6673551	7.8437691	8.0919625	9.4183015
4 C	5.8646413	6.8820927	6.9522668	8.2253960
5 C	4.4580807	5.4846671	5.6335826	6.9477054
6 C	3.7768904	5.0593503	5.5695150	6.9606972
7 C	4.9673957	6.3470692	6.9814245	8.3809786
8 C	5.1742657	6.6308968	7.5038620	8.8967528
9 C	4.3439752	5.7956700	6.8500444	8.2005690
10 C	2.9174988 *	4.3675982	5.4336589	6.7751765
11 C	2.4610796 *	3.8583824	4.6345392	6.0301568
12 N	1.3341364 *	2.5150951 *	3.1730779	4.5715659
13 C	0.0000000	1.4690943 *	2.6166902 *	3.8948373
14 C	1.4690943 *	0.0000000	1.4413629 *	2.5103549 *
15 C	2.6166902 *	1.4413629 *	0.0000000	1.4053170 *
16 C	3.8948373	2.5103549 *	1.4053170 *	0.0000000
17 C	4.3531149	2.8893359 *	2.4328548 *	1.4259478 *
18 C	3.8004482	2.5000981 *	2.8125633 *	2.4703973 *
19 C	2.4792166 *	1.4471909 *	2.4425866 *	2.8501076 *

20	O	3.0694733	2.5035202 *	1.4588385 *	2.4409245 *
21	N	4.1993650	4.8640645	4.6697861	5.8634867
22	H	7.1663729	8.5370758	9.1051208	10.4971468
23	H	7.7554591	8.9055197	9.0908012	10.3915595
24	H	6.5262623	7.3859378	7.2539825	8.4326995
25	H	6.2566573	7.7169024	8.6057184	9.9981658
26	H	4.9900212	6.3910778	7.5591277	8.8606349
27	H	2.6279066 *	3.9547029	5.1933416	6.4418755
28	H	1.1068468 *	2.1660666 *	3.5291164	4.6670913
29	H	4.8042786	3.5116526	2.1970730 *	1.1066258 *
30	H	5.4607843	3.9973705	3.4348894	2.1913474 *
31	H	4.6621833	3.4920108	3.9125082	3.4686033
32	H	2.6607215 *	2.2104006 *	3.4580901	3.9620951
33	H	4.0443072	3.3322782	2.0377279 *	2.4776912 *
34	H	4.3188416	4.8953979	4.6868928	5.7932197
35	H	5.1272573	5.6712896	5.2823413	6.3711850

C C C O

1	CO	5.4343712	5.6002162	4.6943900	1.9464204 *
2	C	10.3869099	10.0676158	8.7605761	7.3474811
3	C	10.4703272	10.3373367	9.1197840	7.1504100
4	C	9.3544728	9.3582614	8.2324959	5.9153987
5	C	8.0198008	7.9681638	6.8263196	4.7066727
6	C	7.8373294	7.5328132	6.2532632	4.9515292
7	C	9.1883038	8.7676299	7.4276237	6.4110060
8	C	9.5200434	8.8957807	7.4984835	7.1691653
9	C	8.6536357	7.8857650	6.4750782	6.7681107
10	C	7.2313691	6.5049461	5.0996324	5.4381102
11	C	6.7278608	6.2602898	4.9238870	4.3579781
12	N	5.3267092	4.9959953	3.7544102	2.9819461 *
13	C	4.3531149	3.8004482	2.4792166 *	3.0694733
14	C	2.8893359 *	2.5000981 *	1.4471909 *	2.5035202 *
15	C	2.4328548 *	2.8125633 *	2.4425866 *	1.4588385 *
16	C	1.4259478 *	2.4703973 *	2.8501076 *	2.4409245 *
17	C	0.0000000	1.4234855 *	2.4586868 *	3.7456335
18	C	1.4234855 *	0.0000000	1.4154168 *	4.2652834
19	C	2.4586868 *	1.4154168 *	0.0000000	3.7873075
20	O	3.7456335	4.2652834	3.7873075	0.0000000
21	N	7.0613294	7.2402861	6.2804051	3.5683791
22	H	11.3600264	10.9662535	9.6257912	8.4076218
23	H	11.4848719	11.3982525	10.1988680	8.0827330
24	H	9.6526081	9.8083737	8.7819492	6.0872649
25	H	10.6053070	9.9463565	8.5418769	8.2565133
26	H	9.1707931	8.2702316	6.8702712	7.6211952
27	H	6.6991797	5.8175751	4.4166600	5.4743464

28 H	4.8450498	3.9910637	2.5772943 *	4.1566615
29 H	2.1987195 *	3.4719250	3.9561939	2.6717380 *
30 H	1.1080681 *	2.2043968 *	3.4659582	4.6249150
31 H	2.1948034 *	1.1016323 *	2.1832850 *	5.3622895
32 H	3.4628766	2.1881290 *	1.1123286 *	4.6995515
33 H	3.8901911	4.6943313	4.4747082	0.9868499 *
34 H	6.9583926	7.1606423	6.2499570	3.7228374
35 H	7.6594613	7.9777625	7.1089465	4.0105362

N H H H

1 CO	1.9679958 *	6.4990947	6.2043580	4.4034792
2 C	4.3414542	1.1061478 *	2.1846269 *	3.4266771
3 C	3.7917762	2.1779995 *	1.1011096 *	2.1836186 *
4 C	2.4432622 *	3.4424473	2.1944535 *	1.1048539 *
5 C	1.5124221 *	3.9440215	3.4654729	2.1787441 *
6 C	2.6272096 *	3.5396996	4.0462862	3.5132107
7 C	3.9079579	2.1996882 *	3.4840951	3.9395398
8 C	5.1566628	2.6563047 *	4.6518809	5.3804560
9 C	5.4597050	4.0533876	5.9154866	6.2602654
10 C	4.6579574	4.8788919	6.2591041	6.0184554
11 C	3.2496782	4.7101230	5.5167538	4.8318683
12 N	3.0312959	6.0410942	6.4681342	5.2431127
13 C	4.1993650	7.1663729	7.7554591	6.5262623
14 C	4.8640645	8.5370758	8.9055197	7.3859378
15 C	4.6697861	9.1051208	9.0908012	7.2539825
16 C	5.8634867	10.4971468	10.3915595	8.4326995
17 C	7.0613294	11.3600264	11.4848719	9.6526081
18 C	7.2402861	10.9662535	11.3982525	9.8083737
19 C	6.2804051	9.6257912	10.1988680	8.7819492
20 O	3.5683791	8.4076218	8.0827330	6.0872649
21 N	0.0000000	5.4471528	4.6369290	2.5932533 *
22 H	5.4471528	0.0000000	2.5285077 *	4.3484273
23 H	4.6369290	2.5285077 *	0.0000000	2.5075201 *
24 H	2.5932533 *	4.3484273	2.5075201 *	0.0000000
25 H	6.0879863	2.3639612 *	4.7482423	5.9476587
26 H	6.5446013	4.7379439	6.8237721	7.3340318
27 H	5.3803568	5.9439398	7.3517892	6.9931698
28 H	5.0365262	7.2370127	8.1478515	7.1927547
29 H	6.0675753	11.0223524	10.6765855	8.5555662
30 H	8.0165247	12.4489972	12.5063806	10.5975531
31 H	8.2963287	11.7994197	12.3631277	10.8498258
32 H	6.7742977	9.5076636	10.3454885	9.1639559
33 H	4.0360759	9.1219957	8.5793147	6.4273956
34 H	1.0426830 *	5.8853508	5.0416282	2.9761118 *
35 H	1.0387349 *	5.7657636	4.5261762	2.1837052 *

	H	H	H	H
1 CO	6.5293058	6.2950041	4.5546573	3.8772001
2 C	2.6559760 *	4.6412121	5.3826257	6.4682136
3 C	4.0548188	5.9097438	6.2772557	7.0490163
4 C	4.8667772	6.2403844	6.0318459	6.4243017
5 C	4.6678888	5.4751888	4.8383147	5.0537342
6 C	3.5315378	4.0213868	3.5129346	4.1169776
7 C	2.1968679 *	3.4713423	3.9409931	5.0705635
8 C	1.1036970 *	2.1740000 *	3.4159284	4.9824806
9 C	2.1784718 *	1.1005974 *	2.1610599 *	3.9387735
10 C	3.4520472	2.1970987 *	1.1002307 *	2.5907522 *
11 C	3.9809978	3.4808279	2.1950943 *	2.6800009 *
12 N	5.4398829	4.6800771	2.7159895 *	2.1035346 *
13 C	6.2566573	4.9900212	2.6279066 *	1.1068468 *
14 C	7.7169024	6.3910778	3.9547029	2.1660666 *
15 C	8.6057184	7.5591277	5.1933416	3.5291164
16 C	9.9981658	8.8606349	6.4418755	4.6670913
17 C	10.6053070	9.1707931	6.6991797	4.8450498
18 C	9.9463565	8.2702316	5.8175751	3.9910637
19 C	8.5418769	6.8702712	4.4166600	2.5772943 *
20 O	8.2565133	7.6211952	5.4743464	4.1566615
21 N	6.0879863	6.5446013	5.3803568	5.0365262
22 H	2.3639612 *	4.7379439	5.9439398	7.2370127
23 H	4.7482423	6.8237721	7.3517892	8.1478515
24 H	5.9476587	7.3340318	6.9931698	7.1927547
25 H	0.0000000	2.5176023 *	4.3289364	6.0045177
26 H	2.5176023 *	0.0000000	2.4752992 *	4.3904268
27 H	4.3289364	2.4752992 *	0.0000000	1.9887522 *
28 H	6.0045177	4.3904268	1.9887522 *	0.0000000
29 H	10.7216246	9.7554587	7.3828461	5.6612699
30 H	11.7132824	10.2549275	7.7816205	5.9268379
31 H	10.6274534	8.7764474	6.3849804	4.6509785
32 H	8.1859048	6.2881770	3.9295781	2.2748825 *
33 H	9.1214095	8.5791827	6.4527007	5.1211534
34 H	6.5047363	6.8974950	5.6750285	5.1086170
35 H	6.7123345	7.3873103	6.3217278	6.0137760

	H	H	H	H
1 CO	4.6149076	6.4173857	6.6610374	5.2925852
2 C	9.9657698	11.4655046	10.9431045	8.7305419
3 C	9.7628257	11.5077550	11.2897892	9.2498323
4 C	8.4880983	10.3560029	10.3613128	8.5052587
5 C	7.3040472	9.0449920	8.9619037	7.1028144

6 C	7.5185501	8.9195020	8.4355752	6.3223430
7 C	8.9756968	10.2836532	9.6028436	7.3371334
8 C	9.6199044	10.6280265	9.6103123	7.2000606
9 C	9.0314792	9.7556158	8.5098411	6.0491289
10 C	7.6219983	8.3351813	7.1824715	4.7710628
11 C	6.7464775	7.8314042	7.1017699	4.9011485
12 N	5.2891604	6.4220122	5.9240826	3.9906278
13 C	4.8042786	5.4607843	4.6621833	2.6607215 *
14 C	3.5116526	3.9973705	3.4920108	2.2104006 *
15 C	2.1970730 *	3.4348894	3.9125082	3.4580901
16 C	1.1066258 *	2.1913474 *	3.4686033	3.9620951
17 C	2.1987195 *	1.1080681 *	2.1948034 *	3.4628766
18 C	3.4719250	2.2043968 *	1.1016323 *	2.1881290 *
19 C	3.9561939	3.4659582	2.1832850 *	1.1123286 *
20 O	2.6717380 *	4.6249150	5.3622895	4.6995515
21 N	6.0675753	8.0165247	8.2963287	6.7742977
22 H	11.0223524	12.4489972	11.7994197	9.5076636
23 H	10.6765855	12.5063806	12.3631277	10.3454885
24 H	8.5555662	10.5975531	10.8498258	9.1639559
25 H	10.7216246	11.7132824	10.6274534	8.1859048
26 H	9.7554587	10.2549275	8.7764474	6.2881770
27 H	7.3828461	7.7816205	6.3849804	3.9295781
28 H	5.6612699	5.9268379	4.6509785	2.2748825 *
29 H	0.0000000	2.5192055 *	4.3818631	5.0678477
30 H	2.5192055 *	0.0000000	2.5416105 *	4.3803341
31 H	4.3818631	2.5416105 *	0.0000000	2.5101549 *
32 H	5.0678477	4.3803341	2.5101549 *	0.0000000
33 H	2.2780242 *	4.5878869	5.7704468	5.4691386
34 H	5.9784945	7.8832504	8.2045139	6.7537221
35 H	6.4153920	8.5537636	9.0569597	7.6754745

H H H

1 CO	2.6442361 *	2.5141239 *	2.5763209 *
2 C	8.0440964	4.8008704	4.6855518
3 C	7.7139779	4.2425713	3.8651997
4 C	6.4100720	2.9314630 *	2.4506232 *
5 C	5.3203315	2.1234418 *	2.0713836 *
6 C	5.7476562	3.1207716	3.4031571
7 C	7.2077140	4.3708341	4.5208498
8 C	8.0461750	5.5755350	5.8576780
9 C	7.7087249	5.8329722	6.2938833
10 C	6.3998805	5.0009281	5.5740877
11 C	5.2802791	3.6299572	4.1807211
12 N	3.9429631	3.3268028	3.9670487
13 C	4.0443072	4.3188416	5.1272573

14 C	3.3322782	4.8953979	5.6712896
15 C	2.0377279 *	4.6868928	5.2823413
16 C	2.4776912 *	5.7932197	6.3711850
17 C	3.8901911	6.9583926	7.6594613
18 C	4.6943313	7.1606423	7.9777625
19 C	4.4747082	6.2499570	7.1089465
20 O	0.9868499 *	3.7228374	4.0105362
21 N	4.0360759	1.0426830 *	1.0387349 *
22 H	9.1219957	5.8853508	5.7657636
23 H	8.5793147	5.0416282	4.5261762
24 H	6.4273956	2.9761118 *	2.1837052 *
25 H	9.1214095	6.5047363	6.7123345
26 H	8.5791827	6.8974950	7.3873103
27 H	6.4527007	5.6750285	6.3217278
28 H	5.1211534	5.1086170	6.0137760
29 H	2.2780242 *	5.9784945	6.4153920
30 H	4.5878869	7.8832504	8.5537636
31 H	5.7704468	8.2045139	9.0569597
32 H	5.4691386	6.7537221	7.6754745
33 H	0.0000000	4.1620439	4.2620135
34 H	4.1620439	0.0000000	1.6632592 *
35 H	4.2620135	1.6632592 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.77 , TOTAL = 2020.8 SECONDS (33.7 MIN)
WALL CLOCK TIME: STEP = 0.79 , TOTAL = 1867.4 SECONDS (31.1 MIN)
CPU UTILIZATION: STEP = 98.07% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.91 , TOTAL = 2021.7 SECONDS (33.7 MIN)
WALL CLOCK TIME: STEP = 0.90 , TOTAL = 1868.3 SECONDS (31.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.629797886	-284.629797886	0.042038620	0.002086435	196577722
11475425						
2	1	-284.630222013	-0.000424127	0.016506968	0.000636190	168020447
13856208						
3	2	-284.630196661	0.000025351	0.013099227	0.000819572	158518134
14649220						
4	3	-284.630256529	-0.000059867	0.002516491	0.000306788	155191649
14906172						
5	4	-284.630251782	0.000004747	0.001896136	0.000642984	143162906
15935459						
6	5	-284.630258342	-0.000006560	0.000615856	0.000083987	139864567
16199760						
7	6	-284.630258269	0.000000073	0.000291604	0.000075326	130094007
16941121						
8	7	-284.630258699	-0.000000431	0.000451723	0.000071040	146605049
15671440						
9	8	-284.630258870	-0.000000171	0.001171661	0.000056999	165058164
14243741						
-----DISABLING FDIFF OPTION-----						
10	9	-284.630259158	-0.000000288	0.001059823	0.000044317	196568784
11476088						
11	10	-284.630259381	-0.000000223	0.000976977	0.000046009	196569092
11476060						
12	11	-284.630259526	-0.000000146	0.000279529	0.000042672	196569276
11476064						
13	12	-284.630259619	-0.000000093	0.000744459	0.000038046	196569267
11476065						
14	13	-284.630259787	-0.000000167	0.000954880	0.000028845	196568898
11476072						
15	14	-284.630259922	-0.000000135	0.001126207	0.000022868	196568759
11476061						
16	15	-284.630259987	-0.000000065	0.000161270	0.000026712	196568393
11476079						
17	16	-284.630260018	-0.000000031	0.000138033	0.000018501	196568396
11476085						
18	17	-284.630260031	-0.000000014	0.000093636	0.000007618	196568220
11476086						
19	18	-284.630260039	-0.000000008	0.000143016	0.000005025	196568385
11476084						
20	19	-284.630260041	-0.000000002	0.000037858	0.000003742	196568428
11476087						
21	20	-284.630260042	-0.000000001	0.000030140	0.000003415	196568431
11476088						
22	21	-284.630260042	0.000000000	0.000020651	0.000002783	196568457
11476083						

23 22	-284.630260043	-0.000000001	0.000055646	0.000002329	196568457
11476083					
24 23	-284.630260044	-0.000000001	0.000043047	0.000002402	196568468
11476085					
25 24	-284.630260044	0.000000000	0.000024453	0.000001870	196568415
11476085					
26 25	-284.630260044	0.000000000	0.000016573	0.000000999	196568454
11476084					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 86.3 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 28.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.8, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 4.3 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6302600444 AFTER 26 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6021059723
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000847216

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 91.35 , TOTAL = 2113.0 SECONDS (35.2 MIN)
WALL CLOCK TIME: STEP = 84.48 , TOTAL = 1952.8 SECONDS (32.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.84 , TOTAL = 2116.8 SECONDS (35.3 MIN)
WALL CLOCK TIME: STEP = 3.83 , TOTAL = 1956.7 SECONDS (32.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.

USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84 , TOTAL = 2119.7 SECONDS (35.3 MIN)
WALL CLOCK TIME: STEP = 2.67 , TOTAL = 1959.3 SECONDS (32.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 16 ENERGY= -284.6302600

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0011610	0.0001863	0.0006538
2 C	6.0	0.0006089	0.0009095	0.0000211
3 C	6.0	-0.0012615	-0.0024522	-0.0006529
4 C	6.0	0.0016530	-0.0024952	-0.0007209
5 C	6.0	-0.0013028	-0.0016050	-0.0001945
6 C	6.0	-0.0019700	0.0007927	-0.0001887
7 C	6.0	0.0011447	0.0012779	-0.0000045
8 C	6.0	0.0014728	0.0022210	0.0007473
9 C	6.0	0.0006292	0.0013440	0.0002628
10 C	6.0	-0.0023634	0.0012106	-0.0000413
11 C	6.0	-0.0020856	-0.0005424	-0.0005739
12 N	7.0	-0.0020837	-0.0009901	-0.0002508
13 C	6.0	0.0014138	0.0022954	-0.0004767
14 C	6.0	0.0020372	0.0011466	-0.0001268
15 C	6.0	-0.0009211	-0.0013870	0.0000648
16 C	6.0	0.0017095	-0.0021984	-0.0016132
17 C	6.0	0.0029136	0.0006089	-0.0005099
18 C	6.0	-0.0009122	-0.0000091	0.0003244
19 C	6.0	-0.0021839	-0.0025786	0.0001166
20 O	8.0	-0.0022306	-0.0021059	0.0018165
21 N	7.0	0.0019218	-0.0014351	-0.0016724
22 H	1.0	0.0010871	0.0000394	0.0002321
23 H	1.0	-0.0019786	0.0005879	0.0002969
24 H	1.0	-0.0001202	0.0019618	0.0005875
25 H	1.0	-0.0006385	-0.0003401	0.0002274
26 H	1.0	0.0013456	-0.0023794	-0.0004397
27 H	1.0	0.0023366	0.0000908	-0.0005795
28 H	1.0	-0.0004579	0.0002253	0.0004422
29 H	1.0	-0.0003445	0.0001449	-0.0019550

30 H	1.0	-0.0016175	-0.0011384	0.0007066
31 H	1.0	0.0014308	-0.0010729	0.0020095
32 H	1.0	-0.0000740	0.0042453	-0.0002248
33 H	1.0	0.0016176	0.0034699	-0.0006713
34 H	1.0	0.0000076	-0.0019113	0.0012834
35 H	1.0	0.0003773	0.0018831	0.0011037

MAXIMUM GRADIENT = 0.0042453 RMS GRADIENT = 0.0014203
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0004930411
 PREDICTED ENERGY CHANGE WAS -0.0004423886 RATIO= 1.114
 GDIIS STEP HAS LENGTH = 0.151235
 RADIUS OF STEP TAKEN= 0.14004 CURRENT TRUST RADIUS= 0.14004

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 2119.7 SECONDS (35.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 1959.3 SECONDS (32.7 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 17

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1084885470	-1.6534527067	1.0391652942
C	6.0	4.9971086337	0.6646712185	0.4252627111
C	6.0	5.2147114387	-0.6943524446	0.1816751675
C	6.0	4.0792714019	-1.5496923315	0.0529645928
C	6.0	2.7688032140	-1.0559909154	0.1734026108
C	6.0	2.4671510232	0.3414295718	0.4557706890
C	6.0	3.6596326466	1.2009015948	0.5615703703
C	6.0	3.5384363383	2.6131855772	0.8214233310
C	6.0	2.2806055993	3.2060575265	0.9797368165
C	6.0	1.1083682293	2.3944214474	0.9090946044
C	6.0	1.1574105419	1.0046180740	0.6517227400
N	7.0	-0.0820001439	0.2242969649	0.6809866987
C	6.0	-1.2936786133	0.7674341876	0.5336104514
C	6.0	-2.5991817316	0.0932326124	0.5868531406
C	6.0	-2.8571083461	-1.3198699101	0.6910116751
C	6.0	-4.1437958932	-1.8841238074	0.5921652526
C	6.0	-5.2700476164	-1.0125270270	0.5117933408
C	6.0	-5.0780071127	0.3996496246	0.5037642217
C	6.0	-3.7684587667	0.9434463494	0.4946924538
O	8.0	-1.7473973444	-2.2393001263	0.9185355609

N	7.0	1.6956463783	-2.1079660729	-0.0256285059
H	1.0	5.8497436001	1.3592721392	0.5270125871
H	1.0	6.2328350371	-1.1080025733	0.0846525157
H	1.0	4.2411540889	-2.6252049306	-0.1619736230
H	1.0	4.4609771660	3.2126758945	0.9053867478
H	1.0	2.1944404905	4.2860837060	1.1902732565
H	1.0	0.1432919178	2.8958191801	1.1078063735
H	1.0	-1.3551864836	1.8506377307	0.3203989592
H	1.0	-4.2871680594	-2.9860208705	0.5887393315
H	1.0	-6.2814675408	-1.4474028800	0.4622817859
H	1.0	-5.9494474640	1.0748126821	0.4871915614
H	1.0	-3.6338346718	2.0410365791	0.4144358273
H	1.0	-2.0657777974	-3.1728128341	1.0244787174
H	1.0	1.4226570700	-2.1692958262	-1.0324317704
H	1.0	2.1278212224	-3.0265624043	0.2050615126

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4451062	5.2658024	4.0927344
2 C	5.4451062	0.0000000	1.3977236 *	2.4257859 *
3 C	5.2658024	1.3977236 *	0.0000000	1.4273741 *
4 C	4.0927344	2.4257859 *	1.4273741 *	0.0000000
5 C	2.8607306 *	2.8265627 *	2.4725125 *	1.4055509 *
6 C	3.1437546	2.5507061 *	2.9490780 *	2.5174445 *
7 C	4.5810544	1.4473993 *	2.4808423 *	2.8285232 *
8 C	5.4787002	2.4660447 *	3.7628425	4.2676204
9 C	5.3232005	3.7610470	4.9456119	5.1682939
10 C	4.1715660	4.2835069	5.1895778	5.0115125
11 C	2.8836937 *	3.8613637	4.4237016	3.9268669
12 N	1.9210731 *	5.1045735	5.3989242	4.5670155
13 C	2.8429477 *	6.2925594	6.6798069	5.8710040
14 C	3.2537631	7.6194672	7.8639294	6.8982589
15 C	3.0045388	8.1054149	8.1120263	6.9694538
16 C	4.2819319	9.4910668	9.4427601	8.2475098
17 C	5.4422016	10.4036041	10.4947790	9.3759712
18 C	5.6037149	10.0789065	10.3557055	9.3733081
19 C	4.6979842	8.7702741	9.1366138	8.2460738
20 O	1.9498926 *	7.3596691	7.1694341	5.9308381
21 N	1.9645453 *	4.3347980	3.7980386	2.4493907 *
22 H	6.5039081	1.1044500 *	2.1771306 *	3.4382216
23 H	6.2222368	2.1875574 *	1.1032205 *	2.1986201 *
24 H	4.4120247	3.4263098	2.1895433 *	1.1086622 *
25 H	6.5300277	2.6476941 *	4.0443472	4.8530891

26 H	6.2969931	4.6427167	5.9113493	6.2371741
27 H	4.5499228	5.3854827	6.2822247	6.0305222
28 H	3.8649217	6.4629069	7.0469694	6.4161591
29 H	4.6152376	9.9775784	9.7827992	8.5057277
30 H	6.4192515	11.4746899	11.5242334	10.3693257
31 H	6.6668355	10.9544120	11.3075961	10.3755377
32 H	5.2957078	8.7400046	9.2646262	8.5156327
33 H	2.6525657 *	8.0603789	7.7368344	6.4296181
34 H	2.5069199 *	4.7888356	4.2460794	2.9359144 *
35 H	2.5804774 *	4.6804385	3.8689329	2.4520270 *

C C C C

1 CO	2.8607306 *	3.1437546	4.5810544	5.4787002
2 C	2.8265627 *	2.5507061 *	1.4473993 *	2.4660447 *
3 C	2.4725125 *	2.9490780 *	2.4808423 *	3.7628425
4 C	1.4055509 *	2.5174445 *	2.8285232 *	4.2676204
5 C	0.0000000	1.4572267 *	2.4571966 *	3.8046185
6 C	1.4572267 *	0.0000000	1.4737361 *	2.5381547 *
7 C	2.4571966 *	1.4737361 *	0.0000000	1.4410962 *
8 C	3.8046185	2.5381547 *	1.4410962 *	0.0000000
9 C	4.3650394	2.9181215 *	2.4692568 *	1.3995351 *
10 C	3.8991836	2.5033116 *	2.8379945 *	2.4414698 *
11 C	2.6592266 *	1.4810929 *	2.5115274 *	2.8784669 *
12 N	3.1660478	2.5617599 *	3.8688283	4.3398239
13 C	4.4674811	3.7856807	4.9723202	5.1806341
14 C	5.5051720	5.0741021	6.3561252	6.6389413
15 C	5.6558317	5.5823823	6.9884875	7.5092559
16 C	6.9746106	6.9768410	8.3911748	8.9047764
17 C	8.0460873	7.8549717	9.2000507	9.5305326
18 C	7.9875190	7.5455354	8.7744911	8.9018957
19 C	6.8437395	6.2647241	7.4328526	7.5023662
20 O	4.7277385	4.9635406	6.4185968	7.1760773
21 N	1.5158927 *	2.6127579 *	3.8923836	5.1383504
22 H	3.9307416	3.5331305	2.1961014 *	2.6459626 *
23 H	3.4655589	4.0520314	3.4899656	4.6529407
24 H	2.1777803 *	3.5113552	3.9371023	5.3760224
25 H	4.6498140	3.5244223	2.1926237 *	1.1034129 *
26 H	5.4682428	4.0217112	3.4728092	2.1773753 *
27 H	4.8356202	3.5143105	3.9415443	3.4189037
28 H	5.0475132	4.1117270	5.0624828	4.9779563
29 H	7.3269537	7.5306330	8.9823549	9.6252449
30 H	9.0633358	8.9296299	10.2882869	10.6323974
31 H	8.9803498	8.4485483	9.6101952	9.6176006
32 H	7.1164210	6.3334350	7.3431697	7.2065571
33 H	5.3458806	5.7637464	7.2196944	8.0576811

34 H	2.1226384 *	3.0999123	4.3477734	5.5484619
35 H	2.0724411 *	3.3943143	4.5105428	5.8460666

	C	C	C	N
--	---	---	---	---

1 CO	5.3232005	4.1715660	2.8836937 *	1.9210731 *
2 C	3.7610470	4.2835069	3.8613637	5.1045735
3 C	4.9456119	5.1895778	4.4237016	5.3989242
4 C	5.1682939	5.0115125	3.9268669	4.5670155
5 C	4.3650394	3.8991836	2.6592266 *	3.1660478
6 C	2.9181215 *	2.5033116 *	1.4810929 *	2.5617599 *
7 C	2.4692568 *	2.8379945 *	2.5115274 *	3.8688283
8 C	1.3995351 *	2.4414698 *	2.8784669 *	4.3398239
9 C	0.0000000	1.4275447 *	2.4930897 *	3.8160259
10 C	1.4275447 *	0.0000000	1.4142839 *	2.4856489 *
11 C	2.4930897 *	1.4142839 *	0.0000000	1.4648878 *
12 N	3.8160259	2.4856489 *	1.4648878 *	0.0000000
13 C	4.3498759	2.9253897 *	2.4653691 *	1.3359950 *
14 C	5.8014103	4.3755270	3.8661114	2.5223485 *
15 C	6.8529910	5.4376948	4.6390893	3.1758113
16 C	8.2056744	6.7817123	6.0374801	4.5772822
17 C	8.6618584	7.2421913	6.7380021	5.3361219
18 C	7.8899719	6.5126529	6.2664433	5.0022237
19 C	6.4765621	5.1049485	4.9287513	3.7605663
20 O	6.7735126	5.4430563	4.3625799	2.9831674 *
21 N	5.4398330	4.6357412	3.2305855	3.0164189
22 H	4.0440477	4.8680757	4.7073689	6.0413128
23 H	5.9188181	6.2615365	5.5267231	6.4813409
24 H	6.2570660	6.0131675	4.8318931	5.2459418
25 H	2.1816489 *	3.4510203	3.9816350	5.4423714
26 H	1.1037240 *	2.1993182 *	3.4833152	4.6839797
27 H	2.1635063 *	1.1055579 *	2.1938757 *	2.7147675 *
28 H	3.9358447	2.5906303 *	2.6718287 *	2.0966667 *
29 H	9.0349524	7.6265063	6.7507483	5.2913219
30 H	9.7586654	8.3407990	7.8348709	6.4246251
31 H	8.5157841	7.1925053	7.1091088	5.9319366
32 H	6.0545390	4.7810100	4.9077998	3.9983898
33 H	7.7190050	6.4095721	5.2895008	3.9488879
34 H	5.8033888	4.9694887	3.6028408	3.3059163
35 H	6.2824371	5.5607565	4.1703260	3.9595330

	C	C	C	C
--	---	---	---	---

1 CO	2.8429477 *	3.2537631	3.0045388	4.2819319
2 C	6.2925594	7.6194672	8.1054149	9.4910668
3 C	6.6798069	7.8639294	8.1120263	9.4427601

4 C	5.8710040	6.8982589	6.9694538	8.2475098
5 C	4.4674811	5.5051720	5.6558317	6.9746106
6 C	3.7856807	5.0741021	5.5823823	6.9768410
7 C	4.9723202	6.3561252	6.9884875	8.3911748
8 C	5.1806341	6.6389413	7.5092559	8.9047764
9 C	4.3498759	5.8014103	6.8529910	8.2056744
10 C	2.9253897 *	4.3755270	5.4376948	6.7817123
11 C	2.4653691 *	3.8661114	4.6390893	6.0374801
12 N	1.3359950 *	2.5223485 *	3.1758113	4.5772822
13 C	0.0000000	1.4702792 *	2.6126473 *	3.8932450
14 C	1.4702792 *	0.0000000	1.4402201 *	2.5091432 *
15 C	2.6126473 *	1.4402201 *	0.0000000	1.4084452 *
16 C	3.8932450	2.5091432 *	1.4084452 *	0.0000000
17 C	4.3566327	2.8916886 *	2.4390274 *	1.4263883 *
18 C	3.8022754	2.4990739 *	2.8149956 *	2.4690457 *
19 C	2.4813367 *	1.4486427 *	2.4477952 *	2.8540378 *
20 O	3.0650415	2.5052463 *	1.4589645 *	2.4444619 *
21 N	4.1853003	4.8647670	4.6757079	5.8762965
22 H	7.1679004	8.5434639	9.1112002	10.5068879
23 H	7.7696354	8.9274684	9.1126083	10.4179846
24 H	6.5290283	7.3987052	7.2675177	8.4513498
25 H	6.2636641	7.7251688	8.6107087	10.0058780
26 H	4.9979071	6.3971033	7.5626797	8.8658014
27 H	2.6314650 *	3.9556346	5.1911611	6.4414954
28 H	1.1056999 *	2.1695610 *	3.5277814	4.6689017
29 H	4.8012960	3.5115671	2.1980877 *	1.1111906 *
30 H	5.4578961	3.9935328	3.4343584	2.1856887 *
31 H	4.6661354	3.4925223	3.9164536	3.4679536
32 H	2.6669451 *	2.2122782 *	3.4605622	3.9621373
33 H	4.0450755	3.3381265	2.0422541 *	2.4830976 *
34 H	4.2959692	4.8904300	4.6912870	5.8056901
35 H	5.1194742	5.6765696	5.2913580	6.3865637

C C C O

1 CO	5.4422016	5.6037149	4.6979842	1.9498926 *
2 C	10.4036041	10.0789065	8.7702741	7.3596691
3 C	10.4947790	10.3557055	9.1366138	7.1694341
4 C	9.3759712	9.3733081	8.2460738	5.9308381
5 C	8.0460873	7.9875190	6.8437395	4.7277385
6 C	7.8549717	7.5455354	6.2647241	4.9635406
7 C	9.2000507	8.7744911	7.4328526	6.4185968
8 C	9.5305326	8.9018957	7.5023662	7.1760773
9 C	8.6618584	7.8899719	6.4765621	6.7735126
10 C	7.2421913	6.5126529	5.1049485	5.4430563
11 C	6.7380021	6.2664433	4.9287513	4.3625799

12 N	5.3361219	5.0022237	3.7605663	2.9831674 *
13 C	4.3566327	3.8022754	2.4813367 *	3.0650415
14 C	2.8916886 *	2.4990739 *	1.4486427 *	2.5052463 *
15 C	2.4390274 *	2.8149956 *	2.4477952 *	1.4589645 *
16 C	1.4263883 *	2.4690457 *	2.8540378 *	2.4444619 *
17 C	0.0000000	1.4251972 *	2.4659467 *	3.7522628
18 C	1.4251972 *	0.0000000	1.4179965 *	4.2695494
19 C	2.4659467 *	1.4179965 *	0.0000000	3.7939699
20 O	3.7522628	4.2695494	3.7939699	0.0000000
21 N	7.0717538	7.2422907	6.2799918	3.5725683
22 H	11.3699349	10.9698291	9.6272412	8.4154360
23 H	11.5112065	11.4185735	10.2177519	8.1030429
24 H	9.6704524	9.8203726	8.7932008	6.0974725
25 H	10.6160303	9.9532225	8.5464430	8.2624530
26 H	9.1790083	8.2743071	6.8711880	7.6284049
27 H	6.7033310	5.8187364	4.4146871	5.4753977
28 H	4.8539141	3.9997978	2.5840390 *	4.1520102
29 H	2.2060487 *	3.4778459	3.9646711	2.6677318 *
30 H	1.1020611 *	2.2049129 *	3.4687784	4.6252634
31 H	2.1952623 *	1.1025099 *	2.1849543 *	5.3690434
32 H	3.4656777	2.1880961 *	1.1087241 *	4.7046833
33 H	3.8983363	4.7018249	4.4859097	0.9919859 *
34 H	6.9652740	7.1566762	6.2425120	3.7229584
35 H	7.6732579	7.9844921	7.1141390	4.0182267

N H H H

1 CO	1.9645453 *	6.5039081	6.2222368	4.4120247
2 C	4.3347980	1.1044500 *	2.1875574 *	3.4263098
3 C	3.7980386	2.1771306 *	1.1032205 *	2.1895433 *
4 C	2.4493907 *	3.4382216	2.1986201 *	1.1086622 *
5 C	1.5158927 *	3.9307416	3.4655589	2.1777803 *
6 C	2.6127579 *	3.5331305	4.0520314	3.5113552
7 C	3.8923836	2.1961014 *	3.4899656	3.9371023
8 C	5.1383504	2.6459626 *	4.6529407	5.3760224
9 C	5.4398330	4.0440477	5.9188181	6.2570660
10 C	4.6357412	4.8680757	6.2615365	6.0131675
11 C	3.2305855	4.7073689	5.5267231	4.8318931
12 N	3.0164189	6.0413128	6.4813409	5.2459418
13 C	4.1853003	7.1679004	7.7696354	6.5290283
14 C	4.8647670	8.5434639	8.9274684	7.3987052
15 C	4.6757079	9.1112002	9.1126083	7.2675177
16 C	5.8762965	10.5068879	10.4179846	8.4513498
17 C	7.0717538	11.3699349	11.5112065	9.6704524
18 C	7.2422907	10.9698291	11.4185735	9.8203726
19 C	6.2799918	9.6272412	10.2177519	8.7932008

20	O	3.5725683	8.4154360	8.1030429	6.0974725
21	N	0.0000000	5.4390879	4.6473831	2.6011028 *
22	H	5.4390879	0.0000000	2.5357220 *	4.3518180
23	H	4.6473831	2.5357220 *	0.0000000	2.5158538 *
24	H	2.6011028 *	4.3518180	2.5158538 *	0.0000000
25	H	6.0682019	2.3466880 *	4.7414499	5.9387232
26	H	6.5277167	4.7294166	6.8284108	7.3337248
27	H	5.3602561	5.9381722	7.3593456	6.9918898
28	H	5.0097765	7.2246209	8.1478340	7.1822614
29	H	6.0780339	11.0291595	10.6982018	8.5688994
30	H	8.0192734	12.4518231	12.5245984	10.6067186
31	H	8.2970190	11.8026867	12.3828400	10.8609348
32	H	6.7684007	9.5087188	10.3622573	9.1717777
33	H	4.0478310	9.1347001	8.6031209	6.4408799
34	H	1.0449580 *	5.8721166	5.0509437	2.9848745 *
35	H	1.0410630 *	5.7612415	4.5328257	2.1821958 *

H H H H

1	CO	6.5300277	6.2969931	4.5499228	3.8649217
2	C	2.6476941 *	4.6427167	5.3854827	6.4629069
3	C	4.0443472	5.9113493	6.2822247	7.0469694
4	C	4.8530891	6.2371741	6.0305222	6.4161591
5	C	4.6498140	5.4682428	4.8356202	5.0475132
6	C	3.5244223	4.0217112	3.5143105	4.1117270
7	C	2.1926237 *	3.4728092	3.9415443	5.0624828
8	C	1.1034129 *	2.1773753 *	3.4189037	4.9779563
9	C	2.1816489 *	1.1037240 *	2.1635063 *	3.9358447
10	C	3.4510203	2.1993182 *	1.1055579 *	2.5906303 *
11	C	3.9816350	3.4833152	2.1938757 *	2.6718287 *
12	N	5.4423714	4.6839797	2.7147675 *	2.0966667 *
13	C	6.2636641	4.9979071	2.6314650 *	1.1056999 *
14	C	7.7251688	6.3971033	3.9556346	2.1695610 *
15	C	8.6107087	7.5626797	5.1911611	3.5277814
16	C	10.0058780	8.8658014	6.4414954	4.6689017
17	C	10.6160303	9.1790083	6.7033310	4.8539141
18	C	9.9532225	8.2743071	5.8187364	3.9997978
19	C	8.5464430	6.8711880	4.4146871	2.5840390 *
20	O	8.2624530	7.6284049	5.4753977	4.1520102
21	N	6.0682019	6.5277167	5.3602561	5.0097765
22	H	2.3466880 *	4.7294166	5.9381722	7.2246209
23	H	4.7414499	6.8284108	7.3593456	8.1478340
24	H	5.9387232	7.3337248	6.9918898	7.1822614
25	H	0.0000000	2.5239955 *	4.3340256	6.0020928
26	H	2.5239955 *	0.0000000	2.4792835 *	4.3918026
27	H	4.3340256	2.4792835 *	0.0000000	1.9894352 *

28 H	6.0020928	4.3918026	1.9894352 *	0.0000000
29 H	10.7263299	9.7599486	7.3820355	5.6623130
30 H	11.7180542	10.2588429	7.7818901	5.9300462
31 H	10.6358962	8.7823400	6.3892645	4.6622911
32 H	8.1938849	6.2937232	3.9342218	2.2885218 *
33 H	9.1316581	8.5913960	6.4587326	5.1220820
34 H	6.4770479	6.8708072	5.6455987	5.0701510
35 H	6.6979226	7.3790158	6.3109356	5.9943078

H H H H

1 CO	4.6152376	6.4192515	6.6668355	5.2957078
2 C	9.9775784	11.4746899	10.9544120	8.7400046
3 C	9.7827992	11.5242334	11.3075961	9.2646262
4 C	8.5057277	10.3693257	10.3755377	8.5156327
5 C	7.3269537	9.0633358	8.9803498	7.1164210
6 C	7.5306330	8.9296299	8.4485483	6.3334350
7 C	8.9823549	10.2882869	9.6101952	7.3431697
8 C	9.6252449	10.6323974	9.6176006	7.2065571
9 C	9.0349524	9.7586654	8.5157841	6.0545390
10 C	7.6265063	8.3407990	7.1925053	4.7810100
11 C	6.7507483	7.8348709	7.1091088	4.9077998
12 N	5.2913219	6.4246251	5.9319366	3.9983898
13 C	4.8012960	5.4578961	4.6661354	2.6669451 *
14 C	3.5115671	3.9935328	3.4925223	2.2122782 *
15 C	2.1980877 *	3.4343584	3.9164536	3.4605622
16 C	1.1111906 *	2.1856887 *	3.4679536	3.9621373
17 C	2.2060487 *	1.1020611 *	2.1952623 *	3.4656777
18 C	3.4778459	2.2049129 *	1.1025099 *	2.1880961 *
19 C	3.9646711	3.4687784	2.1849543 *	1.1087241 *
20 O	2.6677318 *	4.6252634	5.3690434	4.7046833
21 N	6.0780339	8.0192734	8.2970190	6.7684007
22 H	11.0291595	12.4518231	11.8026867	9.5087188
23 H	10.6982018	12.5245984	12.3828400	10.3622573
24 H	8.5688994	10.6067186	10.8609348	9.1717777
25 H	10.7263299	11.7180542	10.6358962	8.1938849
26 H	9.7599486	10.2588429	8.7823400	6.2937232
27 H	7.3820355	7.7818901	6.3892645	3.9342218
28 H	5.6623130	5.9300462	4.6622911	2.2885218 *
29 H	0.0000000	2.5220165 *	4.3890607	5.0723301
30 H	2.5220165 *	0.0000000	2.5440969 *	4.3796642
31 H	4.3890607	2.5440969 *	0.0000000	2.5101682 *
32 H	5.0723301	4.3796642	2.5101682 *	0.0000000
33 H	2.2714169 *	4.5896781	5.7804749	5.4786112
34 H	5.9914388	7.8809158	8.1964273	6.7370938
35 H	6.4265807	8.5601428	9.0632855	7.6760065

	H	H	H
1 CO	2.6525657 *	2.5069199 *	2.5804774 *
2 C	8.0603789	4.7888356	4.6804385
3 C	7.7368344	4.2460794	3.8689329
4 C	6.4296181	2.9359144 *	2.4520270 *
5 C	5.3458806	2.1226384 *	2.0724411 *
6 C	5.7637464	3.0999123	3.3943143
7 C	7.2196944	4.3477734	4.5105428
8 C	8.0576811	5.5484619	5.8460666
9 C	7.7190050	5.8033888	6.2824371
10 C	6.4095721	4.9694887	5.5607565
11 C	5.2895008	3.6028408	4.1703260
12 N	3.9488879	3.3059163	3.9595330
13 C	4.0450755	4.2959692	5.1194742
14 C	3.3381265	4.8904300	5.6765696
15 C	2.0422541 *	4.6912870	5.2913580
16 C	2.4830976 *	5.8056901	6.3865637
17 C	3.8983363	6.9652740	7.6732579
18 C	4.7018249	7.1566762	7.9844921
19 C	4.4859097	6.2425120	7.1141390
20 O	0.9919859 *	3.7229584	4.0182267
21 N	4.0478310	1.0449580 *	1.0410630 *
22 H	9.1347001	5.8721166	5.7612415
23 H	8.6031209	5.0509437	4.5328257
24 H	6.4408799	2.9848745 *	2.1821958 *
25 H	9.1316581	6.4770479	6.6979226
26 H	8.5913960	6.8708072	7.3790158
27 H	6.4587326	5.6455987	6.3109356
28 H	5.1220820	5.0701510	5.9943078
29 H	2.2714169 *	5.9914388	6.4265807
30 H	4.5896781	7.8809158	8.5601428
31 H	5.7804749	8.1964273	9.0632855
32 H	5.4786112	6.7370938	7.6760065
33 H	0.0000000	4.1721823	4.2754072
34 H	4.1721823	0.0000000	1.6623935 *
35 H	4.2754072	1.6623935 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 2120.5 SECONDS (35.3 MIN)

WALL CLOCK TIME: STEP = 0.77 , TOTAL = 1960.1 SECONDS (32.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.17 , TOTAL = 2121.7 SECONDS (35.4 MIN)

WALL CLOCK TIME: STEP = 1.18 , TOTAL = 1961.3 SECONDS (32.7 MIN)

CPU UTILIZATION: STEP = 99.40%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.629915435 -284.629915435 0.113645636 0.003184528 196314275
11493492

2 1 -284.630611113 -0.000695678 0.105993195 0.000342961 169887694
13704208

3 2 -284.630594381 0.000016732 0.019373941 0.000716121 162053455
14421291

4 3 -284.630631322 -0.000036941 0.014212320 0.000279807 152187151
15210861

5 4 -284.630628303 0.000003019 0.002602543 0.000512135 146749761
15672259

6 5 -284.630633070 -0.000004767 0.003195953 0.000099510 137383362
16405922

7 6 -284.630633053 0.000000017 0.000876171 0.000089255 156037329
14920039

8 7 -284.630633614 -0.000000561 0.001139801 0.000080323 168712677
13886138

-----DISABLING FDIFF OPTION-----

9 8 -284.630633991 -0.000000377 0.002779729 0.000067919 196294252
11494773

10 9 -284.630634600 -0.000000609 0.001949578 0.000110762 196294339
11494798

11 10 -284.630635143 -0.000000543 0.001893684 0.000071256 196294723
11494776

12 11 -284.630635522 -0.000000379 0.000522717 0.000072255 196293845
11494789

13 12 -284.630635793 -0.000000271 0.000874888 0.000049841 196293554
11494776

14 13 -284.630635982 -0.000000189 0.000692974 0.000042323 196294182
11494744

15 14	-284.630636184	-0.000000203	0.000978233	0.000041465	196293718
11494764					
16 15	-284.630636260	-0.000000076	0.000173404	0.000033691	196293329
11494766					
17 16	-284.630636314	-0.000000054	0.000164386	0.000025124	196293209
11494780					
18 17	-284.630636330	-0.000000016	0.000125890	0.000017294	196293289
11494779					
19 18	-284.630636346	-0.000000016	0.000183822	0.000007429	196293240
11494775					
20 19	-284.630636350	-0.000000004	0.000048550	0.000003435	196293279
11494775					
21 20	-284.630636350	-0.000000001	0.000044923	0.000001816	196293297
11494773					
22 21	-284.630636351	0.000000000	0.000013108	0.000000945	196293288
11494774					
23 22	-284.630636351	0.000000000	0.000009556	0.000000958	196293288
11494774					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 78.4 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 24.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.8 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6306363509 AFTER 23 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5971333609
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000727088

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 82.40 , TOTAL = 2204.1 SECONDS (36.7 MIN)
WALL CLOCK TIME: STEP = 75.89 , TOTAL = 2037.2 SECONDS (34.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.81, TOTAL = 2207.9 SECONDS (36.8 MIN)
WALL CLOCK TIME: STEP = 3.78, TOTAL = 2041.0 SECONDS (34.0 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.81, TOTAL = 2210.7 SECONDS (36.8 MIN)
WALL CLOCK TIME: STEP = 2.66, TOTAL = 2043.6 SECONDS (34.1 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 17 ENERGY= -284.6306364

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0007159	0.0016410	-0.0005245
2 C	6.0	0.0021901	-0.0012965	-0.0005568
3 C	6.0	-0.0012273	-0.0001349	-0.0000993
4 C	6.0	-0.0010705	0.0015666	0.0002578
5 C	6.0	0.0045967	0.0013652	-0.0001316
6 C	6.0	0.0008727	-0.0017212	-0.0007635
7 C	6.0	-0.0018726	0.0009993	-0.0002350
8 C	6.0	0.0020163	0.0008858	0.0002650
9 C	6.0	-0.0015927	-0.0010781	-0.0001627
10 C	6.0	0.0037895	-0.0015161	-0.0012201
11 C	6.0	-0.0040974	0.0023619	0.0001516
12 N	7.0	-0.0010755	-0.0021703	0.0002773
13 C	6.0	-0.0005573	0.0014385	-0.0005668
14 C	6.0	-0.0003284	-0.0003368	0.0000880
15 C	6.0	0.0026379	-0.0001098	0.0008654
16 C	6.0	-0.0004998	0.0004206	-0.0017659
17 C	6.0	-0.0031740	-0.0014306	-0.0004159
18 C	6.0	-0.0011238	-0.0007686	0.0012752
19 C	6.0	-0.0001560	0.0030409	0.0002648

20 O	8.0	-0.0009413	0.0009995	0.0005157
21 N	7.0	-0.0019560	0.0012287	0.0012838
22 H	1.0	-0.0001229	-0.0003264	0.0003099
23 H	1.0	-0.0005811	-0.0001038	0.0001273
24 H	1.0	0.0000078	-0.0005031	-0.0000457
25 H	1.0	-0.0004307	-0.0009815	0.0002999
26 H	1.0	0.0012897	-0.0002190	0.0000669
27 H	1.0	-0.0008025	0.0013732	0.0000043
28 H	1.0	0.0006569	-0.0006156	0.0004641
29 H	1.0	0.0000090	-0.0028254	-0.0017073
30 H	1.0	0.0023335	-0.0000953	0.0000849
31 H	1.0	0.0009790	-0.0008166	0.0015294
32 H	1.0	-0.0005871	0.0020342	-0.0006754
33 H	1.0	0.0002647	-0.0008597	-0.0000507
34 H	1.0	-0.0001783	-0.0020351	-0.0001024
35 H	1.0	0.0014476	0.0005889	0.0008923

MAXIMUM GRADIENT = 0.0045967 RMS GRADIENT = 0.0013514
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0003763065
 PREDICTED ENERGY CHANGE WAS -0.0004931698 RATIO= 0.763
 GDIIS STEP HAS LENGTH = 0.073754
 RADIUS OF STEP TAKEN= 0.07375 CURRENT TRUST RADIUS= 0.19805

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 2210.7 SECONDS (36.8 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2043.6 SECONDS (34.1 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 18

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1074304164	-1.6558513653	1.0381271751
C	6.0	4.9953485659	0.6657542516	0.4252111454
C	6.0	5.2217345260	-0.6926765961	0.1821780573
C	6.0	4.0843697048	-1.5490799592	0.0531919578
C	6.0	2.7688340027	-1.0547145296	0.1748481810
C	6.0	2.4688676347	0.3424627884	0.4572631734
C	6.0	3.6618367121	1.1978387050	0.5604551708
C	6.0	3.5365746463	2.6089956019	0.8189599301
C	6.0	2.2827031230	3.2049272863	0.9787098860
C	6.0	1.1054467925	2.3925856015	0.9106361649

C	6.0	1.1635393681	0.9994269153	0.6529705862
N	7.0	-0.0807761247	0.2245598322	0.6842748642
C	6.0	-1.2937533213	0.7612267386	0.5358325079
C	6.0	-2.6023018028	0.0917402539	0.5912126445
C	6.0	-2.8632038010	-1.3194339503	0.6955282264
C	6.0	-4.1473413959	-1.8828965769	0.6020779162
C	6.0	-5.2710053251	-1.0093457608	0.5150120718
C	6.0	-5.0786475493	0.4022814157	0.5030855936
C	6.0	-3.7691490802	0.9421676844	0.4966068184
O	8.0	-1.7483378427	-2.2442982708	0.9118868647
N	7.0	1.6980195249	-2.1024568977	-0.0249635656
H	1.0	5.8471415978	1.3631343875	0.5271597942
H	1.0	6.2395939649	-1.1067281741	0.0849373675
H	1.0	4.2426043913	-2.6242932545	-0.1630970087
H	1.0	4.4627514415	3.2089454900	0.9036516868
H	1.0	2.1924680352	4.2855236917	1.1902038181
H	1.0	0.1436155859	2.8905004771	1.1092971919
H	1.0	-1.3517086795	1.8457776178	0.3161694610
H	1.0	-4.2887276664	-2.9832468102	0.6001349023
H	1.0	-6.2852823887	-1.4462667301	0.4550875500
H	1.0	-5.9524552655	1.0780117457	0.4760315232
H	1.0	-3.6340926923	2.0377922065	0.4105285632
H	1.0	-2.0688134653	-3.1749700318	1.0226032280
H	1.0	1.4226198788	-2.1535138950	-1.0309693242
H	1.0	2.1260934879	-3.0227748891	0.1980428765

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4458482	5.2741313	4.0984806
2 C	5.4458482	0.0000000	1.3984456 *	2.4235865 *
3 C	5.2741313	1.3984456 *	0.0000000	1.4295674 *
4 C	4.0984806	2.4235865 *	1.4295674 *	0.0000000
5 C	2.8617626 *	2.8249003 *	2.4794851 *	1.4106139 *
6 C	3.1475464	2.5472830 *	2.9538892 *	2.5201298 *
7 C	4.5831781	1.4421022 *	2.4800046 *	2.8251393 *
8 C	5.4768590	2.4615537 *	3.7611560	4.2633405
9 C	5.3256465	3.7566216	4.9460777	5.1675111
10 C	4.1715863	4.2835639	5.1955095	5.0145707
11 C	2.8834380 *	3.8530473	4.4219688	3.9224828
12 N	1.9226491 *	5.1018436	5.4046316	4.5708318
13 C	2.8386409 *	6.2907992	6.6850945	5.8732160
14 C	3.2552201	7.6211114	7.8738913	6.9060360
15 C	3.0091890	8.1099253	8.1254280	6.9809821

16 C	4.2830797	9.4929280	9.4537042	8.2567413
17 C	5.4423515	10.4025019	10.5027924	9.3823042
18 C	5.6051391	10.0777418	10.3633868	9.3792911
19 C	4.6979587	8.7691460	9.1437175	8.2511023
20 O	1.9509183 *	7.3608807	7.1778767	5.9364268
21 N	1.9645845 *	4.3287445	3.8009151	2.4509185 *
22 H	6.5053553	1.1055695 *	2.1763514 *	3.4370049
23 H	6.2300511	2.1921740 *	1.1031465 *	2.2003805 *
24 H	4.4136700	3.4259514	2.1929555 *	1.1081077 *
25 H	6.5309382	2.6420422 *	4.0397072	4.8482224
26 H	6.2984480	4.6415605	5.9139707	6.2381638
27 H	4.5470528	5.3811507	6.2837887	6.0294922
28 H	3.8615690	6.4567392	7.0478265	6.4144496
29 H	4.6130274	9.9769674	9.7913375	8.5126224
30 H	6.4226660	11.4766790	11.5348956	10.3779466
31 H	6.6717444	10.9556811	11.3174292	10.3835572
32 H	5.2948917	8.7378464	9.2700205	8.5186855
33 H	2.6540535 *	8.0629043	7.7472695	6.4377744
34 H	2.5017097 *	4.7784019	4.2472396	2.9369471 *
35 H	2.5786086 *	4.6786192	3.8746101	2.4551180 *

C C C C

1 CO	2.8617626 *	3.1475464	4.5831781	5.4768590
2 C	2.8249003 *	2.5472830 *	1.4421022 *	2.4615537 *
3 C	2.4794851 *	2.9538892 *	2.4800046 *	3.7611560
4 C	1.4106139 *	2.5201298 *	2.8251393 *	4.2633405
5 C	0.0000000	1.4566546 *	2.4535979 *	3.7982993
6 C	1.4566546 *	0.0000000	1.4715610 *	2.5314015 *
7 C	2.4535979 *	1.4715610 *	0.0000000	1.4400969 *
8 C	3.7982993	2.5314015 *	1.4400969 *	0.0000000
9 C	4.3620024	2.9155217 *	2.4709009 *	1.3974435 *
10 C	3.8977069	2.5034910 *	2.8434444 *	2.4424620 *
11 C	2.6504847 *	1.4743762 *	2.5078708 *	2.8722048 *
12 N	3.1648596	2.5624439 *	3.8690766	4.3346165
13 C	4.4645905	3.7866678	4.9748476	5.1794285
14 C	5.5078869	5.0791302	6.3611187	6.6388438
15 C	5.6622464	5.5901392	6.9950740	7.5103234
16 C	6.9786742	6.9819351	8.3949940	8.9031848
17 C	8.0471601	7.8572485	9.2015974	9.5267121
18 C	7.9883380	7.5478913	8.7768028	8.8989560
19 C	6.8437044	6.2669009	7.4356569	7.5003884
20 O	4.7289721	4.9681825	6.4219779	7.1758900
21 N	1.5114008 *	2.6085210 *	3.8847451	5.1274045
22 H	3.9301520	3.5297863	2.1918003 *	2.6412189 *
23 H	3.4723139	4.0567423	3.4902691	4.6531393

24 H	2.1793998 *	3.5117845	3.9331300	5.3712406
25 H	4.6453533	3.5201645	2.1917570 *	1.1067592 *
26 H	5.4663781	4.0201154	3.4769852	2.1806401 *
27 H	4.8300816	3.5106184	3.9426148	3.4169741
28 H	5.0410017	4.1081220	5.0611400	4.9729884
29 H	7.3286617	7.5329842	8.9830131	9.6206245
30 H	9.0669108	8.9350266	10.2930838	10.6323295
31 H	8.9833245	8.4534055	9.6154093	9.6178584
32 H	7.1145354	6.3342285	7.3456508	7.2049677
33 H	5.3494864	5.7690981	7.2232533	8.0570531
34 H	2.1151001 *	3.0885870	4.3333922	5.5292440
35 H	2.0704866 *	3.3925675	4.5059326	5.8388213

C C C N

1 CO	5.3256465	4.1715863	2.8834380 *	1.9226491 *
2 C	3.7566216	4.2835639	3.8530473	5.1018436
3 C	4.9460777	5.1955095	4.4219688	5.4046316
4 C	5.1675111	5.0145707	3.9224828	4.5708318
5 C	4.3620024	3.8977069	2.6504847 *	3.1648596
6 C	2.9155217 *	2.5034910 *	1.4743762 *	2.5624439 *
7 C	2.4709009 *	2.8434444 *	2.5078708 *	3.8690766
8 C	1.3974435 *	2.4424620 *	2.8722048 *	4.3346165
9 C	0.0000000	1.4319447 *	2.4945672 *	3.8151430
10 C	1.4319447 *	0.0000000	1.4179765 *	2.4816728 *
11 C	2.4945672 *	1.4179765 *	0.0000000	1.4661923 *
12 N	3.8151430	2.4816728 *	1.4661923 *	0.0000000
13 C	4.3541766	2.9254009 *	2.4715882 *	1.3346761 *
14 C	5.8056318	4.3753080	3.8741798	2.5267357 *
15 C	6.8578710	5.4383406	4.6468901	3.1821294
16 C	8.2081226	6.7798776	6.0428332	4.5809477
17 C	8.6621951	7.2380106	6.7422226	5.3375699
18 C	7.8911676	6.5092573	6.2724753	5.0043115
19 C	6.4789983	5.1026285	4.9354983	3.7622168
20 O	6.7784818	5.4447020	4.3666715	2.9879474 *
21 N	5.4330049	4.6294596	3.2197744	3.0136589
22 H	4.0374893	4.8672881	4.6993873	6.0383148
23 H	5.9199820	6.2678898	5.5249327	6.4868029
24 H	6.2549779	6.0136290	4.8247234	5.2464866
25 H	2.1813437 *	3.4551392	3.9786447	5.4404344
26 H	1.1047899 *	2.2006790 *	3.4850747	4.6813492
27 H	2.1660131 *	1.1011379 *	2.1965058 *	2.7089177 *
28 H	3.9363939	2.5865039 *	2.6751107 *	2.0926343 *
29 H	9.0344076	7.6218832	6.7521624	5.2918767
30 H	9.7631021	8.3406948	7.8425455	6.4296257
31 H	8.5202282	7.1924243	7.1186279	5.9370330

32 H	6.0575166	4.7790397	4.9146978	3.9986007
33 H	7.7227400	6.4098472	5.2924780	3.9526652
34 H	5.7871794	4.9535292	3.5838265	3.2950716
35 H	6.2783949	5.5565851	4.1607183	3.9562454

C C C C

1 CO	2.8386409 *	3.2552201	3.0091890	4.2830797
2 C	6.2907992	7.6211114	8.1099253	9.4929280
3 C	6.6850945	7.8738913	8.1254280	9.4537042
4 C	5.8732160	6.9060360	6.9809821	8.2567413
5 C	4.4645905	5.5078869	5.6622464	6.9786742
6 C	3.7866678	5.0791302	5.5901392	6.9819351
7 C	4.9748476	6.3611187	6.9950740	8.3949940
8 C	5.1794285	6.6388438	7.5103234	8.9031848
9 C	4.3541766	5.8056318	6.8578710	8.2081226
10 C	2.9254009 *	4.3753080	5.4383406	6.7798776
11 C	2.4715882 *	3.8741798	4.6468901	6.0428332
12 N	1.3346761 *	2.5267357 *	3.1821294	4.5809477
13 C	0.0000000	1.4709107 *	2.6110968 *	3.8908536
14 C	1.4709107 *	0.0000000	1.4388760 *	2.5072806 *
15 C	2.6110968 *	1.4388760 *	0.0000000	1.4054296 *
16 C	3.8908536	2.5072806 *	1.4054296 *	0.0000000
17 C	4.3536070	2.8879362 *	2.4343888 *	1.4259355 *
18 C	3.8020177	2.4972966 *	2.8123885 *	2.4696496 *
19 C	2.4823099 *	1.4469657 *	2.4444117 *	2.8522170 *
20 O	3.0628817	2.5078202 *	1.4646198 *	2.4457741 *
21 N	4.1792201	4.8669228	4.6836942	5.8829952
22 H	7.1662227	8.5448019	9.1156260	10.5086640
23 H	7.7745664	8.9371003	9.1257324	10.4287247
24 H	6.5269828	7.4026051	7.2754660	8.4573253
25 H	6.2660965	7.7284904	8.6150540	10.0075722
26 H	5.0002610	6.3981582	7.5643950	8.8650146
27 H	2.6322420 *	3.9549378	5.1899630	6.4385482
28 H	1.1080890 *	2.1716996 *	3.5280441	4.6690810
29 H	4.7953194	3.5070867	2.1930553 *	1.1093983 *
30 H	5.4584714	3.9935375	3.4328589	2.1870170 *
31 H	4.6698429	3.4942133	3.9165545	3.4700579
32 H	2.6688029 *	2.2100582 *	3.4563654	3.9587771
33 H	4.0412014	3.3379790	2.0447612 *	2.4832587 *
34 H	4.2812690	4.8859631	4.6951856	5.8107268
35 H	5.1115675	5.6756065	5.2954650	6.3889398

C C C O

1 CO	5.4423515	5.6051391	4.6979587	1.9509183 *
------	-----------	-----------	-----------	-------------

2 C	10.4025019	10.0777418	8.7691460	7.3608807
3 C	10.5027924	10.3633868	9.1437175	7.1778767
4 C	9.3823042	9.3792911	8.2511023	5.9364268
5 C	8.0471601	7.9883380	6.8437044	4.7289721
6 C	7.8572485	7.5478913	6.2669009	4.9681825
7 C	9.2015974	8.7768028	7.4356569	6.4219779
8 C	9.5267121	8.8989560	7.5003884	7.1758900
9 C	8.6621951	7.8911676	6.4789983	6.7784818
10 C	7.2380106	6.5092573	5.1026285	5.4447020
11 C	6.7422226	6.2724753	4.9354983	4.3666715
12 N	5.3375699	5.0043115	3.7622168	2.9879474 *
13 C	4.3536070	3.8020177	2.4823099 *	3.0628817
14 C	2.8879362 *	2.4972966 *	1.4469657 *	2.5078202 *
15 C	2.4343888 *	2.8123885 *	2.4444117 *	1.4646198 *
16 C	1.4259355 *	2.4696496 *	2.8522170 *	2.4457741 *
17 C	0.0000000	1.4247228 *	2.4625831 *	3.7539051
18 C	1.4247228 *	0.0000000	1.4164411 *	4.2734606
19 C	2.4625831 *	1.4164411 *	0.0000000	3.7960112
20 O	3.7539051	4.2734606	3.7960112	0.0000000
21 N	7.0748691	7.2440159	6.2794671	3.5742393
22 H	11.3684652	10.9679846	9.6255490	8.4174161
23 H	11.5190427	11.4260469	10.2245970	8.1107932
24 H	9.6735028	9.8229166	8.7944896	6.0984732
25 H	10.6156037	9.9536984	8.5479912	8.2653231
26 H	9.1757812	8.2716881	6.8702245	7.6319058
27 H	6.6992608	5.8164215	4.4137419	5.4758211
28 H	4.8530562	4.0010864	2.5871000 *	4.1522180
29 H	2.2064453 *	3.4778145	3.9610048	2.6639847 *
30 H	1.1060058 *	2.2080312 *	3.4694769	4.6291885
31 H	2.1961227 *	1.1049359 *	2.1876249 *	5.3760875
32 H	3.4605563	2.1840790 *	1.1072682 *	4.7057125
33 H	3.8989242	4.7037993	4.4853803	0.9905113 *
34 H	6.9644668	7.1520551	6.2346771	3.7199334
35 H	7.6727725	7.9832547	7.1108224	4.0158209

N H H H

1 CO	1.9645845 *	6.5053553	6.2300511	4.4136700
2 C	4.3287445	1.1055695 *	2.1921740 *	3.4259514
3 C	3.8009151	2.1763514 *	1.1031465 *	2.1929555 *
4 C	2.4509185 *	3.4370049	2.2003805 *	1.1081077 *
5 C	1.5114008 *	3.9301520	3.4723139	2.1793998 *
6 C	2.6085210 *	3.5297863	4.0567423	3.5117845
7 C	3.8847451	2.1918003 *	3.4902691	3.9331300
8 C	5.1274045	2.6412189 *	4.6531393	5.3712406
9 C	5.4330049	4.0374893	5.9199820	6.2549779

10 C	4.6294596	4.8672881	6.2678898	6.0136290
11 C	3.2197744	4.6993873	5.5249327	4.8247234
12 N	3.0136589	6.0383148	6.4868029	5.2464866
13 C	4.1792201	7.1662227	7.7745664	6.5269828
14 C	4.8669228	8.5448019	8.9371003	7.4026051
15 C	4.6836942	9.1156260	9.1257324	7.2754660
16 C	5.8829952	10.5086640	10.4287247	8.4573253
17 C	7.0748691	11.3684652	11.5190427	9.6735028
18 C	7.2440159	10.9679846	11.4260469	9.8229166
19 C	6.2794671	9.6255490	10.2245970	8.7944896
20 O	3.5742393	8.4174161	8.1107932	6.0984732
21 N	0.0000000	5.4341860	4.6507475	2.6012124 *
22 H	5.4341860	0.0000000	2.5396458 *	4.3532256
23 H	4.6507475	2.5396458 *	0.0000000	2.5204151 *
24 H	2.6012124 *	4.3532256	2.5204151 *	0.0000000
25 H	6.0594607	2.3377983 *	4.7384071	5.9340620
26 H	6.5213041	4.7261639	6.8320731	7.3334884
27 H	5.3509198	5.9331223	7.3612568	6.9881075
28 H	5.0005769	7.2180958	8.1485357	7.1768774
29 H	6.0833939	11.0286990	10.7066478	8.5729223
30 H	8.0245962	12.4536597	12.5349442	10.6116115
31 H	8.3003700	11.8031519	12.3924214	10.8653021
32 H	6.7648161	9.5059229	10.3674349	9.1709566
33 H	4.0542214	9.1379538	8.6131571	6.4453957
34 H	1.0442698 *	5.8626763	5.0541317	2.9878334 *
35 H	1.0392134 *	5.7611385	4.5392636	2.1837646 *

H H H H

1 CO	6.5309382	6.2984480	4.5470528	3.8615690
2 C	2.6420422 *	4.6415605	5.3811507	6.4567392
3 C	4.0397072	5.9139707	6.2837887	7.0478265
4 C	4.8482224	6.2381638	6.0294922	6.4144496
5 C	4.6453533	5.4663781	4.8300816	5.0410017
6 C	3.5201645	4.0201154	3.5106184	4.1081220
7 C	2.1917570 *	3.4769852	3.9426148	5.0611400
8 C	1.1067592 *	2.1806401 *	3.4169741	4.9729884
9 C	2.1813437 *	1.1047899 *	2.1660131 *	3.9363939
10 C	3.4551392	2.2006790 *	1.1011379 *	2.5865039 *
11 C	3.9786447	3.4850747	2.1965058 *	2.6751107 *
12 N	5.4404344	4.6813492	2.7089177 *	2.0926343 *
13 C	6.2660965	5.0002610	2.6322420 *	1.1080890 *
14 C	7.7284904	6.3981582	3.9549378	2.1716996 *
15 C	8.6150540	7.5643950	5.1899630	3.5280441
16 C	10.0075722	8.8650146	6.4385482	4.6690810
17 C	10.6156037	9.1757812	6.6992608	4.8530562

18 C	9.9536984	8.2716881	5.8164215	4.0010864
19 C	8.5479912	6.8702245	4.4137419	2.5871000 *
20 O	8.2653231	7.6319058	5.4758211	4.1522180
21 N	6.0594607	6.5213041	5.3509198	5.0005769
22 H	2.3377983 *	4.7261639	5.9331223	7.2180958
23 H	4.7384071	6.8320731	7.3612568	8.1485357
24 H	5.9340620	7.3334884	6.9881075	7.1768774
25 H	0.0000000	2.5288969 *	4.3357389	6.0009423
26 H	2.5288969 *	0.0000000	2.4800065 *	4.3906133
27 H	4.3357389	2.4800065 *	0.0000000	1.9890933 *
28 H	6.0009423	4.3906133	1.9890933 *	0.0000000
29 H	10.7249128	9.7564903	7.3760301	5.6591690
30 H	11.7214522	10.2599254	7.7824334	5.9327063
31 H	10.6395615	8.7828213	6.3912613	4.6671072
32 H	8.1959536	6.2935682	3.9352851	2.2923896 *
33 H	9.1339951	8.5933449	6.4569568	5.1206635
34 H	6.4607375	6.8547415	5.6266041	5.0503480
35 H	6.6926970	7.3756367	6.3029698	5.9843016

H H H H

1 CO	4.6130274	6.4226660	6.6717444	5.2948917
2 C	9.9769674	11.4766790	10.9556811	8.7378464
3 C	9.7913375	11.5348956	11.3174292	9.2700205
4 C	8.5126224	10.3779466	10.3835572	8.5186855
5 C	7.3286617	9.0669108	8.9833245	7.1145354
6 C	7.5329842	8.9350266	8.4534055	6.3342285
7 C	8.9830131	10.2930838	9.6154093	7.3456508
8 C	9.6206245	10.6323295	9.6178584	7.2049677
9 C	9.0344076	9.7631021	8.5202282	6.0575166
10 C	7.6218832	8.3406948	7.1924243	4.7790397
11 C	6.7521624	7.8425455	7.1186279	4.9146978
12 N	5.2918767	6.4296257	5.9370330	3.9986007
13 C	4.7953194	5.4584714	4.6698429	2.6688029 *
14 C	3.5070867	3.9935375	3.4942133	2.2100582 *
15 C	2.1930553 *	3.4328589	3.9165545	3.4563654
16 C	1.1093983 *	2.1870170 *	3.4700579	3.9587771
17 C	2.2064453 *	1.1060058 *	2.1961227 *	3.4605563
18 C	3.4778145	2.2080312 *	1.1049359 *	2.1840790 *
19 C	3.9610048	3.4694769	2.1876249 *	1.1072682 *
20 O	2.6639847 *	4.6291885	5.3760875	4.7057125
21 N	6.0833939	8.0245962	8.3003700	6.7648161
22 H	11.0286990	12.4536597	11.8031519	9.5059229
23 H	10.7066478	12.5349442	12.3924214	10.3674349
24 H	8.5729223	10.6116115	10.8653021	9.1709566
25 H	10.7249128	11.7214522	10.6395615	8.1959536

26 H	9.7564903	10.2599254	8.7828213	6.2935682
27 H	7.3760301	7.7824334	6.3912613	3.9352851
28 H	5.6591690	5.9327063	4.6671072	2.2923896 *
29 H	0.0000000	2.5238021 *	4.3905822	5.0670830
30 H	2.5238021 *	0.0000000	2.5462118 *	4.3782941
31 H	4.3905822	2.5462118 *	0.0000000	2.5100347 *
32 H	5.0670830	4.3782941	2.5100347 *	0.0000000
33 H	2.2678749 *	4.5922869	5.7852630	5.4770087
34 H	5.9973701	7.8816446	8.1917973	6.7242327
35 H	6.4275323	8.5616993	9.0640321	7.6703477

H H H

1 CO	2.6540535 *	2.5017097 *	2.5786086 *
2 C	8.0629043	4.7784019	4.6786192
3 C	7.7472695	4.2472396	3.8746101
4 C	6.4377744	2.9369471 *	2.4551180 *
5 C	5.3494864	2.1151001 *	2.0704866 *
6 C	5.7690981	3.0885870	3.3925675
7 C	7.2232533	4.3333922	4.5059326
8 C	8.0570531	5.5292440	5.8388213
9 C	7.7227400	5.7871794	6.2783949
10 C	6.4098472	4.9535292	5.5565851
11 C	5.2924780	3.5838265	4.1607183
12 N	3.9526652	3.2950716	3.9562454
13 C	4.0412014	4.2812690	5.1115675
14 C	3.3379790	4.8859631	5.6756065
15 C	2.0447612 *	4.6951856	5.2954650
16 C	2.4832587 *	5.8107268	6.3889398
17 C	3.8989242	6.9644668	7.6727725
18 C	4.7037993	7.1520551	7.9832547
19 C	4.4853803	6.2346771	7.1108224
20 O	0.9905113 *	3.7199334	4.0158209
21 N	4.0542214	1.0442698 *	1.0392134 *
22 H	9.1379538	5.8626763	5.7611385
23 H	8.6131571	5.0541317	4.5392636
24 H	6.4453957	2.9878334 *	2.1837646 *
25 H	9.1339951	6.4607375	6.6926970
26 H	8.5933449	6.8547415	7.3756367
27 H	6.4569568	5.6266041	6.3029698
28 H	5.1206635	5.0503480	5.9843016
29 H	2.2678749 *	5.9973701	6.4275323
30 H	4.5922869	7.8816446	8.5616993
31 H	5.7852630	8.1917973	9.0640321
32 H	5.4770087	6.7242327	7.6703477
33 H	0.0000000	4.1773963	4.2778859

34 H 4.1773963 0.0000000 1.6616139 *
35 H 4.2778859 1.6616139 * 0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.54, TOTAL = 2211.2 SECONDS (36.9 MIN)
WALL CLOCK TIME: STEP = 0.54, TOTAL = 2044.2 SECONDS (34.1 MIN)

CPU UTILIZATION: STEP = 99.43%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.00, TOTAL = 2212.2 SECONDS (36.9 MIN)
WALL CLOCK TIME: STEP = 0.99, TOTAL = 2045.2 SECONDS (34.1 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.630430120	-284.630430120	0.036526044	0.002272546	196122120
11501911						
2	1	-284.630775161	-0.000345042	0.080757827	0.000843673	165830895
14047562						
3	2	-284.630751222	0.000023939	0.008183044	0.001069889	160896182
14475531						
4	3	-284.630811199	-0.000059977	0.002564099	0.000110925	154868266
14946502						
5	4	-284.630810033	0.000001167	0.001055029	0.000199423	140757006
16097698						
6	5	-284.630812131	-0.000002099	0.000922228	0.000060217	134516633
16591575						
7	6	-284.630812007	0.000000124	0.000333692	0.000081598	129653994
16990659						
8	7	-284.630812258	-0.000000251	0.000284733	0.000046758	145728174
15753209						
9	8	-284.630812296	-0.000000038	0.000295332	0.000039177	141194106
16114893						
10	9	-284.630812373	-0.000000076	0.000585611	0.000021164	158560024
14902075						

-----DISABLING FDIFF OPTION-----

11	10	-284.630812377	-0.000000004	0.000221953	0.000022526	196139556
11500202						
12	11	-284.630812421	-0.000000044	0.000165363	0.000020759	196139713
11500196						
13	12	-284.630812444	-0.000000023	0.000261977	0.000016367	196139825
11500200						
14	13	-284.630812484	-0.000000040	0.000551503	0.000012419	196139976
11500203						
15	14	-284.630812513	-0.000000029	0.000299431	0.000023364	196139615
11500198						
16	15	-284.630812529	-0.000000016	0.000112449	0.000023331	196139453
11500208						
17	16	-284.630812543	-0.000000014	0.000328504	0.000017586	196139382
11500213						
18	17	-284.630812559	-0.000000016	0.000196763	0.000004771	196139272
11500220						
19	18	-284.630812563	-0.000000004	0.000080401	0.000004377	196139340
11500214						
20	19	-284.630812564	-0.000000001	0.000031890	0.000003865	196139414
11500214						
21	20	-284.630812565	-0.000000001	0.000036285	0.000003181	196139390
11500216						
22	21	-284.630812566	-0.000000001	0.000051213	0.000002411	196139411
11500215						
23	22	-284.630812567	-0.000000001	0.000052783	0.000002355	196139482
11500212						
24	23	-284.630812567	-0.000000001	0.000028553	0.000002332	196139470
11500213						
25	24	-284.630812568	0.000000000	0.000022256	0.000001384	196139497
11500210						

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 82.9 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 26.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 4.8 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6308125677 AFTER 25 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5994638703
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000672343

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 88.92 , TOTAL = 2301.2 SECONDS (38.4 MIN)
WALL CLOCK TIME: STEP = 81.26 , TOTAL = 2126.4 SECONDS (35.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.65 , TOTAL = 2304.8 SECONDS (38.4 MIN)
WALL CLOCK TIME: STEP = 3.62 , TOTAL = 2130.1 SECONDS (35.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84 , TOTAL = 2307.7 SECONDS (38.5 MIN)
WALL CLOCK TIME: STEP = 2.68 , TOTAL = 2132.7 SECONDS (35.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 18 ENERGY= -284.6308126

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0002881	0.0015339	-0.0007299
2 C	6.0	-0.0028956	-0.0003792	-0.0002605
3 C	6.0	0.0020735	0.0008690	0.0000494
4 C	6.0	0.0015309	-0.0006613	-0.0002472
5 C	6.0	-0.0009230	0.0018276	-0.0003132
6 C	6.0	-0.0008557	0.0020744	0.0000343

7 C	6.0	0.0014491	-0.0010954	-0.0007270
8 C	6.0	-0.0025021	-0.0014748	-0.0002525
9 C	6.0	0.0038627	-0.0003897	-0.0004692
10 C	6.0	-0.0035864	0.0009388	-0.0000719
11 C	6.0	0.0020891	-0.0039961	-0.0010009
12 N	7.0	-0.0022106	0.0018285	-0.0000062
13 C	6.0	-0.0008229	-0.0028557	0.0003753
14 C	6.0	-0.0018924	0.0002438	0.0001169
15 C	6.0	-0.0015460	0.0014342	0.0002012
16 C	6.0	0.0005387	0.0002768	-0.0011903
17 C	6.0	0.0004586	0.0002856	0.0000120
18 C	6.0	0.0011419	-0.0007684	0.0014892
19 C	6.0	-0.0004770	0.0018858	0.0005259
20 O	8.0	0.0003089	-0.0019888	0.0003506
21 N	7.0	-0.0003533	0.0009333	0.0019493
22 H	1.0	0.0004727	0.0000383	0.0003759
23 H	1.0	-0.0006697	-0.0004480	0.0000655
24 H	1.0	-0.0002816	-0.0001062	-0.0000283
25 H	1.0	0.0014780	0.0000173	0.0005517
26 H	1.0	0.0005531	0.0004330	0.0002871
27 H	1.0	0.0016803	0.0001997	-0.0005209
28 H	1.0	0.0012513	0.0007426	0.0000893
29 H	1.0	0.0005663	-0.0018058	-0.0016449
30 H	1.0	-0.0000316	-0.0013022	-0.0004929
31 H	1.0	-0.0005331	0.0000596	0.0012847
32 H	1.0	-0.0009208	0.0010435	-0.0008217
33 H	1.0	0.0005396	0.0003802	-0.0000495
34 H	1.0	0.0000971	-0.0014832	0.0004109
35 H	1.0	0.0006981	0.0017091	0.0006575

MAXIMUM GRADIENT = 0.0039961 RMS GRADIENT = 0.0012533
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001762168
 PREDICTED ENERGY CHANGE WAS -0.0002211821 RATIO= 0.797
 GDIIS STEP HAS LENGTH = 0.037198
 RADIUS OF STEP TAKEN= 0.03720 CURRENT TRUST RADIUS= 0.10430

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 2307.7 SECONDS (38.5 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2132.8 SECONDS (35.5
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 19

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1088450563	-1.6583218752	1.0391286216
C	6.0	4.9967359078	0.6663302241	0.4258633015
C	6.0	5.2220430864	-0.6928828781	0.1825095480
C	6.0	4.0837619977	-1.5494145666	0.0534107806
C	6.0	2.7681575220	-1.0577212432	0.1754889763
C	6.0	2.4695358390	0.3410754589	0.4581185351
C	6.0	3.6624995687	1.1978091492	0.5613239375
C	6.0	3.5371043222	2.6091593386	0.8185159943
C	6.0	2.2797436883	3.2068667192	0.9793695104
C	6.0	1.1076199688	2.3915258067	0.9118459137
C	6.0	1.1649910436	1.0025011833	0.6545905186
N	7.0	-0.0763646297	0.2241385819	0.6848016652
C	6.0	-1.2922873229	0.7623440055	0.5360601116
C	6.0	-2.6005346598	0.0909866934	0.5913821467
C	6.0	-2.8632437408	-1.3211446920	0.6953252229
C	6.0	-4.1490826761	-1.8826365299	0.6067561402
C	6.0	-5.2706210909	-1.0077313200	0.5159900859
C	6.0	-5.0798276747	0.4042568537	0.5002105529
C	6.0	-3.7686091137	0.9376685500	0.4960094874
O	8.0	-1.7484836217	-2.2434800370	0.9101146442
N	7.0	1.6999388593	-2.1032576834	-0.0277354086
H	1.0	5.8458424218	1.3640031636	0.5263973196
H	1.0	6.2424140901	-1.1061933343	0.0846274814
H	1.0	4.2428850048	-2.6232868278	-0.1631785265
H	1.0	4.4614393768	3.2089843275	0.9023823449
H	1.0	2.1898477214	4.2862640965	1.1900128815
H	1.0	0.1410310011	2.8883692544	1.1103511016
H	1.0	-1.3529306608	1.8436412385	0.3151518898
H	1.0	-4.2892748229	-2.9787187600	0.6057881761
H	1.0	-6.2870592969	-1.4440746152	0.4543576212
H	1.0	-5.9534464805	1.0793025477	0.4708955459
H	1.0	-3.6323310375	2.0338195862	0.4115913316
H	1.0	-2.0705416037	-3.1757567826	1.0222244777
H	1.0	1.4226767434	-2.1477349363	-1.0313891157
H	1.0	2.1235222129	-3.0255856972	0.1945941851

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4471624	5.2735816	4.0967628
2 C	5.4471624	0.0000000	1.3990871 *	2.4252355 *

3 C	5.2735816	1.3990871 *	0.0000000	1.4303835 *
4 C	4.0967628	2.4252355 *	1.4303835 *	0.0000000
5 C	2.8598142 *	2.8287104 *	2.4808689 *	1.4097803 *
6 C	3.1477013	2.5482487 *	2.9531892 *	2.5186240 *
7 C	4.5841294	1.4425692 *	2.4799985 *	2.8253630 *
8 C	5.4784147	2.4615616 *	3.7612505	4.2635616
9 C	5.3278919	3.7606837	4.9497635	5.1705022
10 C	4.1731305	4.2822543	5.1936486	5.0125187
11 C	2.8884759 *	3.8532578	4.4223137	3.9233806
12 N	1.9244499 *	5.0989147	5.4005879	4.5662675
13 C	2.8418081 *	6.2907214	6.6842489	5.8718893
14 C	3.2559631	7.6208226	7.8723790	6.9036332
15 C	3.0108472	8.1118399	8.1258572	6.9803331
16 C	4.2856985	9.4961019	9.4558710	8.2581450
17 C	5.4438587	10.4033276	10.5026825	9.3814649
18 C	5.6095444	10.0802452	10.3649983	9.3801832
19 C	4.6977437	8.7698243	9.1426915	8.2487095
20 O	1.9515954 *	7.3620297	7.1778829	5.9355503
21 N	1.9666586 *	4.3295773	3.7998129	2.4486608 *
22 H	6.5046507	1.1035563 *	2.1767326 *	3.4375350
23 H	6.2319008	2.1931703 *	1.1052436 *	2.2039053 *
24 H	4.4121408	3.4259074	2.1919649 *	1.1069926 *
25 H	6.5310372	2.6417234 *	4.0399632	4.8482732
26 H	6.3001143	4.6439710	5.9161792	6.2397052
27 H	4.5473628	5.3836652	6.2851365	6.0296083
28 H	3.8632468	6.4588376	7.0485338	6.4139663
29 H	4.6124495	9.9774120	9.7912910	8.5120959
30 H	6.4261537	11.4794884	11.5367945	10.3791035
31 H	6.6759909	10.9580595	11.3188062	10.3841226
32 H	5.2935914	8.7367630	9.2675415	8.5150427
33 H	2.6556771 *	8.0662067	7.7492952	6.4388696
34 H	2.5005445 *	4.7766564	4.2456247	2.9353284 *
35 H	2.5771249 *	4.6839178	3.8784636	2.4579573 *

C C C C

1 CO	2.8598142 *	3.1477013	4.5841294	5.4784147
2 C	2.8287104 *	2.5482487 *	1.4425692 *	2.4615616 *
3 C	2.4808689 *	2.9531892 *	2.4799985 *	3.7612505
4 C	1.4097803 *	2.5186240 *	2.8253630 *	4.2635616
5 C	0.0000000	1.4579735 *	2.4568544 *	3.8014176
6 C	1.4579735 *	0.0000000	1.4723473 *	2.5325468 *
7 C	2.4568544 *	1.4723473 *	0.0000000	1.4400629 *
8 C	3.8014176	2.5325468 *	1.4400629 *	0.0000000
9 C	4.3670908	2.9189867 *	2.4744875 *	1.4014577 *
10 C	3.8983217	2.5030042 *	2.8416958 *	2.4409976 *

11 C	2.6540907 *	1.4757786 *	2.5068691 *	2.8696940 *
12 N	3.1613083	2.5586459 *	3.8655383	4.3316696
13 C	4.4642873	3.7861399	4.9739503	5.1781784
14 C	5.5059380	5.0779837	6.3601539	6.6380265
15 C	5.6614752	5.5908658	6.9963141	7.5117855
16 C	6.9795909	6.9837740	8.3971440	8.9049729
17 C	8.0461420	7.8570133	9.2014732	9.5262504
18 C	7.9895992	7.5497452	8.7784820	8.9002489
19 C	6.8420488	6.2667225	7.4359475	7.5014226
20 O	4.7271287	4.9674859	6.4220608	7.1759278
21 N	1.5084886 *	2.6082749 *	3.8853156	5.1281763
22 H	3.9319245	3.5285251	2.1899375 *	2.6393217 *
23 H	3.4757825	4.0581637	3.4916509	4.6541529
24 H	2.1772718 *	3.5097323	3.9322418	5.3703206
25 H	4.6476181	3.5199363	2.1907650 *	1.1050877 *
26 H	5.4700896	4.0222392	3.4788658	2.1830691 *
27 H	4.8319138	3.5122710	3.9446375	3.4200058
28 H	5.0419022	4.1096707	5.0628293	4.9751217
29 H	7.3268506	7.5315577	8.9819863	9.6188276
30 H	9.0677444	8.9367071	10.2948877	10.6336968
31 H	8.9844595	8.4552808	9.6171014	9.6193480
32 H	7.1119352	6.3324819	7.3441056	7.2039855
33 H	5.3493967	5.7704963	7.2255290	8.0593079
34 H	2.1106878 *	3.0836219	4.3296889	5.5245811
35 H	2.0708477 *	3.3946396	4.5099896	5.8427600

C C C N

1 CO	5.3278919	4.1731305	2.8884759 *	1.9244499 *
2 C	3.7606837	4.2822543	3.8532578	5.0989147
3 C	4.9497635	5.1936486	4.4223137	5.4005879
4 C	5.1705022	5.0125187	3.9233806	4.5662675
5 C	4.3670908	3.8983217	2.6540907 *	3.1613083
6 C	2.9189867 *	2.5030042 *	1.4757786 *	2.5586459 *
7 C	2.4744875 *	2.8416958 *	2.5068691 *	3.8655383
8 C	1.4014577 *	2.4409976 *	2.8696940 *	4.3316696
9 C	0.0000000	1.4294105 *	2.4914619 *	3.8124380
10 C	1.4294105 *	0.0000000	1.4138109 *	2.4801081 *
11 C	2.4914619 *	1.4138109 *	0.0000000	1.4655118 *
12 N	3.8124380	2.4801081 *	1.4655118 *	0.0000000
13 C	4.3510482	2.9248937 *	2.4718297 *	1.3380049 *
14 C	5.8031336	4.3755672	3.8747952	2.5294053 *
15 C	6.8581257	5.4404561	4.6505553	3.1866450
16 C	8.2080261	6.7819220	6.0469569	4.5860249
17 C	8.6594206	7.2383430	6.7436895	5.3410019
18 C	7.8897089	6.5117732	6.2753080	5.0101057

19	C	6.4780760	5.1053140	4.9365739	3.7652937
20	O	6.7777350	5.4443190	4.3692129	2.9892958 *
21	N	5.4357939	4.6299820	3.2245117	3.0132601
22	H	4.0396027	4.8636535	4.6965399	6.0329860
23	H	5.9250154	6.2677301	5.5273570	6.4851335
24	H	6.2569985	6.0111488	4.8258177	5.2424059
25	H	2.1830546 *	3.4520186	3.9744862	5.4358358
26	H	1.1034268 *	2.1996879 *	3.4813944	4.6788696
27	H	2.1662615 *	1.1047859 *	2.1937890 *	2.7067468 *
28	H	3.9364821	2.5904692 *	2.6763155 *	2.0950061 *
29	H	9.0306719	7.6196897	6.7528890	5.2927451
30	H	9.7620185	8.3428057	7.8459468	6.4349645
31	H	8.5188318	7.1954865	7.1212215	5.9428236
32	H	6.0540102	4.7796803	4.9129386	3.9993107
33	H	7.7242929	6.4115154	5.2973263	3.9559935
34	H	5.7835519	4.9477582	3.5823061	3.2891062
35	H	6.2836089	5.5580216	4.1660368	3.9548089

C C C C

1	CO	2.8418081 *	3.2559631	3.0108472	4.2856985
2	C	6.2907214	7.6208226	8.1118399	9.4961019
3	C	6.6842489	7.8723790	8.1258572	9.4558710
4	C	5.8718893	6.9036332	6.9803331	8.2581450
5	C	4.4642873	5.5059380	5.6614752	6.9795909
6	C	3.7861399	5.0779837	5.5908658	6.9837740
7	C	4.9739503	6.3601539	6.9963141	8.3971440
8	C	5.1781784	6.6380265	7.5117855	8.9049729
9	C	4.3510482	5.8031336	6.8581257	8.2080261
10	C	2.9248937 *	4.3755672	5.4404561	6.7819220
11	C	2.4718297 *	3.8747952	4.6505553	6.0469569
12	N	1.3380049 *	2.5294053 *	3.1866450	4.5860249
13	C	0.0000000	1.4714932 *	2.6142293 *	3.8938669
14	C	1.4714932 *	0.0000000	1.4401164 *	2.5086702 *
15	C	2.6142293 *	1.4401164 *	0.0000000	1.4058803 *
16	C	3.8938669	2.5086702 *	1.4058803 *	0.0000000
17	C	4.3543896	2.8882913 *	2.4343079 *	1.4253231 *
18	C	3.8045990	2.5006688 *	2.8157281 *	2.4713396 *
19	C	2.4828436 *	1.4458091 *	2.4416491 *	2.8480073 *
20	O	3.0631699	2.5054573 *	1.4627122 *	2.4464485 *
21	N	4.1812625	4.8674518	4.6858460	5.8874703
22	H	7.1634477	8.5420185	9.1151927	10.5093128
23	H	7.7760497	8.9379966	9.1286450	10.4335367
24	H	6.5260680	7.4006105	7.2752779	8.4596976
25	H	6.2630353	7.7259373	8.6148665	10.0076515
26	H	4.9970923	6.3958170	7.5644883	8.8643986

27 H	2.6275835 *	3.9510581	5.1882483	6.4359288
28 H	1.1052971 *	2.1690129 *	3.5272436	4.6678309
29 H	4.7939907	3.5035899	2.1884089 *	1.1050118 *
30 H	5.4610169	3.9957043	3.4344854	2.1878085 *
31 H	4.6723777	3.4976139	3.9194220	3.4709177
32 H	2.6660734 *	2.2071539 *	3.4536626	3.9552181
33 H	4.0435966	3.3373838	2.0432390 *	2.4829633 *
34 H	4.2774392	4.8817508	4.6940290	5.8136305
35 H	5.1120216	5.6733744	5.2937402	6.3891926

C C C O

1 CO	5.4438587	5.6095444	4.6977437	1.9515954 *
2 C	10.4033276	10.0802452	8.7698243	7.3620297
3 C	10.5026825	10.3649983	9.1426915	7.1778829
4 C	9.3814649	9.3801832	8.2487095	5.9355503
5 C	8.0461420	7.9895992	6.8420488	4.7271287
6 C	7.8570133	7.5497452	6.2667225	4.9674859
7 C	9.2014732	8.7784820	7.4359475	6.4220608
8 C	9.5262504	8.9002489	7.5014226	7.1759278
9 C	8.6594206	7.8897089	6.4780760	6.7777350
10 C	7.2383430	6.5117732	5.1053140	5.4443190
11 C	6.7436895	6.2753080	4.9365739	4.3692129
12 N	5.3410019	5.0101057	3.7652937	2.9892958 *
13 C	4.3543896	3.8045990	2.4828436 *	3.0631699
14 C	2.8882913 *	2.5006688 *	1.4458091 *	2.5054573 *
15 C	2.4343079 *	2.8157281 *	2.4416491 *	1.4627122 *
16 C	1.4253231 *	2.4713396 *	2.8480073 *	2.4464485 *
17 C	0.0000000	1.4249076 *	2.4578486 *	3.7533800
18 C	1.4249076 *	0.0000000	1.4155705 *	4.2750889
19 C	2.4578486 *	1.4155705 *	0.0000000	3.7910548
20 O	3.7533800	4.2750889	3.7910548	0.0000000
21 N	7.0770419	7.2478680	6.2790571	3.5764288
22 H	11.3666615	10.9677740	9.6239474	8.4163509
23 H	11.5215341	11.4301062	10.2258101	8.1135255
24 H	9.6735768	9.8244123	8.7919833	6.0985826
25 H	10.6133402	9.9530907	8.5473804	8.2639319
26 H	9.1727471	8.2700658	6.8700757	7.6306196
27 H	6.6946877	5.8138155	4.4122483	5.4723155
28 H	4.8496350	3.9994794	2.5863098 *	4.1490967
29 H	2.2036097 *	3.4757221	3.9523706	2.6624820 *
30 H	1.1078541 *	2.2081304 *	3.4665583	4.6309214
31 H	2.1963594 *	1.1044256 *	2.1895674 *	5.3773144
32 H	3.4562878	2.1814157 *	1.1078110 *	4.7002871
33 H	3.8983479	4.7058261	4.4811386	0.9926882 *
34 H	6.9637796	7.1512952	6.2291340	3.7195244

35 H 7.6712702 7.9840761 7.1074220 4.0144848

N H H H

1 CO	1.9666586 *	6.5046507	6.2319008	4.4121408
2 C	4.3295773	1.1035563 *	2.1931703 *	3.4259074
3 C	3.7998129	2.1767326 *	1.1052436 *	2.1919649 *
4 C	2.4486608 *	3.4375350	2.2039053 *	1.1069926 *
5 C	1.5084886 *	3.9319245	3.4757825	2.1772718 *
6 C	2.6082749 *	3.5285251	4.0581637	3.5097323
7 C	3.8853156	2.1899375 *	3.4916509	3.9322418
8 C	5.1281763	2.6393217 *	4.6541529	5.3703206
9 C	5.4357939	4.0396027	5.9250154	6.2569985
10 C	4.6299820	4.8636535	6.2677301	6.0111488
11 C	3.2245117	4.6965399	5.5273570	4.8258177
12 N	3.0132601	6.0329860	6.4851335	5.2424059
13 C	4.1812625	7.1634477	7.7760497	6.5260680
14 C	4.8674518	8.5420185	8.9379966	7.4006105
15 C	4.6858460	9.1151927	9.1286450	7.2752779
16 C	5.8874703	10.5093128	10.4335367	8.4596976
17 C	7.0770419	11.3666615	11.5215341	9.6735768
18 C	7.2478680	10.9677740	11.4301062	9.8244123
19 C	6.2790571	9.6239474	10.2258101	8.7919833
20 O	3.5764288	8.4163509	8.1135255	6.0985826
21 N	0.0000000	5.4329989	4.6519721	2.5991057 *
22 H	5.4329989	0.0000000	2.5405315 *	4.3524095
23 H	4.6519721	2.5405315 *	0.0000000	2.5221215 *
24 H	2.5991057 *	4.3524095	2.5221215 *	0.0000000
25 H	6.0589536	2.3370691 *	4.7393409	5.9328385
26 H	6.5229526	4.7271865	6.8354786	7.3340291
27 H	5.3518010	5.9337650	7.3644765	6.9875201
28 H	5.0015593	7.2178259	8.1513145	7.1760295
29 H	6.0859235	11.0266105	10.7095486	8.5741118
30 H	8.0286410	12.4538265	12.5394804	10.6137467
31 H	8.3037118	11.8028536	12.3961530	10.8662962
32 H	6.7632476	9.5025053	10.3671200	9.1672258
33 H	4.0582254	9.1391685	8.6178543	6.4474614
34 H	1.0421964 *	5.8586174	5.0557067	2.9888984 *
35 H	1.0390102 *	5.7649156	4.5454846	2.1866743 *

H H H H

1 CO	6.5310372	6.3001143	4.5473628	3.8632468
2 C	2.6417234 *	4.6439710	5.3836652	6.4588376
3 C	4.0399632	5.9161792	6.2851365	7.0485338
4 C	4.8482732	6.2397052	6.0296083	6.4139663

5 C	4.6476181	5.4700896	4.8319138	5.0419022
6 C	3.5199363	4.0222392	3.5122710	4.1096707
7 C	2.1907650 *	3.4788658	3.9446375	5.0628293
8 C	1.1050877 *	2.1830691 *	3.4200058	4.9751217
9 C	2.1830546 *	1.1034268 *	2.1662615 *	3.9364821
10 C	3.4520186	2.1996879 *	1.1047859 *	2.5904692 *
11 C	3.9744862	3.4813944	2.1937890 *	2.6763155 *
12 N	5.4358358	4.6788696	2.7067468 *	2.0950061 *
13 C	6.2630353	4.9970923	2.6275835 *	1.1052971 *
14 C	7.7259373	6.3958170	3.9510581	2.1690129 *
15 C	8.6148665	7.5644883	5.1882483	3.5272436
16 C	10.0076515	8.8643986	6.4359288	4.6678309
17 C	10.6133402	9.1727471	6.6946877	4.8496350
18 C	9.9530907	8.2700658	5.8138155	3.9994794
19 C	8.5473804	6.8700757	4.4122483	2.5863098 *
20 O	8.2639319	7.6306196	5.4723155	4.1490967
21 N	6.0589536	6.5229526	5.3518010	5.0015593
22 H	2.3370691 *	4.7271865	5.9337650	7.2178259
23 H	4.7393409	6.8354786	7.3644765	8.1513145
24 H	5.9328385	7.3340291	6.9875201	7.1760295
25 H	0.0000000	2.5304924 *	4.3372772	6.0013249
26 H	2.5304924 *	0.0000000	2.4815531 *	4.3912489
27 H	4.3372772	2.4815531 *	0.0000000	1.9888992 *
28 H	6.0013249	4.3912489	1.9888992 *	0.0000000
29 H	10.7215035	9.7519395	7.3691869	5.6534717
30 H	11.7210028	10.2584562	7.7795078	5.9307739
31 H	10.6391528	8.7815131	6.3893882	4.6661778
32 H	8.1933514	6.2910422	3.9315113	2.2893524 *
33 H	9.1348813	8.5942321	6.4554198	5.1194994
34 H	6.4550749	6.8497826	5.6206772	5.0446261
35 H	6.6960200	7.3795938	6.3042641	5.9841148

H H H H

1 CO	4.6124495	6.4261537	6.6759909	5.2935914
2 C	9.9774120	11.4794884	10.9580595	8.7367630
3 C	9.7912910	11.5367945	11.3188062	9.2675415
4 C	8.5120959	10.3791035	10.3841226	8.5150427
5 C	7.3268506	9.0677444	8.9844595	7.1119352
6 C	7.5315577	8.9367071	8.4552808	6.3324819
7 C	8.9819863	10.2948877	9.6171014	7.3441056
8 C	9.6188276	10.6336968	9.6193480	7.2039855
9 C	9.0306719	9.7620185	8.5188318	6.0540102
10 C	7.6196897	8.3428057	7.1954865	4.7796803
11 C	6.7528890	7.8459468	7.1212215	4.9129386
12 N	5.2927451	6.4349645	5.9428236	3.9993107

13 C	4.7939907	5.4610169	4.6723777	2.6660734 *
14 C	3.5035899	3.9957043	3.4976139	2.2071539 *
15 C	2.1884089 *	3.4344854	3.9194220	3.4536626
16 C	1.1050118 *	2.1878085 *	3.4709177	3.9552181
17 C	2.2036097 *	1.1078541 *	2.1963594 *	3.4562878
18 C	3.4757221	2.2081304 *	1.1044256 *	2.1814157 *
19 C	3.9523706	3.4665583	2.1895674 *	1.1078110 *
20 O	2.6624820 *	4.6309214	5.3773144	4.7002871
21 N	6.0859235	8.0286410	8.3037118	6.7632476
22 H	11.0266105	12.4538265	11.8028536	9.5025053
23 H	10.7095486	12.5394804	12.3961530	10.3671200
24 H	8.5741118	10.6137467	10.8662962	9.1672258
25 H	10.7215035	11.7210028	10.6391528	8.1933514
26 H	9.7519395	10.2584562	8.7815131	6.2910422
27 H	7.3691869	7.7795078	6.3893882	3.9315113
28 H	5.6534717	5.9307739	4.6661778	2.2893524 *
29 H	0.0000000	2.5237287 *	4.3880748	5.0591331
30 H	2.5237287 *	0.0000000	2.5453886 *	4.3755182
31 H	4.3880748	2.5453886 *	0.0000000	2.5104176 *
32 H	5.0591331	4.3755182	2.5104176 *	0.0000000
33 H	2.2660583 *	4.5934973	5.7867473	5.4728187
34 H	5.9997729	7.8830585	8.1901052	6.7171939
35 H	6.4261375	8.5619236	9.0644290	7.6664540

H H H

1 CO	2.6556771 *	2.5005445 *	2.5771249 *
2 C	8.0662067	4.7766564	4.6839178
3 C	7.7492952	4.2456247	3.8784636
4 C	6.4388696	2.9353284 *	2.4579573 *
5 C	5.3493967	2.1106878 *	2.0708477 *
6 C	5.7704963	3.0836219	3.3946396
7 C	7.2255290	4.3296889	4.5099896
8 C	8.0593079	5.5245811	5.8427600
9 C	7.7242929	5.7835519	6.2836089
10 C	6.4115154	4.9477582	5.5580216
11 C	5.2973263	3.5823061	4.1660368
12 N	3.9559935	3.2891062	3.9548089
13 C	4.0435966	4.2774392	5.1120216
14 C	3.3373838	4.8817508	5.6733744
15 C	2.0432390 *	4.6940290	5.2937402
16 C	2.4829633 *	5.8136305	6.3891926
17 C	3.8983479	6.9637796	7.6712702
18 C	4.7058261	7.1512952	7.9840761
19 C	4.4811386	6.2291340	7.1074220
20 O	0.9926882 *	3.7195244	4.0144848

21 N	4.0582254	1.0421964 *	1.0390102 *
22 H	9.1391685	5.8586174	5.7649156
23 H	8.6178543	5.0557067	4.5454846
24 H	6.4474614	2.9888984 *	2.1866743 *
25 H	9.1348813	6.4550749	6.6960200
26 H	8.5942321	6.8497826	7.3795938
27 H	6.4554198	5.6206772	6.3042641
28 H	5.1194994	5.0446261	5.9841148
29 H	2.2660583 *	5.9997729	6.4261375
30 H	4.5934973	7.8830585	8.5619236
31 H	5.7867473	8.1901052	9.0644290
32 H	5.4728187	6.7171939	7.6664540
33 H	0.0000000	4.1805182	4.2775805
34 H	4.1805182	0.0000000	1.6627812 *
35 H	4.2775805	1.6627812 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.76, TOTAL = 2308.4 SECONDS (38.5 MIN)
WALL CLOCK TIME: STEP = 0.77, TOTAL = 2133.5 SECONDS (35.6 MIN)
CPU UTILIZATION: STEP = 99.10%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.98, TOTAL = 2309.4 SECONDS (38.5 MIN)
WALL CLOCK TIME: STEP = 0.97, TOTAL = 2134.5 SECONDS (35.6 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.630868138	-284.630868138	0.030225241	0.001631758	196113285
11501299						
2	1	-284.630983755	-0.000115617	0.005057714	0.000259505	162408891
14298161						
3	2	-284.630975410	0.000008345	0.007936073	0.000554498	152182934
15142622						

4 3	-284.630991695	-0.000016285	0.001292748	0.000197888	148732278
15432361					
5 4	-284.630990179	0.000001516	0.001415144	0.000346973	139178590
16213775					
6 5	-284.630992386	-0.000002207	0.000464166	0.000043136	135842829
16484909					
7 6	-284.630992298	0.000000088	0.000246243	0.000037786	126169486
17213763					
8 7	-284.630992478	-0.000000180	0.000221102	0.000032831	143611394
15878232					
9 8	-284.630992520	-0.000000042	0.000662837	0.000026260	135724601
16592296					
10 9	-284.630992602	-0.000000081	0.000363829	0.000021601	162319846
14568774					
11 10	-284.630992638	-0.000000036	0.000250575	0.000022080	160713812
14620848					
12 11	-284.630992656	-0.000000019	0.000108892	0.000018870	160428737
14637119					
13 12	-284.630992673	-0.000000017	0.000216468	0.000015099	154604064
15072348					

-----DISABLING FDIFF OPTION-----

14 13	-284.630992701	-0.000000028	0.000327837	0.000012313	196112848
11501271					
15 14	-284.630992724	-0.000000023	0.000530548	0.000013213	196112694
11501277					
16 15	-284.630992738	-0.000000013	0.000093750	0.000013649	196112532
11501278					
17 16	-284.630992746	-0.000000008	0.000070440	0.000011042	196112633
11501280					
18 17	-284.630992750	-0.000000004	0.000094532	0.000007381	196112655
11501276					
19 18	-284.630992754	-0.000000004	0.000119931	0.000003704	196112636
11501282					
20 19	-284.630992756	-0.000000001	0.000033414	0.000004888	196112731
11501272					
21 20	-284.630992756	-0.000000001	0.000025703	0.000004715	196112681
11501275					
22 21	-284.630992757	-0.000000001	0.000044618	0.000003989	196112664
11501280					
23 22	-284.630992758	-0.000000001	0.000085944	0.000002896	196112680
11501276					
24 23	-284.630992759	-0.000000001	0.000036613	0.000002124	196112723
11501274					
25 24	-284.630992759	0.000000000	0.000011427	0.000001068	196112723
11501274					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 83.5 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 26.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 3.9 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6309927594 AFTER 25 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5997960317
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000638003

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 88.36 , TOTAL = 2397.8 SECONDS (40.0 MIN)
WALL CLOCK TIME: STEP = 80.95 , TOTAL = 2215.4 SECONDS (36.9
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.79 , TOTAL = 2401.6 SECONDS (40.0 MIN)
WALL CLOCK TIME: STEP = 3.77 , TOTAL = 2219.2 SECONDS (37.0
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.90 , TOTAL = 2404.5 SECONDS (40.1 MIN)
WALL CLOCK TIME: STEP = 2.72 , TOTAL = 2221.9 SECONDS (37.0
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 19 ENERGY= -284.6309928

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0004427	0.0008140	-0.0003253
2 C	6.0	-0.0013706	0.0010105	0.0000478
3 C	6.0	0.0011386	0.0007185	0.0000118
4 C	6.0	0.0003356	-0.0011778	-0.0004516
5 C	6.0	-0.0014608	-0.0002463	-0.0006300
6 C	6.0	-0.0007850	0.0010763	-0.0001602
7 C	6.0	0.0016133	-0.0005785	-0.0005616
8 C	6.0	0.0013198	-0.0024384	-0.0006688
9 C	6.0	-0.0010829	0.0016657	0.0001657
10 C	6.0	0.0009531	-0.0027988	-0.0010072
11 C	6.0	0.0006640	0.0011747	-0.0001074
12 N	7.0	0.0012711	0.0002419	0.0000806
13 C	6.0	-0.0024862	0.0009632	-0.0001872
14 C	6.0	-0.0016696	0.0018790	0.0001746
15 C	6.0	-0.0015079	-0.0003056	-0.0000814
16 C	6.0	-0.0010144	-0.0024549	-0.0007332
17 C	6.0	0.0028735	0.0006130	0.0002566
18 C	6.0	0.0003204	0.0011860	0.0011217
19 C	6.0	-0.0006837	-0.0014239	0.0007116
20 O	8.0	0.0007172	0.0007693	-0.0000992
21 N	7.0	0.0009389	0.0010202	0.0001782
22 H	1.0	-0.0007214	-0.0006270	0.0002269
23 H	1.0	0.0007452	-0.0007415	-0.0000229
24 H	1.0	-0.0004041	0.0006380	0.0001390
25 H	1.0	0.0005077	-0.0005836	0.0004737
26 H	1.0	0.0006730	-0.0003948	0.0001104
27 H	1.0	-0.0005042	0.0011606	-0.0001501
28 H	1.0	0.0009638	-0.0010487	0.0003120
29 H	1.0	0.0011914	0.0010602	-0.0017086
30 H	1.0	-0.0011865	-0.0015850	-0.0006784
31 H	1.0	-0.0005162	-0.0002819	0.0013124
32 H	1.0	-0.0008936	0.0012515	-0.0007352
33 H	1.0	-0.0003043	-0.0012299	0.0001781
34 H	1.0	0.0004183	-0.0010116	0.0017932
35 H	1.0	0.0003891	0.0016856	0.0010141

MAXIMUM GRADIENT = 0.0028735 RMS GRADIENT = 0.0010426
HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0001801917
PREDICTED ENERGY CHANGE WAS -0.0001600999 RATIO= 1.125
GDIIS STEP HAS LENGTH = 0.061798
RADIUS OF STEP TAKEN= 0.05261 CURRENT TRUST RADIUS= 0.05261

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 2404.5 SECONDS (40.1 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2222.0 SECONDS (37.0 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

INSERCH= 20

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1110359722	-1.6620993612	1.0403452207
C	6.0	4.9995251989	0.6654692793	0.4265556253
C	6.0	5.2209656151	-0.6937722640	0.1829400782
C	6.0	4.0824321257	-1.5491141882	0.0541769203
C	6.0	2.7690926850	-1.0607495159	0.1771814110
C	6.0	2.4706327870	0.3383533166	0.4595123340
C	6.0	3.6616295363	1.1978972670	0.5629888410
C	6.0	3.5344112571	2.6126040765	0.8189327069
C	6.0	2.2790174717	3.2071362047	0.9798793775
C	6.0	1.1074963411	2.3945534788	0.9147902393
C	6.0	1.1662018139	1.0034513223	0.6564067877
N	7.0	-0.0732371576	0.2235064474	0.6851424340
C	6.0	-1.2871534275	0.7620004551	0.5366839693
C	6.0	-2.5958540864	0.0881309497	0.5912022238
C	6.0	-2.8607284327	-1.3228381894	0.6948485607
C	6.0	-4.1498631999	-1.8789172405	0.6131426379
C	6.0	-5.2733148337	-1.0063419431	0.5169187429
C	6.0	-5.0808195530	0.4046317394	0.4954508993
C	6.0	-3.7669895394	0.9341277185	0.4944928388
O	8.0	-1.7493260675	-2.2437044057	0.9071033585
N	7.0	1.7006130912	-2.1053625527	-0.0308033569
H	1.0	5.8448052296	1.3659463865	0.5252378303
H	1.0	6.2441619839	-1.1045260570	0.0842724675
H	1.0	4.2432039680	-2.6225377315	-0.1633846190
H	1.0	4.4593750128	3.2097396315	0.9002403346
H	1.0	2.1855695015	4.2874404590	1.1896276397
H	1.0	0.1387805152	2.8841083997	1.1116516289
H	1.0	-1.3555736128	1.8429666484	0.3138015853
H	1.0	-4.2909265755	-2.9750429386	0.6146495305

H	1.0	-6.2871410518	-1.4394942588	0.4545074912
H	1.0	-5.9536796675	1.0814422262	0.4630767112
H	1.0	-3.6285718993	2.0276058456	0.4139664813
H	1.0	-2.0716030873	-3.1746806434	1.0222212955
H	1.0	1.4221907217	-2.1397095299	-1.0346047646
H	1.0	2.1196383642	-3.0311160325	0.1897315372

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4490036	5.2710703	4.0935658
2 C	5.4490036	0.0000000	1.3985428 *	2.4257175 *
3 C	5.2710703	1.3985428 *	0.0000000	1.4298420 *
4 C	4.0935658	2.4257175 *	1.4298420 *	0.0000000
5 C	2.8586603 *	2.8314039 *	2.4791907 *	1.4065883 *
6 C	3.1475188	2.5501741 *	2.9506111 *	2.5149011 *
7 C	4.5841209	1.4463950 *	2.4808022 *	2.8252498 *
8 C	5.4810228	2.4681679 *	3.7657770	4.2667408
9 C	5.3304085	3.7639607	4.9504806	5.1702173
10 C	4.1791302	4.2867230	5.1955741	5.0143208
11 C	2.8923942 *	3.8550527	4.4210687	3.9220748
12 N	1.9275982 *	5.0985406	5.3964980	4.5617857
13 C	2.8433903 *	6.2883841	6.6783248	5.8657065
14 C	3.2545798	7.6190691	7.8664300	6.8969903
15 C	3.0109550	8.1122706	8.1222874	6.9763271
16 C	4.2877469	9.4984223	9.4552671	8.2578386
17 C	5.4493327	10.4083793	10.5042450	9.3828958
18 C	5.6145927	10.0839542	10.3648894	9.3796070
19 C	4.6986628	8.7708935	9.1395001	8.2446218
20 O	1.9537054 *	7.3648633	7.1771630	5.9345887
21 N	1.9673833 *	4.3323790	3.7988360	2.4473855 *
22 H	6.5046527	1.1022271 *	2.1791706 *	3.4388131
23 H	6.2321904	2.1906990 *	1.1069710 *	2.2071793 *
24 H	4.4097868	3.4250608	2.1899988 *	1.1069863 *
25 H	6.5316535	2.6437570 *	4.0412801	4.8481542
26 H	6.3026184	4.6496560	5.9194197	6.2412103
27 H	4.5468516	5.3868873	6.2842932	6.0269481
28 H	3.8683714	6.4642474	7.0500381	6.4144777
29 H	4.6132756	9.9800402	9.7911522	8.5123756
30 H	6.4287968	11.4813104	11.5354397	10.3778769
31 H	6.6813947	10.9611616	11.3182402	10.3831867
32 H	5.2906466	8.7349662	9.2614030	8.5077587
33 H	2.6555873 *	8.0686073	7.7486036	6.4383015
34 H	2.5005311 *	4.7750748	4.2430933	2.9344732 *

35 H 2.5753124 * 4.6919694 3.8834846 2.4631817 *

C C C C

1 CO 2.8586603 * 3.1475188 4.5841209 5.4810228
2 C 2.8314039 * 2.5501741 * 1.4463950 * 2.4681679 *
3 C 2.4791907 * 2.9506111 * 2.4808022 * 3.7657770
4 C 1.4065883 * 2.5149011 * 2.8252498 * 4.2667408
5 C 0.0000000 1.4581762 * 2.4590557 * 3.8067156
6 C 1.4581762 * 0.0000000 1.4724118 * 2.5363407 *
7 C 2.4590557 * 1.4724118 * 0.0000000 1.4432904 *
8 C 3.8067156 2.5363407 * 1.4432904 * 0.0000000
9 C 4.3702799 2.9218853 * 2.4743595 * 1.3983511 *
10 C 3.9043678 2.5086606 * 2.8424192 * 2.4385756 *
11 C 2.6570362 * 1.4773838 * 2.5047346 * 2.8677872 *
12 N 3.1600913 2.5564376 * 3.8618115 4.3290662
13 C 4.4614787 3.7823788 4.9680128 5.1722224
14 C 5.5021808 5.0743712 6.3551930 6.6336249
15 C 5.6596427 5.5891281 6.9937578 7.5100542
16 C 6.9807887 6.9836135 8.3957562 8.9030437
17 C 8.0497640 7.8600398 9.2029356 9.5270154
18 C 7.9918558 7.5518287 8.7786245 8.8995497
19 C 6.8410959 6.2661075 7.4336160 7.4988664
20 O 4.7273964 4.9674352 6.4219528 7.1770040
21 N 1.5086824 * 2.6086562 * 3.8871198 5.1326481
22 H 3.9331926 3.5277907 2.1899593 * 2.6416533 *
23 H 3.4765867 4.0573672 3.4928207 4.6582755
24 H 2.1744360 * 3.5066915 3.9321204 5.3734574
25 H 4.6494028 3.5205392 2.1903530 * 1.1039655 *
26 H 5.4743660 4.0261171 3.4809060 2.1821700 *
27 H 4.8325646 3.5133587 3.9439579 3.4190214
28 H 5.0460980 4.1139942 5.0646358 4.9758870
29 H 7.3280127 7.5313576 8.9810494 9.6176631
30 H 9.0683916 8.9364070 10.2929898 10.6308606
31 H 8.9865165 8.4570228 9.6165334 9.6174300
32 H 7.1080319 6.3289767 7.3387779 7.1982323
33 H 5.3493114 5.7697449 7.2249767 8.0598627
34 H 2.1087260 * 3.0777284 4.3251602 5.5210109
35 H 2.0746789 * 3.3984265 4.5168143 5.8522691

C C C N

1 CO 5.3304085 4.1791302 2.8923942 * 1.9275982 *
2 C 3.7639607 4.2867230 3.8550527 5.0985406
3 C 4.9504806 5.1955741 4.4210687 5.3964980
4 C 5.1702173 5.0143208 3.9220748 4.5617857

5 C	4.3702799	3.9043678	2.6570362 *	3.1600913
6 C	2.9218853 *	2.5086606 *	1.4773838 *	2.5564376 *
7 C	2.4743595 *	2.8424192 *	2.5047346 *	3.8618115
8 C	1.3983511 *	2.4385756 *	2.8677872 *	4.3290662
9 C	0.0000000	1.4272313 *	2.4898233 *	3.8107766
10 C	1.4272313 *	0.0000000	1.4161121 *	2.4819982 *
11 C	2.4898233 *	1.4161121 *	0.0000000	1.4647009 *
12 N	3.8107766	2.4819982 *	1.4647009 *	0.0000000
13 C	4.3465717	2.9227626 *	2.4681135 *	1.3362666 *
14 C	5.8003135	4.3748255	3.8723543	2.5279928 *
15 C	6.8570328	5.4418915	4.6507277	3.1876925
16 C	8.2056652	6.7818414	6.0473521	4.5874011
17 C	8.6605689	7.2414876	6.7473032	5.3461794
18 C	7.8902410	6.5138996	6.2777199	5.0144462
19 C	6.4773736	5.1058893	4.9363346	3.7663160
20 O	6.7782381	5.4474700	4.3711751	2.9909313 *
21 N	5.4386280	4.6362894	3.2284016	3.0137608
22 H	4.0387524	4.8633198	4.6944582	6.0294249
23 H	5.9257838	6.2704586	5.5278012	6.4833824
24 H	6.2570104	6.0138447	4.8257431	5.2394303
25 H	2.1818130 *	3.4496131	3.9714170	5.4321661
26 H	1.1044384 *	2.1956317 *	3.4796580	4.6767801
27 H	2.1684845 *	1.1030996 *	2.1908248 *	2.7028992 *
28 H	3.9388920	2.5946385 *	2.6798350 *	2.0987930 *
29 H	9.0286708	7.6200801	6.7535480	5.2938258
30 H	9.7594191	8.3422086	7.8460861	6.4367201
31 H	8.5183896	7.1964236	7.1229328	5.9468455
32 H	6.0507158	4.7765906	4.9089230	3.9960876
33 H	7.7238124	6.4136248	5.2984892	3.9566102
34 H	5.7776343	4.9455752	3.5783391	3.2830816
35 H	6.2901134	5.5666894	4.1718774	3.9555913

C C C C

1 CO	2.8433903 *	3.2545798	3.0109550	4.2877469
2 C	6.2883841	7.6190691	8.1122706	9.4984223
3 C	6.6783248	7.8664300	8.1222874	9.4552671
4 C	5.8657065	6.8969903	6.9763271	8.2578386
5 C	4.4614787	5.5021808	5.6596427	6.9807887
6 C	3.7823788	5.0743712	5.5891281	6.9836135
7 C	4.9680128	6.3551930	6.9937578	8.3957562
8 C	5.1722224	6.6336249	7.5100542	8.9030437
9 C	4.3465717	5.8003135	6.8570328	8.2056652
10 C	2.9227626 *	4.3748255	5.4418915	6.7818414
11 C	2.4681135 *	3.8723543	4.6507277	6.0473521
12 N	1.3362666 *	2.5279928 *	3.1876925	4.5874011

13 C	0.0000000	1.4730138 *	2.6168123 *	3.8955615
14 C	1.4730138 *	0.0000000	1.4393522 *	2.5069312 *
15 C	2.6168123 *	1.4393522 *	0.0000000	1.4063315 *
16 C	3.8955615	2.5069312 *	1.4063315 *	0.0000000
17 C	4.3608380	2.8934728 *	2.4397545 *	1.4257595 *
18 C	3.8106844	2.5068694 *	2.8200561 *	2.4688311 *
19 C	2.4861607 *	1.4479715 *	2.4403579 *	2.8414595 *
20 O	3.0635071	2.5007717 *	1.4588564 *	2.4458252 *
21 N	4.1797800	4.8639423	4.6845226	5.8901627
22 H	7.1574937	8.5370893	9.1128836	10.5085805
23 H	7.7723426	8.9345001	9.1279512	10.4362419
24 H	6.5215066	7.3952580	7.2726638	8.4616513
25 H	6.2566916	7.7211530	8.6122217	10.0047907
26 H	4.9914795	6.3917388	7.5620867	8.8596845
27 H	2.6205376 *	3.9454510	5.1835488	6.4286382
28 H	1.1058236 *	2.1667245 *	3.5260471	4.6636980
29 H	4.7952294	3.5009791	2.1867051 *	1.1051664 *
30 H	5.4638089	3.9972395	3.4368119	2.1877418 *
31 H	4.6780261	3.5040086	3.9243636	3.4698706
32 H	2.6644056 *	2.2044232 *	3.4487612	3.9461802
33 H	4.0433360	3.3326500	2.0394147 *	2.4830452 *
34 H	4.2695919	4.8735209	4.6905953	5.8164310
35 H	5.1102191	5.6680464	5.2893676	6.3885436

C C C O

1 CO	5.4493327	5.6145927	4.6986628	1.9537054 *
2 C	10.4083793	10.0839542	8.7708935	7.3648633
3 C	10.5042450	10.3648894	9.1395001	7.1771630
4 C	9.3828958	9.3796070	8.2446218	5.9345887
5 C	8.0497640	7.9918558	6.8410959	4.7273964
6 C	7.8600398	7.5518287	6.2661075	4.9674352
7 C	9.2029356	8.7786245	7.4336160	6.4219528
8 C	9.5270154	8.8995497	7.4988664	7.1770040
9 C	8.6605689	7.8902410	6.4773736	6.7782381
10 C	7.2414876	6.5138996	5.1058893	5.4474700
11 C	6.7473032	6.2777199	4.9363346	4.3711751
12 N	5.3461794	5.0144462	3.7663160	2.9909313 *
13 C	4.3608380	3.8106844	2.4861607 *	3.0635071
14 C	2.8934728 *	2.5068694 *	1.4479715 *	2.5007717 *
15 C	2.4397545 *	2.8200561 *	2.4403579 *	1.4588564 *
16 C	1.4257595 *	2.4688311 *	2.8414595 *	2.4458252 *
17 C	0.0000000	1.4242058 *	2.4566118 *	3.7552372
18 C	1.4242058 *	0.0000000	1.4165155 *	4.2757445
19 C	2.4566118 *	1.4165155 *	0.0000000	3.7867968
20 O	3.7552372	4.2757445	3.7867968	0.0000000

21 N	7.0812087	7.2501616	6.2776680	3.5778328
22 H	11.3683954	10.9678754	9.6215389	8.4170203
23 H	11.5260182	11.4324902	10.2248494	8.1160723
24 H	9.6767263	9.8252345	8.7889631	6.0991701
25 H	10.6135541	9.9522760	8.5449467	8.2636595
26 H	9.1712390	8.2679196	6.8673778	7.6301426
27 H	6.6917925	5.8113452	4.4088943	5.4682036
28 H	4.8485578	3.9974068	2.5833243 *	4.1482440
29 H	2.2023673 *	3.4728000	3.9459553	2.6608492 *
30 H	1.1042462 *	2.2040165 *	3.4622022	4.6306978
31 H	2.1965059 *	1.1049911 *	2.1918719 *	5.3786940
32 H	3.4526248	2.1793825 *	1.1051418 *	4.6924237
33 H	3.8997412	4.7057781	4.4760629	0.9918827 *
34 H	6.9657406	7.1486982	6.2220741	3.7201565
35 H	7.6721912	7.9840104	7.1041133	4.0129198

N H H H

1 CO	1.9673833 *	6.5046527	6.2321904	4.4097868
2 C	4.3323790	1.1022271 *	2.1906990 *	3.4250608
3 C	3.7988360	2.1791706 *	1.1069710 *	2.1899988 *
4 C	2.4473855 *	3.4388131	2.2071793 *	1.1069863 *
5 C	1.5086824 *	3.9331926	3.4765867	2.1744360 *
6 C	2.6086562 *	3.5277907	4.0573672	3.5066915
7 C	3.8871198	2.1899593 *	3.4928207	3.9321204
8 C	5.1326481	2.6416533 *	4.6582755	5.3734574
9 C	5.4386280	4.0387524	5.9257838	6.2570104
10 C	4.6362894	4.8633198	6.2704586	6.0138447
11 C	3.2284016	4.6944582	5.5278012	4.8257431
12 N	3.0137608	6.0294249	6.4833824	5.2394303
13 C	4.1797800	7.1574937	7.7723426	6.5215066
14 C	4.8639423	8.5370893	8.9345001	7.3952580
15 C	4.6845226	9.1128836	9.1279512	7.2726638
16 C	5.8901627	10.5085805	10.4362419	8.4616513
17 C	7.0812087	11.3683954	11.5260182	9.6767263
18 C	7.2501616	10.9678754	11.4324902	9.8252345
19 C	6.2776680	9.6215389	10.2248494	8.7889631
20 O	3.5778328	8.4170203	8.1160723	6.0991701
21 N	0.0000000	5.4344729	4.6538965	2.5980409 *
22 H	5.4344729	0.0000000	2.5410963 *	4.3528534
23 H	4.6538965	2.5410963 *	0.0000000	2.5237921 *
24 H	2.5980409 *	4.3528534	2.5237921 *	0.0000000
25 H	6.0603565	2.3365824 *	4.7396368	5.9324099
26 H	6.5262979	4.7293284	6.8386611	7.3356868
27 H	5.3515740	5.9335837	7.3648079	6.9853533
28 H	5.0048310	7.2192596	8.1545311	7.1773774

29 H	6.0886370	11.0265698	10.7129932	8.5767699
30 H	8.0301384	12.4522938	12.5412453	10.6145913
31 H	8.3058919	11.8020783	12.3979551	10.8668467
32 H	6.7586582	9.4971074	10.3629061	9.1608965
33 H	4.0597927	9.1396831	8.6207446	6.4488225
34 H	1.0422648 *	5.8551047	5.0571630	2.9916991 *
35 H	1.0398256 *	5.7726589	4.5535223	2.1911545 *

H H H H

1 CO	6.5316535	6.3026184	4.5468516	3.8683714
2 C	2.6437570 *	4.6496560	5.3868873	6.4642474
3 C	4.0412801	5.9194197	6.2842932	7.0500381
4 C	4.8481542	6.2412103	6.0269481	6.4144777
5 C	4.6494028	5.4743660	4.8325646	5.0460980
6 C	3.5205392	4.0261171	3.5133587	4.1139942
7 C	2.1903530 *	3.4809060	3.9439579	5.0646358
8 C	1.1039655 *	2.1821700 *	3.4190214	4.9758870
9 C	2.1818130 *	1.1044384 *	2.1684845 *	3.9388920
10 C	3.4496131	2.1956317 *	1.1030996 *	2.5946385 *
11 C	3.9714170	3.4796580	2.1908248 *	2.6798350 *
12 N	5.4321661	4.6767801	2.7028992 *	2.0987930 *
13 C	6.2566916	4.9914795	2.6205376 *	1.1058236 *
14 C	7.7211530	6.3917388	3.9454510	2.1667245 *
15 C	8.6122217	7.5620867	5.1835488	3.5260471
16 C	10.0047907	8.8596845	6.4286382	4.6636980
17 C	10.6135541	9.1712390	6.6917925	4.8485578
18 C	9.9522760	8.2679196	5.8113452	3.9974068
19 C	8.5449467	6.8673778	4.4088943	2.5833243 *
20 O	8.2636595	7.6301426	5.4682036	4.1482440
21 N	6.0603565	6.5262979	5.3515740	5.0048310
22 H	2.3365824 *	4.7293284	5.9335837	7.2192596
23 H	4.7396368	6.8386611	7.3648079	8.1545311
24 H	5.9324099	7.3356868	6.9853533	7.1773774
25 H	0.0000000	2.5328592 *	4.3380027	6.0021335
26 H	2.5328592 *	0.0000000	2.4828947 *	4.3911522
27 H	4.3380027	2.4828947 *	0.0000000	1.9883750 *
28 H	6.0021335	4.3911522	1.9883750 *	0.0000000
29 H	10.7191826	9.7477826	7.3619950	5.6497808
30 H	11.7175791	10.2530487	7.7728918	5.9257662
31 H	10.6373150	8.7780224	6.3865739	4.6631300
32 H	8.1883324	6.2859162	3.9259783	2.2826839 *
33 H	9.1339683	8.5927175	6.4500169	5.1177477
34 H	6.4486216	6.8438450	5.6118005	5.0394329
35 H	6.7027957	7.3868402	6.3058397	5.9874179

	H	H	H	H
1 CO	4.6132756	6.4287968	6.6813947	5.2906466
2 C	9.9800402	11.4813104	10.9611616	8.7349662
3 C	9.7911522	11.5354397	11.3182402	9.2614030
4 C	8.5123756	10.3778769	10.3831867	8.5077587
5 C	7.3280127	9.0683916	8.9865165	7.1080319
6 C	7.5313576	8.9364070	8.4570228	6.3289767
7 C	8.9810494	10.2929898	9.6165334	7.3387779
8 C	9.6176631	10.6308606	9.6174300	7.1982323
9 C	9.0286708	9.7594191	8.5183896	6.0507158
10 C	7.6200801	8.3422086	7.1964236	4.7765906
11 C	6.7535480	7.8460861	7.1229328	4.9089230
12 N	5.2938258	6.4367201	5.9468455	3.9960876
13 C	4.7952294	5.4638089	4.6780261	2.6644056 *
14 C	3.5009791	3.9972395	3.5040086	2.2044232 *
15 C	2.1867051 *	3.4368119	3.9243636	3.4487612
16 C	1.1051664 *	2.1877418 *	3.4698706	3.9461802
17 C	2.2023673 *	1.1042462 *	2.1965059 *	3.4526248
18 C	3.4728000	2.2040165 *	1.1049911 *	2.1793825 *
19 C	3.9459553	3.4622022	2.1918719 *	1.1051418 *
20 O	2.6608492 *	4.6306978	5.3786940	4.6924237
21 N	6.0886370	8.0301384	8.3058919	6.7586582
22 H	11.0265698	12.4522938	11.8020783	9.4971074
23 H	10.7129932	12.5412453	12.3979551	10.3629061
24 H	8.5767699	10.6145913	10.8668467	9.1608965
25 H	10.7191826	11.7175791	10.6373150	8.1883324
26 H	9.7477826	10.2530487	8.7780224	6.2859162
27 H	7.3619950	7.7728918	6.3865739	3.9259783
28 H	5.6497808	5.9257662	4.6631300	2.2826839 *
29 H	0.0000000	2.5235743 *	4.3866609	5.0502953
30 H	2.5235743 *	0.0000000	2.5429099 *	4.3692581
31 H	4.3866609	2.5429099 *	0.0000000	2.5107297 *
32 H	5.0502953	4.3692581	2.5107297 *	0.0000000
33 H	2.2652520 *	4.5939015	5.7877235	5.4642392
34 H	6.0047923	7.8829914	8.1867168	6.7063462
35 H	6.4248768	8.5602165	9.0645638	7.6604745

	H	H	H
1 CO	2.6555873 *	2.5005311 *	2.5753124 *
2 C	8.0686073	4.7750748	4.6919694
3 C	7.7486036	4.2430933	3.8834846
4 C	6.4383015	2.9344732 *	2.4631817 *
5 C	5.3493114	2.1087260 *	2.0746789 *
6 C	5.7697449	3.0777284	3.3984265

7 C	7.2249767	4.3251602	4.5168143
8 C	8.0598627	5.5210109	5.8522691
9 C	7.7238124	5.7776343	6.2901134
10 C	6.4136248	4.9455752	5.5666894
11 C	5.2984892	3.5783391	4.1718774
12 N	3.9566102	3.2830816	3.9555913
13 C	4.0433360	4.2695919	5.1102191
14 C	3.3326500	4.8735209	5.6680464
15 C	2.0394147 *	4.6905953	5.2893676
16 C	2.4830452 *	5.8164310	6.3885436
17 C	3.8997412	6.9657406	7.6721912
18 C	4.7057781	7.1486982	7.9840104
19 C	4.4760629	6.2220741	7.1041133
20 O	0.9918827 *	3.7201565	4.0129198
21 N	4.0597927	1.0422648 *	1.0398256 *
22 H	9.1396831	5.8551047	5.7726589
23 H	8.6207446	5.0571630	4.5535223
24 H	6.4488225	2.9916991 *	2.1911545 *
25 H	9.1339683	6.4486216	6.7027957
26 H	8.5927175	6.8438450	7.3868402
27 H	6.4500169	5.6118005	6.3058397
28 H	5.1177477	5.0394329	5.9874179
29 H	2.2652520 *	6.0047923	6.4248768
30 H	4.5939015	7.8829914	8.5602165
31 H	5.7877235	8.1867168	9.0645638
32 H	5.4642392	6.7063462	7.6604745
33 H	0.0000000	4.1842913	4.2755298
34 H	4.1842913	0.0000000	1.6673446 *
35 H	4.2755298	1.6673446 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.82 , TOTAL = 2405.3 SECONDS (40.1 MIN)
WALL CLOCK TIME: STEP = 0.82 , TOTAL = 2222.8 SECONDS (37.0 MIN)

CPU UTILIZATION: STEP = 99.50%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.19 , TOTAL = 2406.5 SECONDS (40.1 MIN)
WALL CLOCK TIME: STEP = 1.19 , TOTAL = 2224.0 SECONDS (37.1 MIN)

CPU UTILIZATION: STEP = 99.90%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

		NONZERO BLOCKS				
ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD	
INTEGRALS SKIPPED						
-----START SECOND ORDER SCF-----						
1	0	-284.631020407	-284.631020407	0.045796427	0.001808761	196061080 11502431
2	1	-284.631163038	-0.000142632	0.009840586	0.000499720	163249696 14245680
3	2	-284.631153044	0.000009994	0.012602018	0.000585752	154431005 14960849
4	3	-284.631180208	-0.000027164	0.001687485	0.000226065	152263077 15143044
5	4	-284.631177735	0.000002473	0.001265853	0.000475307	140114544 16167010
6	5	-284.631181079	-0.000003344	0.000594345	0.000044215	136813375 16425835
7	6	-284.631180976	0.000000103	0.000330281	0.000048134	127581991 17095481
8	7	-284.631181175	-0.000000199	0.000145176	0.000024837	145152261 15729111
9	8	-284.631181185	-0.000000011	0.000212622	0.000018862	133467653 16718982
10	9	-284.631181206	-0.000000021	0.000365558	0.000010709	152072975 15399251
-----DISABLING FDIFF OPTION-----						
11	10	-284.631181231	-0.000000025	0.000129374	0.000013171	196058000 11502491
12	11	-284.631181236	-0.000000005	0.000075510	0.000011762	196057858 11502498
13	12	-284.631181241	-0.000000004	0.000104939	0.000010486	196057899 11502497
14	13	-284.631181246	-0.000000005	0.000145045	0.000007271	196058036 11502495
15	14	-284.631181252	-0.000000006	0.000208829	0.000004592	196057954 11502493
16	15	-284.631181255	-0.000000003	0.000036093	0.000007849	196057858 11502497
17	16	-284.631181257	-0.000000002	0.000053564	0.000006785	196057915 11502497
18	17	-284.631181259	-0.000000002	0.000078103	0.000004574	196057939 11502496
19	18	-284.631181261	-0.000000002	0.000109643	0.000003020	196057910 11502498

20 19 -284.631181262 -0.000000001 0.000016174 0.000002045 196057842
11502499
21 20 -284.631181262 0.000000000 0.000015291 0.000001904 196057836
11502499

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 70.8 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 22.6 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6311812625 AFTER 21 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6010358767
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000617611

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 74.52 , TOTAL = 2481.0 SECONDS (41.4 MIN)
WALL CLOCK TIME: STEP = 68.29 , TOTAL = 2292.3 SECONDS (38.2
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.86 , TOTAL = 2484.9 SECONDS (41.4 MIN)
WALL CLOCK TIME: STEP = 3.84 , TOTAL = 2296.1 SECONDS (38.3
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.97, TOTAL = 2487.8 SECONDS (41.5 MIN)
WALL CLOCK TIME: STEP = 2.81, TOTAL = 2298.9 SECONDS (38.3 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 20 ENERGY= -284.6311813

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000920	-0.0000253	0.0000949
2 C	6.0	0.0028119	-0.0002456	-0.0001500
3 C	6.0	-0.0012604	0.0002276	-0.0000672
4 C	6.0	-0.0017335	0.0005583	-0.0002548
5 C	6.0	0.0005376	-0.0011172	-0.0007076
6 C	6.0	-0.0000368	-0.0012102	-0.0007122
7 C	6.0	-0.0003506	-0.0009385	-0.0004249
8 C	6.0	-0.0010047	0.0019952	0.0001385
9 C	6.0	0.0006698	-0.0018925	-0.0005799
10 C	6.0	0.0011437	0.0018132	0.0000385
11 C	6.0	-0.0004010	0.0010815	-0.0001798
12 N	7.0	0.0003915	0.0004632	-0.0003438
13 C	6.0	0.0009393	0.0013306	0.0002173
14 C	6.0	0.0000170	0.0005615	0.0005011
15 C	6.0	0.0001035	-0.0018711	-0.0003932
16 C	6.0	-0.0007570	-0.0012530	-0.0000553
17 C	6.0	-0.0002616	-0.0002312	0.0001851
18 C	6.0	-0.0007127	0.0006397	0.0007307
19 C	6.0	-0.0013608	0.0001199	0.0004654
20 O	8.0	-0.0008210	0.0015686	-0.0005271
21 N	7.0	0.0012196	0.0007708	-0.0003558
22 H	1.0	-0.0017476	-0.0007639	0.0001325
23 H	1.0	0.0020151	-0.0006335	-0.0000358
24 H	1.0	-0.0003655	0.0006583	0.0001565
25 H	1.0	0.0000476	-0.0012238	0.0003536
26 H	1.0	0.0002311	0.0001705	0.0002278
27 H	1.0	0.0000216	0.0000809	-0.0004816
28 H	1.0	0.0001390	-0.0007574	0.0001146
29 H	1.0	0.0011939	0.0010949	-0.0017956
30 H	1.0	0.0008648	-0.0002721	-0.0006803
31 H	1.0	-0.0009683	-0.0001996	0.0013264
32 H	1.0	-0.0009749	-0.0006209	-0.0003881
33 H	1.0	-0.0001545	-0.0004391	0.0001892

34 H 1.0 0.0003375 -0.0003772 0.0015810
35 H 1.0 0.0003186 0.0009372 0.0016798

MAXIMUM GRADIENT = 0.0028119 RMS GRADIENT = 0.0008833
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0001885031
PREDICTED ENERGY CHANGE WAS -0.0002725261 RATIO= 0.692
GDIIS STEP HAS LENGTH = 0.079119
RADIUS OF STEP TAKEN= 0.05261 CURRENT TRUST RADIUS= 0.05261

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 2487.9 SECONDS (41.5 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2298.9 SECONDS (38.3
MIN)
CPU UTILIZATION: STEP = 99.45%, TOTAL = 100.00%

INSERCH= 21

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1119288593	-1.6657386267	1.0413993289
C	6.0	4.9999465095	0.6659360902	0.4270381073
C	6.0	5.2234878066	-0.6942865795	0.1833234145
C	6.0	4.0852528639	-1.5492562483	0.0549308120
C	6.0	2.7708593644	-1.0610500125	0.1793195448
C	6.0	2.4725923619	0.3376196579	0.4612978896
C	6.0	3.6619694164	1.1986790070	0.5641183165
C	6.0	3.5348288005	2.6123112572	0.8184762171
C	6.0	2.2775751131	3.2091436159	0.9805952371
C	6.0	1.1072118760	2.3935836835	0.9167723055
C	6.0	1.1676267845	1.0025384306	0.6583024084
N	7.0	-0.0708872789	0.2210289102	0.6871507935
C	6.0	-1.2858192844	0.7594790828	0.5372393375
C	6.0	-2.5938211431	0.0861118717	0.5922672021
C	6.0	-2.8608494569	-1.3225290147	0.6974384008
C	6.0	-4.1521489852	-1.8754533165	0.6201344201
C	6.0	-5.2759248208	-1.0047556183	0.5179957840
C	6.0	-5.0819674552	0.4049416398	0.4914105983
C	6.0	-3.7654696833	0.9312357381	0.4935457320
O	8.0	-1.7499591811	-2.2454191445	0.9052783770
N	7.0	1.7004376032	-2.1054952257	-0.0323647729
H	1.0	5.8458633308	1.3690154272	0.5244345734
H	1.0	6.2458221425	-1.1022891784	0.0843250175
H	1.0	4.2451599298	-2.6224614332	-0.1640269886

H	1.0	4.4588183274	3.2105161588	0.8980516229
H	1.0	2.1828775519	4.2873334285	1.1889962915
H	1.0	0.1374045976	2.8800694738	1.1136640470
H	1.0	-1.3564785321	1.8413481443	0.3110393446
H	1.0	-4.2948955303	-2.9733737708	0.6256400278
H	1.0	-6.2899589127	-1.4359803429	0.4528808760
H	1.0	-5.9541261299	1.0837187183	0.4535370137
H	1.0	-3.6259719700	2.0243638485	0.4141111562
H	1.0	-2.0741880918	-3.1758966794	1.0204922941
H	1.0	1.4212340370	-2.1292875093	-1.0380580033
H	1.0	2.1175661796	-3.0345964839	0.1821302731

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4504003	5.2733337	4.0956064
2 C	5.4504003	0.0000000	1.3998476 *	2.4253258 *
3 C	5.2733337	1.3998476 *	0.0000000	1.4293483 *
4 C	4.0956064	2.4253258 *	1.4293483 *	0.0000000
5 C	2.8598499 *	2.8306669 *	2.4799028 *	1.4076392 *
6 C	3.1500308	2.5488202 *	2.9511906 *	2.5151757 *
7 C	4.5864445	1.4466474 *	2.4832767 *	2.8265861 *
8 C	5.4833976	2.4674217 *	3.7667728	4.2666863
9 C	5.3346225	3.7663824	4.9548775	5.1736759
10 C	4.1814134	4.2869556	5.1977512	5.0157238
11 C	2.8949894 *	3.8540185	4.4220842	3.9227867
12 N	1.9284205 *	5.0969556	5.3964852	4.5614814
13 C	2.8442148 *	6.2874276	6.6790546	5.8661142
14 C	3.2545019	7.6176639	7.8668021	6.8973320
15 C	3.0122272	8.1129047	8.1249930	6.9794383
16 C	4.2899655	9.5003578	9.4598374	8.2632106
17 C	5.4534225	10.4111966	10.5093321	9.3884268
18 C	5.6184307	10.0854971	10.3684921	9.3833540
19 C	4.6987912	8.7696823	9.1400174	8.2449420
20 O	1.9547853 *	7.3665412	7.1802642	5.9377970
21 N	1.9671592 *	4.3334330	3.8013042	2.4503808 *
22 H	6.5080711	1.1042563 *	2.1819540 *	3.4404204
23 H	6.2336276	2.1900409 *	1.1051852 *	2.2065138 *
24 H	4.4104388	3.4252911	2.1898941 *	1.1069246 *
25 H	6.5340537	2.6437778 *	4.0426526	4.8482819
26 H	6.3047347	4.6509114	5.9222653	6.2426689
27 H	4.5464538	5.3868503	6.2856819	6.0270514
28 H	3.8716022	6.4652292	7.0527804	6.4167149
29 H	4.6155029	9.9838924	9.7974233	8.5194311

30 H	6.4329861	11.4839316	11.5404604	10.3834587
31 H	6.6859645	10.9620688	11.3213679	10.3865574
32 H	5.2898251	8.7322370	9.2605217	8.5066303
33 H	2.6570890 *	8.0718800	7.7534066	6.4433672
34 H	2.5006600 *	4.7714740	4.2435992	2.9373555 *
35 H	2.5757904 *	4.6970243	3.8889331	2.4686446 *

C C C C

1 CO	2.8598499 *	3.1500308	4.5864445	5.4833976
2 C	2.8306669 *	2.5488202 *	1.4466474 *	2.4674217 *
3 C	2.4799028 *	2.9511906 *	2.4832767 *	3.7667728
4 C	1.4076392 *	2.5151757 *	2.8265861 *	4.2666863
5 C	0.0000000	1.4576529 *	2.4593744 *	3.8060154
6 C	1.4576529 *	0.0000000	1.4719419 *	2.5357730 *
7 C	2.4593744 *	1.4719419 *	0.0000000	1.4419497 *
8 C	3.8060154	2.5357730 *	1.4419497 *	0.0000000
9 C	4.3726337	2.9246113 *	2.4762812 *	1.4011346 *
10 C	3.9046195	2.5097229 *	2.8423490 *	2.4394319 *
11 C	2.6567229 *	1.4777899 *	2.5038145 *	2.8671710 *
12 N	3.1586616	2.5561478 *	3.8607196	4.3285871
13 C	4.4608379	3.7827755	4.9673164	5.1721107
14 C	5.5014819	5.0743428	6.3540155	6.6327373
15 C	5.6615336	5.5908369	6.9943856	7.5101477
16 C	6.9846700	6.9864239	8.3972539	8.9033139
17 C	8.0541049	7.8641404	9.2056072	9.5290525
18 C	7.9945870	7.5549198	8.7801901	8.9010466
19 C	6.8404341	6.2663257	7.4325876	7.4983967
20 O	4.7294341	4.9698239	6.4239531	7.1787230
21 N	1.5104565 *	2.6093555 *	3.8885687	5.1328958
22 H	3.9344595	3.5279910	2.1908861 *	2.6406676 *
23 H	3.4765056	4.0561939	3.4929860	4.6569002
24 H	2.1747309 *	3.5064379	3.9333727	5.3733349
25 H	4.6488772	3.5198554	2.1895133 *	1.1036023 *
26 H	5.4745205	4.0266262	3.4810877	2.1842062 *
27 H	4.8312013	3.5132228	3.9435557	3.4207194
28 H	5.0473937	4.1164986	5.0657568	4.9776263
29 H	7.3335582	7.5358197	8.9845150	9.6198569
30 H	9.0726973	8.9402479	10.2953718	10.6324399
31 H	8.9889154	8.4596873	9.6174185	9.6182140
32 H	7.1059381	6.3277025	7.3360989	7.1962672
33 H	5.3530022	5.7732753	7.2283257	8.0625822
34 H	2.1082286 *	3.0723042	4.3200955	5.5133258
35 H	2.0788664 *	3.4023257	4.5223575	5.8567172

C C C N

1	CO	5.3346225	4.1814134	2.8949894 *	1.9284205 *
2	C	3.7663824	4.2869556	3.8540185	5.0969556
3	C	4.9548775	5.1977512	4.4220842	5.3964852
4	C	5.1736759	5.0157238	3.9227867	4.5614814
5	C	4.3726337	3.9046195	2.6567229 *	3.1586616
6	C	2.9246113 *	2.5097229 *	1.4777899 *	2.5561478 *
7	C	2.4762812 *	2.8423490 *	2.5038145 *	3.8607196
8	C	1.4011346 *	2.4394319 *	2.8671710 *	4.3285871
9	C	0.0000000	1.4279221 *	2.4909766 *	3.8118519
10	C	1.4279221 *	0.0000000	1.4161439 *	2.4820632 *
11	C	2.4909766 *	1.4161439 *	0.0000000	1.4647547 *
12	N	3.8118519	2.4820632 *	1.4647547 *	0.0000000
13	C	4.3468610	2.9224889 *	2.4684270 *	1.3373338 *
14	C	5.7995368	4.3734855	3.8720394	2.5283198 *
15	C	6.8570870	5.4408742	4.6514612	3.1885053
16	C	8.2051453	6.7803796	6.0484963	4.5887282
17	C	8.6617727	7.2423868	6.7504276	5.3501006
18	C	7.8908629	6.5147195	6.2803187	5.0182729
19	C	6.4764552	5.1049591	4.9363620	3.7672026
20	O	6.7807787	5.4482938	4.3729319	2.9916932 *
21	N	5.4410074	4.6362149	3.2281236	3.0113135
22	H	4.0406479	4.8639990	4.6944779	6.0292858
23	H	5.9277936	6.2705192	5.5270080	6.4819278
24	H	6.2601252	6.0146117	4.8257704	5.2381490
25	H	2.1828049 *	3.4497819	3.9704643	5.4313669
26	H	1.1022213 *	2.1948692 *	3.4788286	4.6761242
27	H	2.1694070 *	1.1027062 *	2.1894828 *	2.7010731 *
28	H	3.9402431	2.5964682 *	2.6824058 *	2.1022938 *
29	H	9.0303314	7.6204826	6.7563374	5.2962475
30	H	9.7600358	8.3425950	7.8488315	6.4402961
31	H	8.5179884	7.1967234	7.1251585	5.9507402
32	H	6.0478488	4.7740990	4.9073766	3.9956470
33	H	7.7271065	6.4149182	5.3009306	3.9577057
34	H	5.7712328	4.9372396	3.5707547	3.2751731
35	H	6.2966213	5.5700677	4.1746357	3.9551828

C C C C

1	CO	2.8442148 *	3.2545019	3.0122272	4.2899655
2	C	6.2874276	7.6176639	8.1129047	9.5003578
3	C	6.6790546	7.8668021	8.1249930	9.4598374
4	C	5.8661142	6.8973320	6.9794383	8.2632106
5	C	4.4608379	5.5014819	5.6615336	6.9846700
6	C	3.7827755	5.0743428	5.5908369	6.9864239
7	C	4.9673164	6.3540155	6.9943856	8.3972539

8 C	5.1721107	6.6327373	7.5101477	8.9033139
9 C	4.3468610	5.7995368	6.8570870	8.2051453
10 C	2.9224889 *	4.3734855	5.4408742	6.7803796
11 C	2.4684270 *	3.8720394	4.6514612	6.0484963
12 N	1.3373338 *	2.5283198 *	3.1885053	4.5887282
13 C	0.0000000	1.4721822 *	2.6155576 *	3.8943018
14 C	1.4721822 *	0.0000000	1.4375793 *	2.5053743 *
15 C	2.6155576 *	1.4375793 *	0.0000000	1.4068247 *
16 C	3.8943018	2.5053743 *	1.4068247 *	0.0000000
17 C	4.3627785	2.8964095 *	2.4424923 *	1.4252785 *
18 C	3.8129435	2.5105172 *	2.8213414 *	2.4660360 *
19 C	2.4859758 *	1.4480126 *	2.4370814 *	2.8360270 *
20 O	3.0627262	2.4992231 *	1.4591096 *	2.4471816 *
21 N	4.1773505	4.8614777	4.6851882	5.8933390
22 H	7.1576948	8.5369032	9.1148883	10.5117071
23 H	7.7715465	8.9336216	9.1299442	10.4404348
24 H	6.5208149	7.3945935	7.2751162	8.4668605
25 H	6.2560874	7.7197882	8.6119847	10.0046530
26 H	4.9902306	6.3893035	7.5598524	8.8564161
27 H	2.6181549 *	3.9417823	5.1792476	6.4233043
28 H	1.1075197 *	2.1658625 *	3.5245645	4.6611078
29 H	4.7954713	3.5007457	2.1879057 *	1.1071749 *
30 H	5.4652147	3.9997034	3.4396906	2.1889133 *
31 H	4.6803019	3.5080073	3.9265604	3.4686561
32 H	2.6629699 *	2.2031558 *	3.4449062	3.9405433
33 H	4.0425538	3.3307799	2.0391595 *	2.4838198 *
34 H	4.2608299	4.8668905	4.6903141	5.8203636
35 H	5.1092215	5.6660571	5.2897391	6.3909928

C C C O

1 CO	5.4534225	5.6184307	4.6987912	1.9547853 *
2 C	10.4111966	10.0854971	8.7696823	7.3665412
3 C	10.5093321	10.3684921	9.1400174	7.1802642
4 C	9.3884268	9.3833540	8.2449420	5.9377970
5 C	8.0541049	7.9945870	6.8404341	4.7294341
6 C	7.8641404	7.5549198	6.2663257	4.9698239
7 C	9.2056072	8.7801901	7.4325876	6.4239531
8 C	9.5290525	8.9010466	7.4983967	7.1787230
9 C	8.6617727	7.8908629	6.4764552	6.7807787
10 C	7.2423868	6.5147195	5.1049591	5.4482938
11 C	6.7504276	6.2803187	4.9363620	4.3729319
12 N	5.3501006	5.0182729	3.7672026	2.9916932 *
13 C	4.3627785	3.8129435	2.4859758 *	3.0627262
14 C	2.8964095 *	2.5105172 *	1.4480126 *	2.4992231 *
15 C	2.4424923 *	2.8213414 *	2.4370814 *	1.4591096 *

16 C	1.4252785 *	2.4660360 *	2.8360270 *	2.4471816 *
17 C	0.0000000	1.4232261 *	2.4556333 *	3.7578807
18 C	1.4232261 *	0.0000000	1.4177999 *	4.2776136
19 C	2.4556333 *	1.4177999 *	0.0000000	3.7845664
20 O	3.7578807	4.2776136	3.7845664	0.0000000
21 N	7.0840777	7.2510449	6.2749071	3.5782665
22 H	11.3722910	10.9703243	9.6213475	8.4205522
23 H	11.5303181	11.4348713	10.2239253	8.1186963
24 H	9.6815898	9.8280249	8.7881370	6.1013956
25 H	10.6149980	9.9530497	8.5438667	8.2653615
26 H	9.1700698	8.2666538	6.8651204	7.6305017
27 H	6.6896055	5.8099313	4.4062373	5.4659126
28 H	4.8482158	3.9968819	2.5816374 *	4.1484472
29 H	2.2021497 *	3.4713851	3.9425520	2.6617319 *
30 H	1.1038387 *	2.2022084 *	3.4609842	4.6337298
31 H	2.1967788 *	1.1058180 *	2.1943265 *	5.3816586
32 H	3.4508986	2.1790884 *	1.1048523 *	4.6895326
33 H	3.9009581	4.7062796	4.4728786	0.9920620 *
34 H	6.9669084	7.1451537	6.2140573	3.7210898
35 H	7.6744230	7.9849459	7.1017544	4.0129162

N H H H

1 CO	1.9671592 *	6.5080711	6.2336276	4.4104388
2 C	4.3334330	1.1042563 *	2.1900409 *	3.4252911
3 C	3.8013042	2.1819540 *	1.1051852 *	2.1898941 *
4 C	2.4503808 *	3.4404204	2.2065138 *	1.1069246 *
5 C	1.5104565 *	3.9344595	3.4765056	2.1747309 *
6 C	2.6093555 *	3.5279910	4.0561939	3.5064379
7 C	3.8885687	2.1908861 *	3.4929860	3.9333727
8 C	5.1328958	2.6406676 *	4.6569002	5.3733349
9 C	5.4410074	4.0406479	5.9277936	6.2601252
10 C	4.6362149	4.8639990	6.2705192	6.0146117
11 C	3.2281236	4.6944779	5.5270080	4.8257704
12 N	3.0113135	6.0292858	6.4819278	5.2381490
13 C	4.1773505	7.1576948	7.7715465	6.5208149
14 C	4.8614777	8.5369032	8.9336216	7.3945935
15 C	4.6851882	9.1148883	9.1299442	7.2751162
16 C	5.8933390	10.5117071	10.4404348	8.4668605
17 C	7.0840777	11.3722910	11.5303181	9.6815898
18 C	7.2510449	10.9703243	11.4348713	9.8280249
19 C	6.2749071	9.6213475	10.2239253	8.7881370
20 O	3.5782665	8.4205522	8.1186963	6.1013956
21 N	0.0000000	5.4375366	4.6562388	2.6000386 *
22 H	5.4375366	0.0000000	2.5418517 *	4.3552403
23 H	4.6562388	2.5418517 *	0.0000000	2.5249261 *

24 H	2.6000386 *	4.3552403	2.5249261 *	0.0000000
25 H	6.0608841	2.3355103 *	4.7387576	5.9327303
26 H	6.5263105	4.7302946	6.8392872	7.3368212
27 H	5.3490475	5.9343893	7.3642029	6.9845540
28 H	5.0040219	7.2209670	8.1554507	7.1784147
29 H	6.0934557	11.0318438	10.7191748	8.5836624
30 H	8.0330660	12.4559746	12.5456363	10.6196536
31 H	8.3065957	11.8036508	12.3997454	10.8693419
32 H	6.7546810	9.4951207	10.3603589	9.1587088
33 H	4.0622736	9.1449174	8.6254755	6.4531803
34 H	1.0440017 *	5.8529352	5.0587666	2.9969498 *
35 H	1.0407851 *	5.7800666	4.5591528	2.1946151 *

H H H H

1 CO	6.5340537	6.3047347	4.5464538	3.8716022
2 C	2.6437778 *	4.6509114	5.3868503	6.4652292
3 C	4.0426526	5.9222653	6.2856819	7.0527804
4 C	4.8482819	6.2426689	6.0270514	6.4167149
5 C	4.6488772	5.4745205	4.8312013	5.0473937
6 C	3.5198554	4.0266262	3.5132228	4.1164986
7 C	2.1895133 *	3.4810877	3.9435557	5.0657568
8 C	1.1036023 *	2.1842062 *	3.4207194	4.9776263
9 C	2.1828049 *	1.1022213 *	2.1694070 *	3.9402431
10 C	3.4497819	2.1948692 *	1.1027062 *	2.5964682 *
11 C	3.9704643	3.4788286	2.1894828 *	2.6824058 *
12 N	5.4313669	4.6761242	2.7010731 *	2.1022938 *
13 C	6.2560874	4.9902306	2.6181549 *	1.1075197 *
14 C	7.7197882	6.3893035	3.9417823	2.1658625 *
15 C	8.6119847	7.5598524	5.1792476	3.5245645
16 C	10.0046530	8.8564161	6.4233043	4.6611078
17 C	10.6149980	9.1700698	6.6896055	4.8482158
18 C	9.9530497	8.2666538	5.8099313	3.9968819
19 C	8.5438667	6.8651204	4.4062373	2.5816374 *
20 O	8.2653615	7.6305017	5.4659126	4.1484472
21 N	6.0608841	6.5263105	5.3490475	5.0040219
22 H	2.3355103 *	4.7302946	5.9343893	7.2209670
23 H	4.7387576	6.8392872	7.3642029	8.1554507
24 H	5.9327303	7.3368212	6.9845540	7.1784147
25 H	0.0000000	2.5345790 *	4.3393894	6.0030727
26 H	2.5345790 *	0.0000000	2.4839538 *	4.3909787
27 H	4.3393894	2.4839538 *	0.0000000	1.9886768 *
28 H	6.0030727	4.3909787	1.9886768 *	0.0000000
29 H	10.7211104	9.7466293	7.3584135	5.6493199
30 H	11.7185459	10.2512021	7.7701945	5.9245447
31 H	10.6372117	8.7758120	6.3850913	4.6618313

32 H	8.1856576	6.2820547	3.9223220	2.2791926 *
33 H	9.1368175	8.5936491	6.4478329	5.1177315
34 H	6.4411910	6.8346833	5.6010520	5.0300793
35 H	6.7078638	7.3911232	6.3065100	5.9883587

H H H H

1 CO	4.6155029	6.4329861	6.6859645	5.2898251
2 C	9.9838924	11.4839316	10.9620688	8.7322370
3 C	9.7974233	11.5404604	11.3213679	9.2605217
4 C	8.5194311	10.3834587	10.3865574	8.5066303
5 C	7.3335582	9.0726973	8.9889154	7.1059381
6 C	7.5358197	8.9402479	8.4596873	6.3277025
7 C	8.9845150	10.2953718	9.6174185	7.3360989
8 C	9.6198569	10.6324399	9.6182140	7.1962672
9 C	9.0303314	9.7600358	8.5179884	6.0478488
10 C	7.6204826	8.3425950	7.1967234	4.7740990
11 C	6.7563374	7.8488315	7.1251585	4.9073766
12 N	5.2962475	6.4402961	5.9507402	3.9956470
13 C	4.7954713	5.4652147	4.6803019	2.6629699 *
14 C	3.5007457	3.9997034	3.5080073	2.2031558 *
15 C	2.1879057 *	3.4396906	3.9265604	3.4449062
16 C	1.1071749 *	2.1889133 *	3.4686561	3.9405433
17 C	2.2021497 *	1.1038387 *	2.1967788 *	3.4508986
18 C	3.4713851	2.2022084 *	1.1058180 *	2.1790884 *
19 C	3.9425520	3.4609842	2.1943265 *	1.1048523 *
20 O	2.6617319 *	4.6337298	5.3816586	4.6895326
21 N	6.0934557	8.0330660	8.3065957	6.7546810
22 H	11.0318438	12.4559746	11.8036508	9.4951207
23 H	10.7191748	12.5456363	12.3997454	10.3603589
24 H	8.5836624	10.6196536	10.8693419	9.1587088
25 H	10.7211104	11.7185459	10.6372117	8.1856576
26 H	9.7466293	10.2512021	8.7758120	6.2820547
27 H	7.3584135	7.7701945	6.3850913	3.9223220
28 H	5.6493199	5.9245447	4.6618313	2.2791926 *
29 H	0.0000000	2.5246192 *	4.3866462	5.0467400
30 H	2.5246192 *	0.0000000	2.5419810 *	4.3671858
31 H	4.3866462	2.5419810 *	0.0000000	2.5113083 *
32 H	5.0467400	4.3671858	2.5113083 *	0.0000000
33 H	2.2646115 *	4.5958911	5.7896184	5.4606264
34 H	6.0128620	7.8845463	8.1819437	6.6959617
35 H	6.4280724	8.5624388	9.0656714	7.6573576

H H H

1 CO	2.6570890 *	2.5006600 *	2.5757904 *
------	-------------	-------------	-------------

2 C	8.0718800	4.7714740	4.6970243
3 C	7.7534066	4.2435992	3.8889331
4 C	6.4433672	2.9373555 *	2.4686446 *
5 C	5.3530022	2.1082286 *	2.0788664 *
6 C	5.7732753	3.0723042	3.4023257
7 C	7.2283257	4.3200955	4.5223575
8 C	8.0625822	5.5133258	5.8567172
9 C	7.7271065	5.7712328	6.2966213
10 C	6.4149182	4.9372396	5.5700677
11 C	5.3009306	3.5707547	4.1746357
12 N	3.9577057	3.2751731	3.9551828
13 C	4.0425538	4.2608299	5.1092215
14 C	3.3307799	4.8668905	5.6660571
15 C	2.0391595 *	4.6903141	5.2897391
16 C	2.4838198 *	5.8203636	6.3909928
17 C	3.9009581	6.9669084	7.6744230
18 C	4.7062796	7.1451537	7.9849459
19 C	4.4728786	6.2140573	7.1017544
20 O	0.9920620 *	3.7210898	4.0129162
21 N	4.0622736	1.0440017 *	1.0407851 *
22 H	9.1449174	5.8529352	5.7800666
23 H	8.6254755	5.0587666	4.5591528
24 H	6.4531803	2.9969498 *	2.1946151 *
25 H	9.1368175	6.4411910	6.7078638
26 H	8.5936491	6.8346833	7.3911232
27 H	6.4478329	5.6010520	6.3065100
28 H	5.1177315	5.0300793	5.9883587
29 H	2.2646115 *	6.0128620	6.4280724
30 H	4.5958911	7.8845463	8.5624388
31 H	5.7896184	8.1819437	9.0656714
32 H	5.4606264	6.6959617	7.6573576
33 H	0.0000000	4.1893909	4.2771042
34 H	4.1893909	0.0000000	1.6713235 *
35 H	4.2771042	1.6713235 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.60 , TOTAL = 2488.5 SECONDS (41.5 MIN)
WALL CLOCK TIME: STEP = 0.60 , TOTAL = 2299.5 SECONDS (38.3 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.02 , TOTAL = 2489.5 SECONDS (41.5 MIN)
 WALL CLOCK TIME: STEP = 1.01 , TOTAL = 2300.5 SECONDS (38.3 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
 INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.631230449	-284.631230449	0.021749686	0.001449650	195993063
11506720						
2	1	-284.631314648	-0.000084199	0.004882161	0.000156475	158776673
14604041						
3	2	-284.631309662	0.000004986	0.002783619	0.000397260	147453132
15522420						
4	3	-284.631318814	-0.000009152	0.001598344	0.000183863	143301462
15875539						
5	4	-284.631317697	0.000001117	0.000910570	0.000293335	136340313
16432605						
6	5	-284.631319344	-0.000001647	0.000298083	0.000021641	132787554
16712906						
7	6	-284.631319296	0.000000048	0.000220342	0.000027664	122667679
17473093						
8	7	-284.631319376	-0.000000081	0.000169967	0.000018254	140376651
16133821						
9	8	-284.631319389	-0.000000013	0.000201283	0.000016222	135433314
16548280						
10	9	-284.631319416	-0.000000027	0.000644682	0.000016764	153383983
15255270						

-----DISABLING FDIFF OPTION-----

11	10	-284.631319449	-0.000000033	0.000184851	0.000018998	195988012
11507253						
12	11	-284.631319464	-0.000000015	0.000126926	0.000016433	195988126
11507254						
13	12	-284.631319477	-0.000000012	0.000220915	0.000010967	195988089
11507255						
14	13	-284.631319493	-0.000000016	0.000324447	0.000008675	195988059
11507253						
15	14	-284.631319501	-0.000000008	0.000087950	0.000010089	195988204
11507251						
16	15	-284.631319505	-0.000000004	0.000055073	0.000008967	195988174
11507250						

17 16	-284.631319507	-0.000000002	0.000050120	0.000006870	195988138
11507254					
18 17	-284.631319510	-0.000000003	0.000096488	0.000004330	195988165
11507250					
19 18	-284.631319512	-0.000000002	0.000046641	0.000002984	195988198
11507249					
20 19	-284.631319512	-0.000000001	0.000015944	0.000003007	195988182
11507253					
21 20	-284.631319513	0.000000000	0.000026586	0.000002882	195988186
11507251					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 70.7 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 22.6 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.2 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6313195127 AFTER 21 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5976435982
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000577063

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 74.10 , TOTAL = 2563.6 SECONDS (42.7 MIN)
WALL CLOCK TIME: STEP = 68.05 , TOTAL = 2368.6 SECONDS (39.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.56 , TOTAL = 2567.1 SECONDS (42.8 MIN)
WALL CLOCK TIME: STEP = 3.54 , TOTAL = 2372.1 SECONDS (39.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.88 , TOTAL = 2570.0 SECONDS (42.8 MIN)
WALL CLOCK TIME: STEP = 2.71 , TOTAL = 2374.8 SECONDS (39.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 21 ENERGY= -284.6313195

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0001179	-0.0002312	0.0001586
2 C	6.0	0.0014852	-0.0004941	-0.0000918
3 C	6.0	0.0000903	-0.0017205	-0.0004657
4 C	6.0	-0.0006643	0.0007837	-0.0003065
5 C	6.0	0.0001258	-0.0001804	-0.0005336
6 C	6.0	0.0008619	-0.0016335	-0.0008726
7 C	6.0	-0.0009802	0.0002004	-0.0001724
8 C	6.0	0.0013357	-0.0001502	-0.0003344
9 C	6.0	-0.0008985	0.0015632	0.0001006
10 C	6.0	0.0005540	0.0015152	0.0001124
11 C	6.0	-0.0005943	0.0015873	-0.0001692
12 N	7.0	0.0013857	-0.0001332	-0.0002748
13 C	6.0	0.0000466	0.0004310	0.0004533
14 C	6.0	0.0008262	0.0000031	0.0006095
15 C	6.0	0.0005832	-0.0007127	-0.0005689
16 C	6.0	-0.0010616	0.0011448	0.0001925
17 C	6.0	-0.0004648	-0.0003226	0.0002710
18 C	6.0	-0.0016756	-0.0004951	0.0005944
19 C	6.0	-0.0004526	-0.0004354	0.0004958
20 O	8.0	-0.0005378	0.0016847	-0.0007866
21 N	7.0	0.0006919	0.0003897	0.0007253
22 H	1.0	-0.0007944	0.0001969	0.0002226
23 H	1.0	0.0009662	-0.0001057	0.0000876
24 H	1.0	-0.0004048	0.0007121	0.0001323
25 H	1.0	-0.0002318	-0.0012848	0.0003148
26 H	1.0	0.0002043	-0.0012781	-0.0000634
27 H	1.0	0.0001880	-0.0001633	-0.0005657

28 H	1.0	-0.0002633	0.0003172	-0.0001928
29 H	1.0	0.0009175	-0.0001648	-0.0017682
30 H	1.0	0.0009825	0.0001047	-0.0008267
31 H	1.0	-0.0015301	0.0000444	0.0012396
32 H	1.0	-0.0009825	-0.0008673	-0.0002425
33 H	1.0	-0.0002924	-0.0005166	0.0002412
34 H	1.0	0.0000611	0.0000879	0.0002444
35 H	1.0	0.0004051	0.0001235	0.0020399

MAXIMUM GRADIENT = 0.0020399 RMS GRADIENT = 0.0007693
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001382502
 PREDICTED ENERGY CHANGE WAS -0.0001969182 RATIO= 0.702
 GDIIS STEP HAS LENGTH = 0.144614
 RADIUS OF STEP TAKEN= 0.05261 CURRENT TRUST RADIUS= 0.05261

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 2570.0 SECONDS (42.8 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2374.9 SECONDS (39.6 MIN)
 CPU UTILIZATION: STEP = 96.93% , TOTAL = 100.00%

INSERCH= 22

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1121614242	-1.6690937188	1.0421340001
C	6.0	5.0006787292	0.6669773278	0.4274240371
C	6.0	5.2254293533	-0.6930999389	0.1840358291
C	6.0	4.0881078591	-1.5494371240	0.0558401755
C	6.0	2.7730819470	-1.0613006327	0.1815822137
C	6.0	2.4740644994	0.3376783028	0.4633762146
C	6.0	3.6626505969	1.1987810315	0.5649773863
C	6.0	3.5343349346	2.6127681839	0.8182271967
C	6.0	2.2768555449	3.2083266469	0.9807816951
C	6.0	1.1074132656	2.3915624501	0.9183699456
C	6.0	1.1690660830	1.0007550933	0.6602529358
N	7.0	-0.0699274739	0.2185230789	0.6894752712
C	6.0	-1.2845073769	0.7572179415	0.5375342529
C	6.0	-2.5930614200	0.0845375630	0.5934760197
C	6.0	-2.8618522386	-1.3224409933	0.7008780516
C	6.0	-4.1540341285	-1.8740564089	0.6269580491
C	6.0	-5.2782533090	-1.0031095032	0.5190159506
C	6.0	-5.0820329649	0.4061776123	0.4876318163

C	6.0	-3.7644011161	0.9291716187	0.4926894041
O	8.0	-1.7505591510	-2.2478521411	0.9035580485
N	7.0	1.7001970211	-2.1049121179	-0.0345173279
H	1.0	5.8465940683	1.3715594855	0.5236382973
H	1.0	6.2479013421	-1.1002359804	0.0843831641
H	1.0	4.2474634515	-2.6228320712	-0.1647969712
H	1.0	4.4586145666	3.2113138839	0.8958188856
H	1.0	2.1805986554	4.2880237707	1.1885110048
H	1.0	0.1360931559	2.8763412421	1.1159596989
H	1.0	-1.3565942641	1.8387195757	0.3083266597
H	1.0	-4.2991675776	-2.9712291156	0.6372665205
H	1.0	-6.2933191591	-1.4330041583	0.4511247762
H	1.0	-5.9536121179	1.0857450338	0.4435512647
H	1.0	-3.6233843396	2.0222120991	0.4136811656
H	1.0	-2.0766972467	-3.1772328593	1.0185728691
H	1.0	1.4204060881	-2.1186912963	-1.0404732758
H	1.0	2.1156882980	-3.0367588814	0.1736217747

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4527697	5.2758322	4.0982000
2 C	5.4527697	0.0000000	1.3998431 *	2.4255624 *
3 C	5.2758322	1.3998431 *	0.0000000	1.4294221 *
4 C	4.0982000	2.4255624 *	1.4294221 *	0.0000000
5 C	2.8618979 *	2.8301184 *	2.4798358 *	1.4083258 *
6 C	3.1528845	2.5482366 *	2.9513630 *	2.5164312 *
7 C	4.5889386	1.4463939 *	2.4832655 *	2.8271784 *
8 C	5.4859591	2.4675886 *	3.7670629	4.2675346
9 C	5.3365620	3.7661484	4.9547978	5.1742118
10 C	4.1826753	4.2863432	5.1973498	5.0159720
11 C	2.8967177 *	3.8531639	4.4215394	3.9229581
12 N	1.9288913 *	5.0971393	5.3969741	4.5625031
13 C	2.8446956 *	6.2867982	6.6788966	5.8666584
14 C	3.2549573	7.6178539	7.8677290	6.8990542
15 C	3.0135330	8.1149218	8.1281806	6.9835196
16 C	4.2912475	9.5029171	9.4638879	8.2682802
17 C	5.4565336	10.4141261	10.5135944	9.3937068
18 C	5.6208433	10.0862638	10.3703597	9.3862855
19 C	4.6990009	8.7692434	9.1402453	8.2459830
20 O	1.9554776 *	7.3689991	7.1832710	5.9410808
21 N	1.9674788 *	4.3347365	3.8037143	2.4533314 *
22 H	6.5113844	1.1051090 *	2.1826575 *	3.4414140
23 H	6.2360396	2.1900420 *	1.1050518 *	2.2061968 *

24 H	4.4121448	3.4265004	2.1913393 *	1.1073625 *
25 H	6.5369290	2.6432699 *	4.0421637	4.8484626
26 H	6.3077022	4.6523201	5.9238128	6.2447966
27 H	4.5460974	5.3869809	6.2857565	6.0274197
28 H	3.8730441	6.4654531	7.0532683	6.4177984
29 H	4.6172825	9.9883793	9.8037359	8.5267777
30 H	6.4370189	11.4875965	11.5455776	10.3896022
31 H	6.6888748	10.9623042	11.3226590	10.3889675
32 H	5.2891392	8.7299092	9.2588963	8.5059885
33 H	2.6582214 *	8.0756832	7.7581197	6.4483638
34 H	2.5001790 *	4.7679161	4.2438114	2.9398276 *
35 H	2.5766143 *	4.7016218	3.8940127	2.4731432 *

C C C C

1 CO	2.8618979 *	3.1528845	4.5889386	5.4859591
2 C	2.8301184 *	2.5482366 *	1.4463939 *	2.4675886 *
3 C	2.4798358 *	2.9513630 *	2.4832655 *	3.7670629
4 C	1.4083258 *	2.5164312 *	2.8271784 *	4.2675346
5 C	0.0000000	1.4580677 *	2.4589212 *	3.8057331
6 C	1.4580677 *	0.0000000	1.4712436 *	2.5349806 *
7 C	2.4589212 *	1.4712436 *	0.0000000	1.4422067 *
8 C	3.8057331	2.5349806 *	1.4422067 *	0.0000000
9 C	4.3720336	2.9235632 *	2.4762057 *	1.4008456 *
10 C	3.9037894	2.5086241 *	2.8419802 *	2.4390386 *
11 C	2.6559492 *	1.4769740 *	2.5032490 *	2.8667122 *
12 N	3.1588933	2.5567976 *	3.8611584	4.3289368
13 C	4.4606886	3.7826413	4.9669008	5.1713728
14 C	5.5025536	5.0751129	6.3542335	6.6323035
15 C	5.6648341	5.5932469	6.9960108	7.5107158
16 C	6.9888389	6.9892933	8.3992102	8.9038867
17 C	8.0586132	7.8676070	9.2081593	9.5302576
18 C	7.9968737	7.5564469	8.7808709	8.9005691
19 C	6.8408663	6.2665123	7.4322952	7.4974676
20 O	4.7320696	4.9725419	6.4262553	7.1807393
21 N	1.5122520 *	2.6101756 *	3.8890881	5.1330052
22 H	3.9347538	3.5279594	2.1911573 *	2.6408188 *
23 H	3.4763966	4.0562394	3.4928458	4.6570774
24 H	2.1753528 *	3.5077296	3.9343746	5.3746069
25 H	4.6482673	3.5189810	2.1893614 *	1.1038887 *
26 H	5.4754190	4.0270550	3.4826273	2.1854504 *
27 H	4.8302996	3.5123759	3.9439063	3.4214270
28 H	5.0478121	4.1171728	5.0663804	4.9779854
29 H	7.3397676	7.5402771	8.9880342	9.6217220
30 H	9.0780199	8.9444107	10.2985722	10.6341818
31 H	8.9907520	8.4608351	9.6176936	9.6173448

32 H	7.1046957	6.3260577	7.3339781	7.1934247
33 H	5.3570590	5.7768743	7.2315531	8.0652299
34 H	2.1074218 *	3.0668405	4.3140184	5.5054674
35 H	2.0819858 *	3.4057624	4.5261518	5.8604804

C C C N

1 CO	5.3365620	4.1826753	2.8967177 *	1.9288913 *
2 C	3.7661484	4.2863432	3.8531639	5.0971393
3 C	4.9547978	5.1973498	4.4215394	5.3969741
4 C	5.1742118	5.0159720	3.9229581	4.5625031
5 C	4.3720336	3.9037894	2.6559492 *	3.1588933
6 C	2.9235632 *	2.5086241 *	1.4769740 *	2.5567976 *
7 C	2.4762057 *	2.8419802 *	2.5032490 *	3.8611584
8 C	1.4008456 *	2.4390386 *	2.8667122 *	4.3289368
9 C	0.0000000	1.4277935 *	2.4906442 *	3.8119779
10 C	1.4277935 *	0.0000000	1.4158992 *	2.4820605 *
11 C	2.4906442 *	1.4158992 *	0.0000000	1.4655531 *
12 N	3.8119779	2.4820605 *	1.4655531 *	0.0000000
13 C	4.3459991	2.9218833 *	2.4686824 *	1.3373416 *
14 C	5.7986339	4.3728061	3.8726628	2.5285120 *
15 C	6.8565676	5.4402383	4.6526544	3.1889723
16 C	8.2043983	6.7796205	6.0498798	4.5894144
17 C	8.6619335	7.2429289	6.7530251	5.3523920
18 C	7.8897703	6.5143329	6.2816845	5.0196769
19 C	6.4753041	5.1043478	4.9368310	3.7673441
20 O	6.7820292	5.4490727	4.3745694	2.9922167 *
21 N	5.4400251	4.6344007	3.2264492	3.0092951
22 H	4.0405107	4.8637489	4.6941908	6.0301096
23 H	5.9276004	6.2699927	5.5263331	6.4823007
24 H	6.2608352	6.0147584	4.8257250	5.2386014
25 H	2.1834148 *	3.4500799	3.9702885	5.4320408
26 H	1.1037041 *	2.1957387 *	3.4797112	4.6770440
27 H	2.1705647 *	1.1034106 *	2.1891837 *	2.6996909 *
28 H	3.9408092	2.5979071 *	2.6842125 *	2.1037639 *
29 H	9.0304481	7.6203457	6.7586068	5.2975199
30 H	9.7606548	8.3436484	7.8520133	6.4432102
31 H	8.5167228	7.1964360	7.1264807	5.9523355
32 H	6.0449402	4.7719573	4.9062973	3.9945478
33 H	7.7285329	6.4156123	5.3027310	3.9581042
34 H	5.7616055	4.9272122	3.5618236	3.2674741
35 H	6.2990932	5.5711705	4.1754548	3.9547290

C C C C

1 CO	2.8446956 *	3.2549573	3.0135330	4.2912475
------	-------------	-----------	-----------	-----------

2 C	6.2867982	7.6178539	8.1149218	9.5029171
3 C	6.6788966	7.8677290	8.1281806	9.4638879
4 C	5.8666584	6.8990542	6.9835196	8.2682802
5 C	4.4606886	5.5025536	5.6648341	6.9888389
6 C	3.7826413	5.0751129	5.5932469	6.9892933
7 C	4.9669008	6.3542335	6.9960108	8.3992102
8 C	5.1713728	6.6323035	7.5107158	8.9038867
9 C	4.3459991	5.7986339	6.8565676	8.2043983
10 C	2.9218833 *	4.3728061	5.4402383	6.7796205
11 C	2.4686824 *	3.8726628	4.6526544	6.0498798
12 N	1.3373416 *	2.5285120 *	3.1889723	4.5894144
13 C	0.0000000	1.4723933 *	2.6152781 *	3.8943273
14 C	1.4723933 *	0.0000000	1.4364443 *	2.5047649 *
15 C	2.6152781 *	1.4364443 *	0.0000000	1.4069391 *
16 C	3.8943273	2.5047649 *	1.4069391 *	0.0000000
17 C	4.3645277	2.8980642 *	2.4441850 *	1.4262078 *
18 C	3.8140425	2.5118986 *	2.8218431 *	2.4657779 *
19 C	2.4862526 *	1.4476192 *	2.4346861 *	2.8333601 *
20 O	3.0629437	2.4992004 *	1.4602867 *	2.4480447 *
21 N	4.1746248	4.8600549	4.6867218	5.8960043
22 H	7.1575287	8.5375106	9.1173510	10.5146213
23 H	7.7712716	8.9345110	9.1332936	10.4447809
24 H	6.5207905	7.3957832	7.2789271	8.4718772
25 H	6.2557497	7.7197329	8.6129071	10.0055482
26 H	4.9897215	6.3883639	7.5591939	8.8551762
27 H	2.6159827 *	3.9389645	5.1758808	6.4195477
28 H	1.1078711 *	2.1650210 *	3.5231853	4.6596031
29 H	4.7957732	3.5000608	2.1882468 *	1.1067782 *
30 H	5.4674249	4.0018876	3.4423199	2.1913432 *
31 H	4.6815918	3.5097286	3.9274109	3.4687957
32 H	2.6619345 *	2.2019251 *	3.4422547	3.9380178
33 H	4.0421363	3.3296375	2.0390319 *	2.4833364 *
34 H	4.2517665	4.8612683	4.6908480	5.8236206
35 H	5.1076436	5.6649001	5.2908218	6.3927154

C C C O

1 CO	5.4565336	5.6208433	4.6990009	1.9554776 *
2 C	10.4141261	10.0862638	8.7692434	7.3689991
3 C	10.5135944	10.3703597	9.1402453	7.1832710
4 C	9.3937068	9.3862855	8.2459830	5.9410808
5 C	8.0586132	7.9968737	6.8408663	4.7320696
6 C	7.8676070	7.5564469	6.2665123	4.9725419
7 C	9.2081593	8.7808709	7.4322952	6.4262553
8 C	9.5302576	8.9005691	7.4974676	7.1807393
9 C	8.6619335	7.8897703	6.4753041	6.7820292

10 C	7.2429289	6.5143329	5.1043478	5.4490727
11 C	6.7530251	6.2816845	4.9368310	4.3745694
12 N	5.3523920	5.0196769	3.7673441	2.9922167 *
13 C	4.3645277	3.8140425	2.4862526 *	3.0629437
14 C	2.8980642 *	2.5118986 *	1.4476192 *	2.4992004 *
15 C	2.4441850 *	2.8218431 *	2.4346861 *	1.4602867 *
16 C	1.4262078 *	2.4657779 *	2.8333601 *	2.4480447 *
17 C	0.0000000	1.4232279 *	2.4548222 *	3.7605695
18 C	1.4232279 *	0.0000000	1.4176396 *	4.2796713
19 C	2.4548222 *	1.4176396 *	0.0000000	3.7838938
20 O	3.7605695	4.2796713	3.7838938	0.0000000
21 N	7.0865462	7.2509899	6.2725947	3.5788455
22 H	11.3754694	10.9712418	9.6212210	8.4238481
23 H	11.5347553	11.4367523	10.2240603	8.1217880
24 H	9.6866083	9.8305680	8.7885717	6.1039551
25 H	10.6164938	9.9528570	8.5433409	8.2677924
26 H	9.1694486	8.2647310	6.8636053	7.6323570
27 H	6.6874231	5.8073526	4.4038382	5.4646070
28 H	4.8476584	3.9953999	2.5804653 *	4.1484427
29 H	2.2013829 *	3.4701794	3.9395436	2.6626285 *
30 H	1.1044353 *	2.2025296 *	3.4607844	4.6373852
31 H	2.1966151 *	1.1060765 *	2.1953530 *	5.3842484
32 H	3.4499649	2.1782314 *	1.1049278 *	4.6883795
33 H	3.9020931	4.7068856	4.4707332	0.9916365 *
34 H	6.9676802	7.1408530	6.2066321	3.7216879
35 H	7.6762881	7.9849612	7.0997085	4.0128606

N H H H

1 CO	1.9674788 *	6.5113844	6.2360396	4.4121448
2 C	4.3347365	1.1051090 *	2.1900420 *	3.4265004
3 C	3.8037143	2.1826575 *	1.1050518 *	2.1913393 *
4 C	2.4533314 *	3.4414140	2.2061968 *	1.1073625 *
5 C	1.5122520 *	3.9347538	3.4763966	2.1753528 *
6 C	2.6101756 *	3.5279594	4.0562394	3.5077296
7 C	3.8890881	2.1911573 *	3.4928458	3.9343746
8 C	5.1330052	2.6408188 *	4.6570774	5.3746069
9 C	5.4400251	4.0405107	5.9276004	6.2608352
10 C	4.6344007	4.8637489	6.2699927	6.0147584
11 C	3.2264492	4.6941908	5.5263331	4.8257250
12 N	3.0092951	6.0301096	6.4823007	5.2386014
13 C	4.1746248	7.1575287	7.7712716	6.5207905
14 C	4.8600549	8.5375106	8.9345110	7.3957832
15 C	4.6867218	9.1173510	9.1332936	7.2789271
16 C	5.8960043	10.5146213	10.4447809	8.4718772
17 C	7.0865462	11.3754694	11.5347553	9.6866083

18 C	7.2509899	10.9712418	11.4367523	9.8305680
19 C	6.2725947	9.6212210	10.2240603	8.7885717
20 O	3.5788455	8.4238481	8.1217880	6.1039551
21 N	0.0000000	5.4396692	4.6588761	2.6026487 *
22 H	5.4396692	0.0000000	2.5423936 *	4.3573301
23 H	4.6588761	2.5423936 *	0.0000000	2.5262900 *
24 H	2.6026487 *	4.3573301	2.5262900 *	0.0000000
25 H	6.0610768	2.3344596 *	4.7380837	5.9335276
26 H	6.5265775	4.7315264	6.8407158	7.3391621
27 H	5.3462981	5.9350681	7.3642050	6.9845981
28 H	5.0013744	7.2215317	8.1557320	7.1787709
29 H	6.0987027	11.0367207	10.7259945	8.5912507
30 H	8.0363928	12.4598687	12.5509938	10.6255893
31 H	8.3060001	11.8039387	12.4009857	10.8713189
32 H	6.7508929	9.4929411	10.3585906	9.1575825
33 H	4.0649479	9.1495911	8.6305022	6.4577653
34 H	1.0442319 *	5.8497381	5.0603620	3.0022026
35 H	1.0412940 *	5.7857964	4.5643476	2.1978007 *

H H H H

1 CO	6.5369290	6.3077022	4.5460974	3.8730441
2 C	2.6432699 *	4.6523201	5.3869809	6.4654531
3 C	4.0421637	5.9238128	6.2857565	7.0532683
4 C	4.8484626	6.2447966	6.0274197	6.4177984
5 C	4.6482673	5.4754190	4.8302996	5.0478121
6 C	3.5189810	4.0270550	3.5123759	4.1171728
7 C	2.1893614 *	3.4826273	3.9439063	5.0663804
8 C	1.1038887 *	2.1854504 *	3.4214270	4.9779854
9 C	2.1834148 *	1.1037041 *	2.1705647 *	3.9408092
10 C	3.4500799	2.1957387 *	1.1034106 *	2.5979071 *
11 C	3.9702885	3.4797112	2.1891837 *	2.6842125 *
12 N	5.4320408	4.6770440	2.6996909 *	2.1037639 *
13 C	6.2557497	4.9897215	2.6159827 *	1.1078711 *
14 C	7.7197329	6.3883639	3.9389645	2.1650210 *
15 C	8.6129071	7.5591939	5.1758808	3.5231853
16 C	10.0055482	8.8551762	6.4195477	4.6596031
17 C	10.6164938	9.1694486	6.6874231	4.8476584
18 C	9.9528570	8.2647310	5.8073526	3.9953999
19 C	8.5433409	6.8636053	4.4038382	2.5804653 *
20 O	8.2677924	7.6323570	5.4646070	4.1484427
21 N	6.0610768	6.5265775	5.3462981	5.0013744
22 H	2.3344596 *	4.7315264	5.9350681	7.2215317
23 H	4.7380837	6.8407158	7.3642050	8.1557320
24 H	5.9335276	7.3391621	6.9845981	7.1787709
25 H	0.0000000	2.5365980 *	4.3410667	6.0038168

26 H	2.5365980 *	0.0000000	2.4855812 *	4.3915315
27 H	4.3410667	2.4855812 *	0.0000000	1.9892324 *
28 H	6.0038168	4.3915315	1.9892324 *	0.0000000
29 H	10.7233127	9.7461784	7.3549143	5.6482338
30 H	11.7205598	10.2509113	7.7685138	5.9241725
31 H	10.6365903	8.7735363	6.3830148	4.6602392
32 H	8.1832222	6.2785733	3.9187246	2.2766437 *
33 H	9.1399616	8.5955514	6.4460596	5.1169109
34 H	6.4334200	6.8258524	5.5901711	5.0191725
35 H	6.7118764	7.3950426	6.3064690	5.9870846

H H H H

1 CO	4.6172825	6.4370189	6.6888748	5.2891392
2 C	9.9883793	11.4875965	10.9623042	8.7299092
3 C	9.8037359	11.5455776	11.3226590	9.2588963
4 C	8.5267777	10.3896022	10.3889675	8.5059885
5 C	7.3397676	9.0780199	8.9907520	7.1046957
6 C	7.5402771	8.9444107	8.4608351	6.3260577
7 C	8.9880342	10.2985722	9.6176936	7.3339781
8 C	9.6217220	10.6341818	9.6173448	7.1934247
9 C	9.0304481	9.7606548	8.5167228	6.0449402
10 C	7.6203457	8.3436484	7.1964360	4.7719573
11 C	6.7586068	7.8520133	7.1264807	4.9062973
12 N	5.2975199	6.4432102	5.9523355	3.9945478
13 C	4.7957732	5.4674249	4.6815918	2.6619345 *
14 C	3.5000608	4.0018876	3.5097286	2.2019251 *
15 C	2.1882468 *	3.4423199	3.9274109	3.4422547
16 C	1.1067782 *	2.1913432 *	3.4687957	3.9380178
17 C	2.2013829 *	1.1044353 *	2.1966151 *	3.4499649
18 C	3.4701794	2.2025296 *	1.1060765 *	2.1782314 *
19 C	3.9395436	3.4607844	2.1953530 *	1.1049278 *
20 O	2.6626285 *	4.6373852	5.3842484	4.6883795
21 N	6.0987027	8.0363928	8.3060001	6.7508929
22 H	11.0367207	12.4598687	11.8039387	9.4929411
23 H	10.7259945	12.5509938	12.4009857	10.3585906
24 H	8.5912507	10.6255893	10.8713189	9.1575825
25 H	10.7233127	11.7205598	10.6365903	8.1832222
26 H	9.7461784	10.2509113	8.7735363	6.2785733
27 H	7.3549143	7.7685138	6.3830148	3.9187246
28 H	5.6482338	5.9241725	4.6602392	2.2766437 *
29 H	0.0000000	2.5253565 *	4.3856301	5.0439200
30 H	2.5253565 *	0.0000000	2.5415656 *	4.3667463
31 H	4.3856301	2.5415656 *	0.0000000	2.5115382 *
32 H	5.0439200	4.3667463	2.5115382 *	0.0000000
33 H	2.2643336 *	4.5982857	5.7908634	5.4582381

34 H	6.0212253	7.8864814	8.1759945	6.6859156
35 H	6.4319232	8.5650711	9.0654018	7.6542649

H H H

1 CO	2.6582214 *	2.5001790 *	2.5766143 *
2 C	8.0756832	4.7679161	4.7016218
3 C	7.7581197	4.2438114	3.8940127
4 C	6.4483638	2.9398276 *	2.4731432 *
5 C	5.3570590	2.1074218 *	2.0819858 *
6 C	5.7768743	3.0668405	3.4057624
7 C	7.2315531	4.3140184	4.5261518
8 C	8.0652299	5.5054674	5.8604804
9 C	7.7285329	5.7616055	6.2990932
10 C	6.4156123	4.9272122	5.5711705
11 C	5.3027310	3.5618236	4.1754548
12 N	3.9581042	3.2674741	3.9547290
13 C	4.0421363	4.2517665	5.1076436
14 C	3.3296375	4.8612683	5.6649001
15 C	2.0390319 *	4.6908480	5.2908218
16 C	2.4833364 *	5.8236206	6.3927154
17 C	3.9020931	6.9676802	7.6762881
18 C	4.7068856	7.1408530	7.9849612
19 C	4.4707332	6.2066321	7.0997085
20 O	0.9916365 *	3.7216879	4.0128606
21 N	4.0649479	1.0442319 *	1.0412940 *
22 H	9.1495911	5.8497381	5.7857964
23 H	8.6305022	5.0603620	4.5643476
24 H	6.4577653	3.0022026	2.1978007 *
25 H	9.1399616	6.4334200	6.7118764
26 H	8.5955514	6.8258524	7.3950426
27 H	6.4460596	5.5901711	6.3064690
28 H	5.1169109	5.0191725	5.9870846
29 H	2.2643336 *	6.0212253	6.4319232
30 H	4.5982857	7.8864814	8.5650711
31 H	5.7908634	8.1759945	9.0654018
32 H	5.4582381	6.6859156	7.6542649
33 H	0.0000000	4.1940330	4.2789919
34 H	4.1940330	0.0000000	1.6734074 *
35 H	4.2789919	1.6734074 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.75 , TOTAL = 2570.8 SECONDS (42.8 MIN)
WALL CLOCK TIME: STEP = 0.76 , TOTAL = 2375.6 SECONDS (39.6 MIN)
CPU UTILIZATION: STEP = 98.97%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.87 , TOTAL = 2571.7 SECONDS (42.9 MIN)
WALL CLOCK TIME: STEP = 0.87 , TOTAL = 2376.5 SECONDS (39.6 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.631371734	-284.631371734	0.020839914	0.001292291	195937295
						11510344
2	1	-284.631440131	-0.000068397	0.003883121	0.000181335	156513015
						14845002
3	2	-284.631436623	0.000003508	0.002169339	0.000367725	144719478
						15766071
4	3	-284.631442420	-0.000005797	0.000745878	0.000088742	140150431
						16127124
5	4	-284.631442058	0.000000362	0.000555795	0.000178416	130576531
						16914256
6	5	-284.631442568	-0.000000510	0.000165572	0.000020152	126127651
						17270241
7	6	-284.631442552	0.000000016	0.000132582	0.000026066	117200584
						17879694
8	7	-284.631442586	-0.000000034	0.000098790	0.000014493	135771948
						16495945
9	8	-284.631442602	-0.000000016	0.000249835	0.000013126	130579822
						16964257
10	9	-284.631442621	-0.000000019	0.000236315	0.000014907	156092836
						15069095
11	10	-284.631442636	-0.000000015	0.000235995	0.000015484	155809751
						15042340
12	11	-284.631442650	-0.000000015	0.000170452	0.000014531	156508422
						14999486
13	12	-284.631442661	-0.000000011	0.000255965	0.000009898	153953075
						15172469

-----DISABLING FDIFF OPTION-----

14 13	-284.631442665	-0.000000004	0.000128078	0.000006595	195931205
11510748					
15 14	-284.631442667	-0.000000003	0.000048163	0.000005305	195931133
11510748					
16 15	-284.631442669	-0.000000002	0.000029139	0.000004996	195931239
11510742					
17 16	-284.631442670	-0.000000001	0.000042473	0.000004314	195931205
11510743					
18 17	-284.631442671	-0.000000001	0.000090833	0.000003404	195931210
11510745					
19 18	-284.631442672	-0.000000001	0.000048546	0.000003213	195931183
11510749					
20 19	-284.631442673	0.000000000	0.000020187	0.000002938	195931086
11510748					
21 20	-284.631442673	-0.000000001	0.000039137	0.000002297	195931074
11510750					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 70.1 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 22.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6314426733 AFTER 21 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5954386949
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000544385

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 73.29 , TOTAL = 2644.9 SECONDS (44.1 MIN)
WALL CLOCK TIME: STEP = 67.26 , TOTAL = 2443.7 SECONDS (40.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 4.09 , TOTAL = 2649.0 SECONDS (44.2 MIN)
 WALL CLOCK TIME: STEP = 4.07 , TOTAL = 2447.8 SECONDS (40.8 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
 USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.83 , TOTAL = 2651.9 SECONDS (44.2 MIN)
 WALL CLOCK TIME: STEP = 2.70 , TOTAL = 2450.5 SECONDS (40.8 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 22 ENERGY= -284.6314427

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0001710	-0.0002628	0.0002348
2 C	6.0	0.0008914	-0.0008316	-0.0001025
3 C	6.0	0.0001428	-0.0015831	-0.0004664
4 C	6.0	0.0001721	0.0008420	-0.0003550
5 C	6.0	0.0002707	0.0002915	-0.0003405
6 C	6.0	0.0007569	-0.0006641	-0.0007141
7 C	6.0	-0.0009793	-0.0002826	-0.0002811
8 C	6.0	0.0008285	0.0000087	-0.0002552
9 C	6.0	-0.0006726	0.0003412	-0.0001385
10 C	6.0	0.0011943	0.0012995	0.0000097
11 C	6.0	-0.0000047	0.0016079	-0.0002247
12 N	7.0	0.0011743	-0.0004008	-0.0002188
13 C	6.0	0.0003012	0.0003224	0.0004862
14 C	6.0	0.0007684	-0.0002615	0.0006315
15 C	6.0	0.0004159	0.0004266	-0.0005736
16 C	6.0	-0.0003747	0.0007864	0.0003893
17 C	6.0	-0.0009081	-0.0000353	0.0003055
18 C	6.0	-0.0015194	-0.0001833	0.0005406
19 C	6.0	-0.0004551	-0.0014753	0.0005682
20 O	8.0	-0.0002172	0.0009772	-0.0009731
21 N	7.0	0.0000132	-0.0001124	0.0006925

22 H	1.0	-0.0003746	0.0005963	0.0002517
23 H	1.0	0.0008632	-0.0001038	0.0000920
24 H	1.0	-0.0004640	0.0003967	0.0000275
25 H	1.0	-0.0000053	-0.0012618	0.0002733
26 H	1.0	0.0000679	-0.0002834	0.0001142
27 H	1.0	-0.0003116	-0.0000711	-0.0004882
28 H	1.0	-0.0005283	0.0005126	-0.0002830
29 H	1.0	0.0007840	0.0001227	-0.0016938
30 H	1.0	0.0005320	0.0001003	-0.0009933
31 H	1.0	-0.0017841	0.0000349	0.0011213
32 H	1.0	-0.0009522	-0.0008583	-0.0001342
33 H	1.0	-0.0002905	-0.0001154	0.0002228
34 H	1.0	0.0000559	0.0004531	0.0000259
35 H	1.0	0.0004379	-0.0003333	0.0022489

MAXIMUM GRADIENT = 0.0022489 RMS GRADIENT = 0.0006877
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001231606
 PREDICTED ENERGY CHANGE WAS -0.0001976415 RATIO= 0.623
 GDIIS STEP HAS LENGTH = 0.211340
 RADIUS OF STEP TAKEN= 0.05261 CURRENT TRUST RADIUS= 0.05261

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 2651.9 SECONDS (44.2 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2450.5 SECONDS (40.8 MIN)
 CPU UTILIZATION: STEP = 95.25% , TOTAL = 100.00%

INSERCH= 23

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1122923199	-1.6723039999	1.0427097507
C	6.0	5.0014818314	0.6685195304	0.4278573817
C	6.0	5.2270803426	-0.6915646958	0.1848911811
C	6.0	4.0902870074	-1.5497251914	0.0569507049
C	6.0	2.7750638986	-1.0619078262	0.1838592533
C	6.0	2.4754456051	0.3372457647	0.4655716345
C	6.0	3.6633981822	1.1994484239	0.5660635622
C	6.0	3.5340903036	2.6131073781	0.8180500123
C	6.0	2.2760126195	3.2080601151	0.9811830501
C	6.0	1.1068776777	2.3892442343	0.9200095705
C	6.0	1.1699691238	0.9984546841	0.6623127474
N	7.0	-0.0692916946	0.2163296682	0.6917924143

C	6.0	-1.2834251613	0.7549390173	0.5376167339
C	6.0	-2.5924438218	0.0830824022	0.5943963571
C	6.0	-2.8627868199	-1.3231351910	0.7044711261
C	6.0	-4.1560063083	-1.8725723622	0.6333721442
C	6.0	-5.2800489251	-1.0017542013	0.5198347029
C	6.0	-5.0816662327	0.4071936108	0.4836665594
C	6.0	-3.7630185443	0.9284286393	0.4915241691
O	8.0	-1.7512451860	-2.2501643970	0.9023879577
N	7.0	1.7002852445	-2.1040973621	-0.0368982677
H	1.0	5.8472819353	1.3735811509	0.5227245024
H	1.0	6.2495272209	-1.0980986329	0.0844166476
H	1.0	4.2499911199	-2.6232464633	-0.1655074775
H	1.0	4.4581398766	3.2126121312	0.8935272836
H	1.0	2.1784316237	4.2881151234	1.1878506048
H	1.0	0.1352903496	2.8726465880	1.1183618369
H	1.0	-1.3564365179	1.8359092935	0.3058214708
H	1.0	-4.3036819439	-2.9693860450	0.6493206835
H	1.0	-6.2964474651	-1.4300090405	0.4499753102
H	1.0	-5.9521551861	1.0876693539	0.4333888784
H	1.0	-3.6204787278	2.0203369439	0.4133099682
H	1.0	-2.0790212874	-3.1786208410	1.0166096834
H	1.0	1.4195563279	-2.1086818372	-1.0428030911
H	1.0	2.1136482118	-3.0385509664	0.1642679529

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4554260	5.2781397	4.1001449
2 C	5.4554260	0.0000000	1.3999130 *	2.4266144 *
3 C	5.2781397	1.3999130 *	0.0000000	1.4300725 *
4 C	4.1001449	2.4266144 *	1.4300725 *	0.0000000
5 C	2.8636620 *	2.8303446 *	2.4798266 *	1.4085040 *
6 C	3.1552927	2.5479450 *	2.9510551 *	2.5170108 *
7 C	4.5917868	1.4461861 *	2.4832086 *	2.8283185 *
8 C	5.4885266	2.4671664 *	3.7666912	4.2682317
9 C	5.3388599	3.7661145	4.9547911	5.1751636
10 C	4.1833515	4.2861461	5.1969080	5.0160823
11 C	2.8976428 *	3.8528322	4.4208877	3.9227465
12 N	1.9295214 *	5.0977330	5.3974788	4.5633396
13 C	2.8451107 *	6.2864594	6.6785830	5.8667964
14 C	3.2554514	7.6182792	7.8684643	6.9002753
15 C	3.0145348	8.1172609	8.1311005	6.9868349
16 C	4.2925561	9.5057337	9.4677468	8.2727169
17 C	5.4589724	10.4167245	10.5170419	9.3977513

18 C	5.6226368	10.0866883	10.3714412	9.3880959
19 C	4.6995372	8.7685844	9.1400372	8.2464846
20 O	1.9561147 *	7.3717852	7.1861716	5.9438100
21 N	1.9681770 *	4.3360467	3.8056173	2.4552484 *
22 H	6.5144383	1.1052101 *	2.1825693 *	3.4423388
23 H	6.2380838	2.1900933 *	1.1048813 *	2.2061367 *
24 H	4.4141400	3.4281983	2.1929152 *	1.1078993 *
25 H	6.5399581	2.6428159 *	4.0417857	4.8492301
26 H	6.3100391	4.6528136	5.9243057	6.2461592
27 H	4.5456383	5.3865380	6.2850056	6.0271025
28 H	3.8739811	6.4653552	7.0530450	6.4180413
29 H	4.6193079	9.9934717	9.8101781	8.5337597
30 H	6.4406511	11.4911931	11.5502062	10.3948571
31 H	6.6907584	10.9616550	11.3226645	10.3898124
32 H	5.2882247	8.7273035	9.2566672	8.5046013
33 H	2.6592343 *	8.0796437	7.7624948	6.4524888
34 H	2.4997457 *	4.7650687	4.2441363	2.9418860 *
35 H	2.5775407 *	4.7065310	3.8990037	2.4769376 *

C C C C

1 CO	2.8636620 *	3.1552927	4.5917868	5.4885266
2 C	2.8303446 *	2.5479450 *	1.4461861 *	2.4671664 *
3 C	2.4798266 *	2.9510551 *	2.4832086 *	3.7666912
4 C	1.4085040 *	2.5170108 *	2.8283185 *	4.2682317
5 C	0.0000000	1.4583428 *	2.4594613 *	3.8057924
6 C	1.4583428 *	0.0000000	1.4712999 *	2.5346628 *
7 C	2.4594613 *	1.4712999 *	0.0000000	1.4417522 *
8 C	3.8057924	2.5346628 *	1.4417522 *	0.0000000
9 C	4.3723453	2.9235601 *	2.4762237 *	1.4011926 *
10 C	3.9032311	2.5080251 *	2.8419516 *	2.4396458 *
11 C	2.6552478 *	1.4765409 *	2.5033679 *	2.8671286 *
12 N	3.1594692	2.5576326 *	3.8620337	4.3295319
13 C	4.4606513	3.7826932	4.9668359	5.1710625
14 C	5.5036063	5.0758938	6.3547333	6.6321541
15 C	5.6678600	5.5955932	6.9981194	7.5117869
16 C	6.9927801	6.9919674	8.4014837	8.9046625
17 C	8.0623409	7.8704232	9.2104656	9.5312752
18 C	7.9985219	7.5574572	8.7812646	8.8999510
19 C	6.8412440	6.2664668	7.4317342	7.4961696
20 O	4.7345233	4.9749789	6.4289428	7.1828474
21 N	1.5132885 *	2.6102693 *	3.8898316	5.1328158
22 H	3.9350934	3.5279651	2.1912436 *	2.6409275 *
23 H	3.4760745	4.0557594	3.4926737	4.6567012
24 H	2.1760620 *	3.5088156	3.9360238	5.3758070
25 H	4.6484292	3.5188001	2.1889895 *	1.1040699 *

26 H	5.4760126	4.0273158	3.4830456	2.1863700 *
27 H	4.8293289	3.5115124	3.9436240	3.4218984
28 H	5.0479218	4.1176247	5.0667099	4.9783198
29 H	7.3460037	7.5448093	8.9922455	9.6241039
30 H	9.0828759	8.9481585	10.3017498	10.6358705
31 H	8.9915127	8.4610062	9.6171183	9.6158088
32 H	7.1032279	6.3242249	7.3315793	7.1904832
33 H	5.3606054	5.7799766	7.2350441	8.0678723
34 H	2.1066175 *	3.0614798	4.3089447	5.4981198
35 H	2.0844598 *	3.4084725	4.5303205	5.8639857

C C C N

1 CO	5.3388599	4.1833515	2.8976428 *	1.9295214 *
2 C	3.7661145	4.2861461	3.8528322	5.0977330
3 C	4.9547911	5.1969080	4.4208877	5.3974788
4 C	5.1751636	5.0160823	3.9227465	4.5633396
5 C	4.3723453	3.9032311	2.6552478 *	3.1594692
6 C	2.9235601 *	2.5080251 *	1.4765409 *	2.5576326 *
7 C	2.4762237 *	2.8419516 *	2.5033679 *	3.8620337
8 C	1.4011926 *	2.4396458 *	2.8671286 *	4.3295319
9 C	0.0000000	1.4286631 *	2.4914587 *	3.8124336
10 C	1.4286631 *	0.0000000	1.4158686 *	2.4813333 *
11 C	2.4914587 *	1.4158686 *	0.0000000	1.4657271 *
12 N	3.8124336	2.4813333 *	1.4657271 *	0.0000000
13 C	4.3455899	2.9207406 *	2.4686013 *	1.3371575 *
14 C	5.7980133	4.3714284	3.8727600	2.5285445 *
15 C	6.8567893	5.4393432	4.6534586	3.1896282
16 C	8.2039421	6.7781406	6.0505907	4.5900066
17 C	8.6619539	7.2423644	6.7545443	5.3539974
18 C	7.8884608	6.5128331	6.2820736	5.0203231
19 C	6.4735140	5.1023006	4.9364400	3.7670692
20 O	6.7836000	5.4491549	4.3754606	2.9928099 *
21 N	5.4393905	4.6322698	3.2242767	3.0077856
22 H	4.0409729	4.8642409	4.6944073	6.0310578
23 H	5.9275637	6.2694992	5.5255235	6.4825998
24 H	6.2622382	6.0151951	4.8258202	5.2396908
25 H	2.1838919 *	3.4510280	3.9708967	5.4328668
26 H	1.1039712 *	2.1967424 *	3.4806684	4.6773679
27 H	2.1711776 *	1.1031788 *	2.1888664 *	2.6981169 *
28 H	3.9412686	2.5983309 *	2.6853569 *	2.1044604 *
29 H	9.0312432	7.6198652	6.7605314	5.2991178
30 H	9.7611956	8.3436713	7.8542918	6.4456478
31 H	8.5146275	7.1945008	7.1263609	5.9526539
32 H	6.0416700	4.7687247	4.9045526	3.9928591
33 H	7.7302826	6.4156376	5.3037180	3.9585614

34 H	5.7530672	4.9174933	3.5530284	3.2605473
35 H	6.3018936	5.5718662	4.1756429	3.9544603

	C	C	C	C
--	---	---	---	---

1 CO	2.8451107 *	3.2554514	3.0145348	4.2925561
2 C	6.2864594	7.6182792	8.1172609	9.5057337
3 C	6.6785830	7.8684643	8.1311005	9.4677468
4 C	5.8667964	6.9002753	6.9868349	8.2727169
5 C	4.4606513	5.5036063	5.6678600	6.9927801
6 C	3.7826932	5.0758938	5.5955932	6.9919674
7 C	4.9668359	6.3547333	6.9981194	8.4014837
8 C	5.1710625	6.6321541	7.5117869	8.9046625
9 C	4.3455899	5.7980133	6.8567893	8.2039421
10 C	2.9207406 *	4.3714284	5.4393432	6.7781406
11 C	2.4686013 *	3.8727600	4.6534586	6.0505907
12 N	1.3371575 *	2.5285445 *	3.1896282	4.5900066
13 C	0.0000000	1.4724623 *	2.6154571 *	3.8941890
14 C	1.4724623 *	0.0000000	1.4361928 *	2.5041630 *
15 C	2.6154571 *	1.4361928 *	0.0000000	1.4068948 *
16 C	3.8941890	2.5041630 *	1.4068948 *	0.0000000
17 C	4.3656945	2.8992501 *	2.4455127 *	1.4264245 *
18 C	3.8145082	2.5126753 *	2.8224490 *	2.4650742 *
19 C	2.4860826 *	1.4475628 *	2.4341946 *	2.8319899 *
20 O	3.0630965	2.4993028 *	1.4608487 *	2.4490450 *
21 N	4.1721319	4.8589928	4.6884067	5.8990692
22 H	7.1575082	8.5381201	9.1197921	10.5173918
23 H	7.7707471	8.9350837	9.1361576	10.4487458
24 H	6.5211361	7.3973364	7.2827716	8.4771760
25 H	6.2555894	7.7197258	8.6142158	10.0065127
26 H	4.9890470	6.3871543	7.5586817	8.8536219
27 H	2.6143267 *	3.9365901	5.1734280	6.4161940
28 H	1.1079515 *	2.1641145 *	3.5224388	4.6580808
29 H	4.7963555	3.4998452	2.1884611 *	1.1068255 *
30 H	5.4691930	4.0037415	3.4447374	2.1933958 *
31 H	4.6817318	3.5103816	3.9280607	3.4683101
32 H	2.6605457 *	2.2005916 *	3.4405926	3.9357287
33 H	4.0416953	3.3287497	2.0382703 *	2.4832439 *
34 H	4.2431309	4.8559652	4.6913232	5.8268525
35 H	5.1058851	5.6636479	5.2914437	6.3943829

	C	C	C	O
--	---	---	---	---

1 CO	5.4589724	5.6226368	4.6995372	1.9561147 *
2 C	10.4167245	10.0866883	8.7685844	7.3717852
3 C	10.5170419	10.3714412	9.1400372	7.1861716

4 C	9.3977513	9.3880959	8.2464846	5.9438100
5 C	8.0623409	7.9985219	6.8412440	4.7345233
6 C	7.8704232	7.5574572	6.2664668	4.9749789
7 C	9.2104656	8.7812646	7.4317342	6.4289428
8 C	9.5312752	8.8999510	7.4961696	7.1828474
9 C	8.6619539	7.8884608	6.4735140	6.7836000
10 C	7.2423644	6.5128331	5.1023006	5.4491549
11 C	6.7545443	6.2820736	4.9364400	4.3754606
12 N	5.3539974	5.0203231	3.7670692	2.9928099 *
13 C	4.3656945	3.8145082	2.4860826 *	3.0630965
14 C	2.8992501 *	2.5126753 *	1.4475628 *	2.4993028 *
15 C	2.4455127 *	2.8224490 *	2.4341946 *	1.4608487 *
16 C	1.4264245 *	2.4650742 *	2.8319899 *	2.4490450 *
17 C	0.0000000	1.4233052 *	2.4551555 *	3.7626229
18 C	1.4233052 *	0.0000000	1.4179490 *	4.2811895
19 C	2.4551555 *	1.4179490 *	0.0000000	3.7841108
20 O	3.7626229	4.2811895	3.7841108	0.0000000
21 N	7.0887359	7.2506852	6.2708159	3.5800358
22 H	11.3780367	10.9716607	9.6206554	8.4269384
23 H	11.5381973	11.4377118	10.2236795	8.1245733
24 H	9.6912638	9.8328441	8.7894488	6.1069164
25 H	10.6175727	9.9521987	8.5420458	8.2703367
26 H	9.1683093	8.2623512	6.8609907	7.6336720
27 H	6.6854406	5.8049920	4.4011045	5.4634104
28 H	4.8469444	3.9937694	2.5786903 *	4.1482242
29 H	2.2003714 *	3.4690043	3.9382961	2.6638799 *
30 H	1.1051464 *	2.2027578 *	3.4615339	4.6407107
31 H	2.1965633 *	1.1060407 *	2.1956905 *	5.3859762
32 H	3.4494283	2.1776709 *	1.1039469 *	4.6872607
33 H	3.9028338	4.7072253	4.4698341	0.9912190 *
34 H	6.9679148	7.1362198	6.1997808	3.7226023
35 H	7.6773515	7.9842170	7.0978332	4.0129510

N H H H

1 CO	1.9681770 *	6.5144383	6.2380838	4.4141400
2 C	4.3360467	1.1052101 *	2.1900933 *	3.4281983
3 C	3.8056173	2.1825693 *	1.1048813 *	2.1929152 *
4 C	2.4552484 *	3.4423388	2.2061367 *	1.1078993 *
5 C	1.5132885 *	3.9350934	3.4760745	2.1760620 *
6 C	2.6102693 *	3.5279651	4.0557594	3.5088156
7 C	3.8898316	2.1912436 *	3.4926737	3.9360238
8 C	5.1328158	2.6409275 *	4.6567012	5.3758070
9 C	5.4393905	4.0409729	5.9275637	6.2622382
10 C	4.6322698	4.8642409	6.2694992	6.0151951
11 C	3.2242767	4.6944073	5.5255235	4.8258202

12 N	3.0077856	6.0310578	6.4825998	5.2396908
13 C	4.1721319	7.1575082	7.7707471	6.5211361
14 C	4.8589928	8.5381201	8.9350837	7.3973364
15 C	4.6884067	9.1197921	9.1361576	7.2827716
16 C	5.8990692	10.5173918	10.4487458	8.4771760
17 C	7.0887359	11.3780367	11.5381973	9.6912638
18 C	7.2506852	10.9716607	11.4377118	9.8328441
19 C	6.2708159	9.6206554	10.2236795	8.7894488
20 O	3.5800358	8.4269384	8.1245733	6.1069164
21 N	0.0000000	5.4410483	4.6607245	2.6051979 *
22 H	5.4410483	0.0000000	2.5422659 *	4.3588568
23 H	4.6607245	2.5422659 *	0.0000000	2.5271887 *
24 H	2.6051979 *	4.3588568	2.5271887 *	0.0000000
25 H	6.0612584	2.3343619 *	4.7377163	5.9348232
26 H	6.5260259	4.7325853	6.8412488	7.3409710
27 H	5.3433899	5.9353878	7.3634063	6.9845489
28 H	4.9984655	7.2217971	8.1552503	7.1790147
29 H	6.1046902	11.0417145	10.7327097	8.5993651
30 H	8.0398492	12.4633693	12.5556871	10.6315569
31 H	8.3047209	11.8032387	12.4008232	10.8725969
32 H	6.7471605	9.4904561	10.3561493	9.1565382
33 H	4.0678788	9.1538379	8.6349451	6.4623711
34 H	1.0443535 *	5.8465192	5.0616718	3.0076212
35 H	1.0414127 *	5.7909776	4.5691604	2.2011794 *

H H H H

1 CO	6.5399581	6.3100391	4.5456383	3.8739811
2 C	2.6428159 *	4.6528136	5.3865380	6.4653552
3 C	4.0417857	5.9243057	6.2850056	7.0530450
4 C	4.8492301	6.2461592	6.0271025	6.4180413
5 C	4.6484292	5.4760126	4.8293289	5.0479218
6 C	3.5188001	4.0273158	3.5115124	4.1176247
7 C	2.1889895 *	3.4830456	3.9436240	5.0667099
8 C	1.1040699 *	2.1863700 *	3.4218984	4.9783198
9 C	2.1838919 *	1.1039712 *	2.1711776 *	3.9412686
10 C	3.4510280	2.1967424 *	1.1031788 *	2.5983309 *
11 C	3.9708967	3.4806684	2.1888664 *	2.6853569 *
12 N	5.4328668	4.6773679	2.6981169 *	2.1044604 *
13 C	6.2555894	4.9890470	2.6143267 *	1.1079515 *
14 C	7.7197258	6.3871543	3.9365901	2.1641145 *
15 C	8.6142158	7.5586817	5.1734280	3.5224388
16 C	10.0065127	8.8536219	6.4161940	4.6580808
17 C	10.6175727	9.1683093	6.6854406	4.8469444
18 C	9.9521987	8.2623512	5.8049920	3.9937694
19 C	8.5420458	6.8609907	4.4011045	2.5786903 *

20	O	8.2703367	7.6336720	5.4634104	4.1482242
21	N	6.0612584	6.5260259	5.3433899	4.9984655
22	H	2.3343619 *	4.7325853	5.9353878	7.2217971
23	H	4.7377163	6.8412488	7.3634063	8.1552503
24	H	5.9348232	7.3409710	6.9845489	7.1790147
25	H	0.0000000	2.5377948 *	4.3420220	6.0041658
26	H	2.5377948 *	0.0000000	2.4865249 *	4.3916491
27	H	4.3420220	2.4865249 *	0.0000000	1.9900490 *
28	H	6.0041658	4.3916491	1.9900490 *	0.0000000
29	H	10.7259620	9.7457239	7.3521303	5.6475756
30	H	11.7222787	10.2501209	7.7670353	5.9237413
31	H	10.6349120	8.7703197	6.3806210	4.6579788
32	H	8.1802327	6.2745591	3.9152690	2.2740832 *
33	H	9.1431660	8.5969398	6.4444835	5.1159419
34	H	6.4263936	6.8169435	5.5797496	5.0084652
35	H	6.7160629	7.3981048	6.3060647	5.9851390

H H H H

1	CO	4.6193079	6.4406511	6.6907584	5.2882247
2	C	9.9934717	11.4911931	10.9616550	8.7273035
3	C	9.8101781	11.5502062	11.3226645	9.2566672
4	C	8.5337597	10.3948571	10.3898124	8.5046013
5	C	7.3460037	9.0828759	8.9915127	7.1032279
6	C	7.5448093	8.9481585	8.4610062	6.3242249
7	C	8.9922455	10.3017498	9.6171183	7.3315793
8	C	9.6241039	10.6358705	9.6158088	7.1904832
9	C	9.0312432	9.7611956	8.5146275	6.0416700
10	C	7.6198652	8.3436713	7.1945008	4.7687247
11	C	6.7605314	7.8542918	7.1263609	4.9045526
12	N	5.2991178	6.4456478	5.9526539	3.9928591
13	C	4.7963555	5.4691930	4.6817318	2.6605457 *
14	C	3.4998452	4.0037415	3.5103816	2.2005916 *
15	C	2.1884611 *	3.4447374	3.9280607	3.4405926
16	C	1.1068255 *	2.1933958 *	3.4683101	3.9357287
17	C	2.2003714 *	1.1051464 *	2.1965633 *	3.4494283
18	C	3.4690043	2.2027578 *	1.1060407 *	2.1776709 *
19	C	3.9382961	3.4615339	2.1956905 *	1.1039469 *
20	O	2.6638799 *	4.6407107	5.3859762	4.6872607
21	N	6.1046902	8.0398492	8.3047209	6.7471605
22	H	11.0417145	12.4633693	11.8032387	9.4904561
23	H	10.7327097	12.5556871	12.4008232	10.3561493
24	H	8.5993651	10.6315569	10.8725969	9.1565382
25	H	10.7259620	11.7222787	10.6349120	8.1802327
26	H	9.7457239	10.2501209	8.7703197	6.2745591
27	H	7.3521303	7.7670353	6.3806210	3.9152690

28 H	5.6475756	5.9237413	4.6579788	2.2740832 *
29 H	0.0000000	2.5259720 *	4.3844942	5.0418055
30 H	2.5259720 *	0.0000000	2.5411645 *	4.3665822
31 H	4.3844942	2.5411645 *	0.0000000	2.5113716 *
32 H	5.0418055	4.3665822	2.5113716 *	0.0000000
33 H	2.2644636 *	4.6005871	5.7915926	5.4561180
34 H	6.0298881	7.8883267	8.1693289	6.6761527
35 H	6.4360070	8.5673068	9.0639563	7.6507895

H H H

1 CO	2.6592343 *	2.4997457 *	2.5775407 *
2 C	8.0796437	4.7650687	4.7065310
3 C	7.7624948	4.2441363	3.8990037
4 C	6.4524888	2.9418860 *	2.4769376 *
5 C	5.3606054	2.1066175 *	2.0844598 *
6 C	5.7799766	3.0614798	3.4084725
7 C	7.2350441	4.3089447	4.5303205
8 C	8.0678723	5.4981198	5.8639857
9 C	7.7302826	5.7530672	6.3018936
10 C	6.4156376	4.9174933	5.5718662
11 C	5.3037180	3.5530284	4.1756429
12 N	3.9585614	3.2605473	3.9544603
13 C	4.0416953	4.2431309	5.1058851
14 C	3.3287497	4.8559652	5.6636479
15 C	2.0382703 *	4.6913232	5.2914437
16 C	2.4832439 *	5.8268525	6.3943829
17 C	3.9028338	6.9679148	7.6773515
18 C	4.7072253	7.1362198	7.9842170
19 C	4.4698341	6.1997808	7.0978332
20 O	0.9912190 *	3.7226023	4.0129510
21 N	4.0678788	1.0443535 *	1.0414127 *
22 H	9.1538379	5.8465192	5.7909776
23 H	8.6349451	5.0616718	4.5691604
24 H	6.4623711	3.0076212	2.2011794 *
25 H	9.1431660	6.4263936	6.7160629
26 H	8.5969398	6.8169435	7.3981048
27 H	6.4444835	5.5797496	6.3060647
28 H	5.1159419	5.0084652	5.9851390
29 H	2.2644636 *	6.0298881	6.4360070
30 H	4.6005871	7.8883267	8.5673068
31 H	5.7915926	8.1693289	9.0639563
32 H	5.4561180	6.6761527	7.6507895
33 H	0.0000000	4.1983325	4.2807223
34 H	4.1983325	0.0000000	1.6743478 *
35 H	4.2807223	1.6743478 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.69 , TOTAL = 2652.6 SECONDS (44.2 MIN)
WALL CLOCK TIME: STEP = 0.69 , TOTAL = 2451.2 SECONDS (40.9 MIN)

CPU UTILIZATION: STEP = 99.30%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.89 , TOTAL = 2653.5 SECONDS (44.2 MIN)
WALL CLOCK TIME: STEP = 0.89 , TOTAL = 2452.1 SECONDS (40.9 MIN)

CPU UTILIZATION: STEP = 99.46%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.631497707	-284.631497707	0.013115982	0.001164608	195895087
11512478						
2	1	-284.631561201	-0.000063494	0.003131247	0.000101582	155098141
14980255						
3	2	-284.631559173	0.000002028	0.001240046	0.000236264	142415061
15946599						
4	3	-284.631562725	-0.000003553	0.000577743	0.000070791	137196991
16356387						
5	4	-284.631562491	0.000000235	0.000397303	0.000139826	128629953
17049901						
6	5	-284.631562810	-0.000000319	0.000199261	0.000019351	123721098
17431940						
7	6	-284.631562796	0.000000013	0.000118278	0.000017525	115757390
17981301						
8	7	-284.631562820	-0.000000024	0.000177310	0.000014294	132775204
16751223						
9	8	-284.631562836	-0.000000016	0.000287477	0.000014843	156490505
14924253						
-----DISABLING FDIFF OPTION-----						
10	9	-284.631562915	-0.000000078	0.000225453	0.000016478	195889408
11512905						

11 10	-284.631562931	-0.000000016	0.000271144	0.000015796	195889499
11512894					
12 11	-284.631562947	-0.000000016	0.000167405	0.000012730	195889536
11512895					
13 12	-284.631562957	-0.000000010	0.000255907	0.000008314	195889577
11512895					
14 13	-284.631562967	-0.000000010	0.000109484	0.000005970	195889605
11512901					
15 14	-284.631562968	-0.000000001	0.000058239	0.000006093	195889566
11512903					
16 15	-284.631562971	-0.000000002	0.000035219	0.000005438	195889620
11512899					
17 16	-284.631562972	-0.000000001	0.000062001	0.000004429	195889702
11512895					
18 17	-284.631562973	-0.000000001	0.000065622	0.000002572	195889766
11512890					
19 18	-284.631562974	-0.000000001	0.000045718	0.000003390	195889742
11512892					
20 19	-284.631562975	-0.000000001	0.000017567	0.000002689	195889666
11512895					
21 20	-284.631562975	0.000000000	0.000031939	0.000002282	195889644
11512898					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 70.4 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 22.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.8 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6315629754 AFTER 21 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5938853528
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000516696

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 73.23 , TOTAL = 2726.7 SECONDS (45.4 MIN)
WALL CLOCK TIME: STEP = 67.46 , TOTAL = 2519.6 SECONDS (42.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.99 , TOTAL = 2730.7 SECONDS (45.5 MIN)
WALL CLOCK TIME: STEP = 3.96 , TOTAL = 2523.6 SECONDS (42.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.81 , TOTAL = 2733.5 SECONDS (45.6 MIN)
WALL CLOCK TIME: STEP = 2.65 , TOTAL = 2526.2 SECONDS (42.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 23 ENERGY= -284.6315630

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0001475	-0.0003363	0.0003294
2 C	6.0	0.0006838	-0.0006228	-0.0000581
3 C	6.0	0.0005317	-0.0012734	-0.0004440
4 C	6.0	0.0001787	0.0007594	-0.0003795
5 C	6.0	0.0004704	0.0005063	-0.0001516
6 C	6.0	0.0006446	-0.0002549	-0.0006475
7 C	6.0	-0.0007709	0.0000126	-0.0002628
8 C	6.0	0.0010215	-0.0005587	-0.0003168
9 C	6.0	-0.0003476	0.0007872	-0.0000758
10 C	6.0	0.0004906	0.0008704	-0.0000371
11 C	6.0	0.0002138	0.0012705	-0.0002811
12 N	7.0	0.0009332	-0.0001710	-0.0001712
13 C	6.0	0.0005787	0.0002391	0.0004510
14 C	6.0	0.0008312	-0.0002927	0.0006035
15 C	6.0	0.0002735	0.0004835	-0.0004097

16 C	6.0	-0.0000412	0.0012493	0.0004329
17 C	6.0	-0.0008999	-0.0002370	0.0003535
18 C	6.0	-0.0017315	-0.0001492	0.0005244
19 C	6.0	-0.0001929	-0.0009265	0.0005328
20 O	8.0	0.0000470	0.0004685	-0.0011512
21 N	7.0	-0.0001892	-0.0005462	0.0006637
22 H	1.0	-0.0003092	0.0006283	0.0002380
23 H	1.0	0.0007291	-0.0000991	0.0000921
24 H	1.0	-0.0004628	0.0000273	-0.0000958
25 H	1.0	0.0001106	-0.0012142	0.0002268
26 H	1.0	0.0000303	-0.0000951	0.0001275
27 H	1.0	-0.0001949	-0.0001720	-0.0005039
28 H	1.0	-0.0007222	0.0005392	-0.0003116
29 H	1.0	0.0006363	0.0001357	-0.0015838
30 H	1.0	-0.0000003	0.0000679	-0.0011270
31 H	1.0	-0.0017948	-0.0000204	0.0009969
32 H	1.0	-0.0009826	-0.0015241	0.0000435
33 H	1.0	-0.0003030	0.0003066	0.0001849
34 H	1.0	0.0000655	0.0006807	-0.0000815
35 H	1.0	0.0003250	-0.0005390	0.0022893

MAXIMUM GRADIENT = 0.0022893 RMS GRADIENT = 0.0006604
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001203021
 PREDICTED ENERGY CHANGE WAS -0.0001883597 RATIO= 0.639
 GDIIS STEP HAS LENGTH = 0.258058
 RADIUS OF STEP TAKEN= 0.05261 CURRENT TRUST RADIUS= 0.05261

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 2733.5 SECONDS (45.6 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2526.2 SECONDS (42.1
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 24

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1124730984	-1.6753008112	1.0431174532
C	6.0	5.0019404184	0.6700512653	0.4283040705
C	6.0	5.2282309329	-0.6900176684	0.1858452779
C	6.0	4.0923459725	-1.5500999021	0.0582308742
C	6.0	2.7766129245	-1.0626918391	0.1860970124
C	6.0	2.4767673335	0.3365551524	0.4679189208

C	6.0	3.6640575632	1.2000550160	0.5673080033
C	6.0	3.5336323921	2.6139106792	0.8180491447
C	6.0	2.2748716654	3.2075228968	0.9816628322
C	6.0	1.1065105583	2.3869654111	0.9217089080
C	6.0	1.1706751569	0.9960679933	0.6644838359
N	7.0	-0.0688604397	0.2140262693	0.6940421771
C	6.0	-1.2826524628	0.7526648660	0.5375560648
C	6.0	-2.5919751831	0.0814851471	0.5950017845
C	6.0	-2.8635936094	-1.3237731078	0.7079246146
C	6.0	-4.1578641575	-1.8714746593	0.6394302520
C	6.0	-5.2816189522	-1.0002838601	0.5204197185
C	6.0	-5.0805892733	0.4080697146	0.4794594363
C	6.0	-3.7615227609	0.9276511250	0.4901069716
O	8.0	-1.7520072022	-2.2523226423	0.9018339127
N	7.0	1.7004171243	-2.1030907338	-0.0394206359
H	1.0	5.8482533038	1.3753865347	0.5217229574
H	1.0	6.2506286243	-1.0958721386	0.0844195723
H	1.0	4.2526486841	-2.6235162033	-0.1660905447
H	1.0	4.4574018311	3.2144359561	0.8912025884
H	1.0	2.1762603017	4.2880208776	1.1871063405
H	1.0	0.1345532401	2.8691250421	1.1209056852
H	1.0	-1.3560795322	1.8331384381	0.3035196828
H	1.0	-4.3083476848	-2.9677523057	0.6616585477
H	1.0	-6.2990852724	-1.4269271817	0.4495227250
H	1.0	-5.9499951279	1.0895708457	0.4231622297
H	1.0	-3.6171626405	2.0193261132	0.4129933051
H	1.0	-2.0811233331	-3.1801707137	1.0146822300
H	1.0	1.4186517833	-2.0993535399	-1.0452563109
H	1.0	2.1115417228	-3.0402770365	0.1542573623

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4576151	5.2798368	4.1018368
2 C	5.4576151	0.0000000	1.3999218 *	2.4276300 *
3 C	5.2798368	1.3999218 *	0.0000000	1.4304760 *
4 C	4.1018368	2.4276300 *	1.4304760 *	0.0000000
5 C	2.8648586 *	2.8307500 *	2.4797816 *	1.4089251 *
6 C	3.1572623	2.5474081 *	2.9502490 *	2.5174205 *
7 C	4.5943245	1.4457374 *	2.4828465 *	2.8294774 *
8 C	5.4911130	2.4670669 *	3.7666017	4.2694811
9 C	5.3405722	3.7658827	4.9544403	5.1759940
10 C	4.1838807	4.2855124	5.1959502	5.0161031
11 C	2.8981660 *	3.8523579	4.4199252	3.9225851

12 N	1.9298425 *	5.0981955	5.3976603	4.5642125
13 C	2.8455202 *	6.2860853	6.6780713	5.8671191
14 C	3.2559400	7.6185138	7.8688150	6.9014739
15 C	3.0154434	8.1191224	8.1333780	6.9898799
16 C	4.2938593	9.5082043	9.4710275	8.2768981
17 C	5.4612352	10.4187378	10.5197505	9.4014432
18 C	5.6237034	10.0860625	10.3712959	9.3890683
19 C	4.6998961	8.7674662	9.1392067	8.2467582
20 O	1.9568347 *	7.3743005	7.1886828	5.9465323
21 N	1.9688726 *	4.3369504	3.8069660	2.4569612 *
22 H	6.5174934	1.1056538 *	2.1824610 *	3.4433278
23 H	6.2395346	2.1899690 *	1.1046728 *	2.2057182 *
24 H	4.4161465	3.4296253	2.1940912 *	1.1082597 *
25 H	6.5430123	2.6428566 *	4.0418393	4.8505577
26 H	6.3119851	4.6529510	5.9243494	6.2473513
27 H	4.5451452	5.3858222	6.2838990	6.0268524
28 H	3.8746352	6.4647321	7.0521846	6.4180845
29 H	4.6216445	9.9984766	9.8163540	8.5408148
30 H	6.4437664	11.4939528	11.5538556	10.3995252
31 H	6.6919639	10.9599688	11.3214837	10.3898822
32 H	5.2874859	8.7240882	9.2538169	8.5031277
33 H	2.6603209 *	8.0831826	7.7662406	6.4562879
34 H	2.4994456 *	4.7624511	4.2443765	2.9441474 *
35 H	2.5786639 *	4.7112676	3.9036481	2.4806117 *

C C C C

1 CO	2.8648586 *	3.1572623	4.5943245	5.4911130
2 C	2.8307500 *	2.5474081 *	1.4457374 *	2.4670669 *
3 C	2.4797816 *	2.9502490 *	2.4828465 *	3.7666017
4 C	1.4089251 *	2.5174205 *	2.8294774 *	4.2694811
5 C	0.0000000	1.4585003 *	2.4602649 *	3.8065533
6 C	1.4585003 *	0.0000000	1.4714511 *	2.5349365 *
7 C	2.4602649 *	1.4714511 *	0.0000000	1.4418286 *
8 C	3.8065533	2.5349365 *	1.4418286 *	0.0000000
9 C	4.3725740	2.9235510 *	2.4761774 *	1.4012935 *
10 C	3.9026276	2.5075309 *	2.8417254 *	2.4399119 *
11 C	2.6545022 *	1.4763034 *	2.5035993 *	2.8678501 *
12 N	3.1598633	2.5585867 *	3.8630287	4.3304477
13 C	4.4605693	3.7830191	4.9669894	5.1710262
14 C	5.5043694	5.0767471	6.3553058	6.6321940
15 C	5.6703084	5.5976556	6.9999794	7.5127879
16 C	6.9961856	6.9945083	8.4036870	8.9055997
17 C	8.0654056	7.8728935	9.2124274	9.5320324
18 C	7.9990517	7.5577038	8.7808773	8.8986062
19 C	6.8411333	6.2662708	7.4309762	7.4946852

20	O	4.7366550	4.9772587	6.4315299	7.1850701
21	N	1.5137653 *	2.6099780 *	3.8903438	5.1328389
22	H	3.9359682	3.5283117	2.1916957 *	2.6418216 *
23	H	3.4756617	4.0547440	3.4921072	4.6564761
24	H	2.1768992 *	3.5096645	3.9375132	5.3773744
25	H	4.6493061	3.5191306	2.1890714 *	1.1042337 *
26	H	5.4765472	4.0276068	3.4832777	2.1866200 *
27	H	4.8284087	3.5108786	3.9433065	3.4220747
28	H	5.0476498	4.1179490	5.0667697	4.9783158
29	H	7.3520120	7.5494217	8.9965974	9.6268412
30	H	9.0868233	8.9513014	10.3043255	10.6370353
31	H	8.9912248	8.4604587	9.6157680	9.6134665
32	H	7.1014564	6.3222399	7.3287916	7.1868958
33	H	5.3635689	5.7827916	7.2383441	8.0706583
34	H	2.1059337 *	3.0566254	4.3044521	5.4918039
35	H	2.0866664 *	3.4109777	4.5344605	5.8679468

C C C N

1	CO	5.3405722	4.1838807	2.8981660 *	1.9298425 *
2	C	3.7658827	4.2855124	3.8523579	5.0981955
3	C	4.9544403	5.1959502	4.4199252	5.3976603
4	C	5.1759940	5.0161031	3.9225851	4.5642125
5	C	4.3725740	3.9026276	2.6545022 *	3.1598633
6	C	2.9235510 *	2.5075309 *	1.4763034 *	2.5585867 *
7	C	2.4761774 *	2.8417254 *	2.5035993 *	3.8630287
8	C	1.4012935 *	2.4399119 *	2.8678501 *	4.3304477
9	C	0.0000000	1.4289775 *	2.4920645 *	3.8127192
10	C	1.4289775 *	0.0000000	1.4159370 *	2.4809260 *
11	C	2.4920645 *	1.4159370 *	0.0000000	1.4659166 *
12	N	3.8127192	2.4809260 *	1.4659166 *	0.0000000
13	C	4.3450589	2.9200362 *	2.4686377 *	1.3371277 *
14	C	5.7972249	4.3704432	3.8728319	2.5285340 *
15	C	6.8564861	5.4384751	4.6539096	3.1899143
16	C	8.2032572	6.7769930	6.0511784	4.5904518
17	C	8.6613471	7.2417325	6.7556106	5.3551419
18	C	7.8861874	6.5108999	6.2815828	5.0200722
19	C	6.4712827	5.1003556	4.9357537	3.7665110
20	O	6.7846915	5.4492671	4.3761226	2.9931651 *
21	N	5.4383110	4.6300215	3.2219393	3.0062172
22	H	4.0419457	4.8649157	4.6951039	6.0324694
23	H	5.9271323	6.2684258	5.5243656	6.4825470
24	H	6.2633822	6.0155148	4.8259511	5.2408889
25	H	2.1844150 *	3.4516823	3.9717918	5.4340023
26	H	1.1042677 *	2.1974558 *	3.4815642	4.6777250
27	H	2.1713739 *	1.1031130 *	2.1886553 *	2.6968758 *

28 H	3.9411442	2.5986982 *	2.6861629 *	2.1049858 *
29 H	9.0318992	7.6197978	6.7625122	5.3007561
30 H	9.7608421	8.3433558	7.8558535	6.4473420
31 H	8.5115262	7.1920827	7.1253719	5.9521172
32 H	6.0374883	4.7651903	4.9024173	3.9910581
33 H	7.7316500	6.4158132	5.3045077	3.9588616
34 H	5.7449501	4.9085071	3.5449031	3.2541632
35 H	6.3044651	5.5726143	4.1758403	3.9542397

C C C C

1 CO	2.8455202 *	3.2559400	3.0154434	4.2938593
2 C	6.2860853	7.6185138	8.1191224	9.5082043
3 C	6.6780713	7.8688150	8.1333780	9.4710275
4 C	5.8671191	6.9014739	6.9898799	8.2768981
5 C	4.4605693	5.5043694	5.6703084	6.9961856
6 C	3.7830191	5.0767471	5.5976556	6.9945083
7 C	4.9669894	6.3553058	6.9999794	8.4036870
8 C	5.1710262	6.6321940	7.5127879	8.9055997
9 C	4.3450589	5.7972249	6.8564861	8.2032572
10 C	2.9200362 *	4.3704432	5.4384751	6.7769930
11 C	2.4686377 *	3.8728319	4.6539096	6.0511784
12 N	1.3371277 *	2.5285340 *	3.1899143	4.5904518
13 C	0.0000000	1.4724497 *	2.6153384 *	3.8940119
14 C	1.4724497 *	0.0000000	1.4357155 *	2.5036042 *
15 C	2.6153384 *	1.4357155 *	0.0000000	1.4070553 *
16 C	3.8940119	2.5036042 *	1.4070553 *	0.0000000
17 C	4.3663321	2.8999949 *	2.4467632 *	1.4268713 *
18 C	3.8139802	2.5126097 *	2.8225070 *	2.4644137 *
19 C	2.4854918 *	1.4473567 *	2.4336459 *	2.8309873 *
20 O	3.0631589	2.4992701 *	1.4613108 *	2.4499079 *
21 N	4.1697657	4.8579312	4.6899952	5.9020288
22 H	7.1580619	8.5391456	9.1223029	10.5203778
23 H	7.7699901	8.9352396	9.1383666	10.4520964
24 H	6.5217541	7.3989979	7.2865725	8.4824028
25 H	6.2556859	7.7198984	8.6154458	10.0076313
26 H	4.9884602	6.3860473	7.5579081	8.8521448
27 H	2.6130772 *	3.9346497	5.1710572	6.4132637
28 H	1.1079656 *	2.1634900 *	3.5216804	4.6569294
29 H	4.7970550	3.4997467	2.1890917 *	1.1067809 *
30 H	5.4701892	4.0048892	3.4467398	2.1951117 *
31 H	4.6808844	3.5102797	3.9282557	3.4678950
32 H	2.6589254 *	2.1998555 *	3.4396458	3.9347125
33 H	4.0413365	3.3279874	2.0377861 *	2.4832140 *
34 H	4.2351327	4.8509414	4.6917794	5.8298909
35 H	5.1043002	5.6623958	5.2919661	6.3958535

	C	C	C	O
1 CO	5.4612352	5.6237034	4.6998961	1.9568347 *
2 C	10.4187378	10.0860625	8.7674662	7.3743005
3 C	10.5197505	10.3712959	9.1392067	7.1886828
4 C	9.4014432	9.3890683	8.2467582	5.9465323
5 C	8.0654056	7.9990517	6.8411333	4.7366550
6 C	7.8728935	7.5577038	6.2662708	4.9772587
7 C	9.2124274	8.7808773	7.4309762	6.4315299
8 C	9.5320324	8.8986062	7.4946852	7.1850701
9 C	8.6613471	7.8861874	6.4712827	6.7846915
10 C	7.2417325	6.5108999	5.1003556	5.4492671
11 C	6.7556106	6.2815828	4.9357537	4.3761226
12 N	5.3551419	5.0200722	3.7665110	2.9931651 *
13 C	4.3663321	3.8139802	2.4854918 *	3.0631589
14 C	2.8999949 *	2.5126097 *	1.4473567 *	2.4992701 *
15 C	2.4467632 *	2.8225070 *	2.4336459 *	1.4613108 *
16 C	1.4268713 *	2.4644137 *	2.8309873 *	2.4499079 *
17 C	0.0000000	1.4232183 *	2.4553095 *	3.7644703
18 C	1.4232183 *	0.0000000	1.4177499 *	4.2820026
19 C	2.4553095 *	1.4177499 *	0.0000000	3.7841650
20 O	3.7644703	4.2820026	3.7841650	0.0000000
21 N	7.0907286	7.2496352	6.2688582	3.5815449
22 H	11.3805917	10.9716493	9.6202527	8.4302264
23 H	11.5408824	11.4374121	10.2226417	8.1269751
24 H	9.6957949	9.8344587	8.7902405	6.1101669
25 H	10.6183741	9.9508039	8.5405494	8.2729876
26 H	9.1668207	8.2593372	6.8582185	7.6347075
27 H	6.6833996	5.8022373	4.3984811	5.4622641
28 H	4.8461518	3.9917100	2.5769903 *	4.1479791
29 H	2.1995767 *	3.4678131	3.9373361	2.6654081 *
30 H	1.1055716 *	2.2029168 *	3.4619228	4.6434666
31 H	2.1962874 *	1.1061102 *	2.1954751 *	5.3870661
32 H	3.4496376	2.1776553 *	1.1038753 *	4.6866569
33 H	3.9037641	4.7073059	4.4691299	0.9909360 *
34 H	6.9679928	7.1310633	6.1930853	3.7239278
35 H	7.6781815	7.9827063	7.0957829	4.0133220

	N	H	H	H
1 CO	1.9688726 *	6.5174934	6.2395346	4.4161465
2 C	4.3369504	1.1056538 *	2.1899690 *	3.4296253
3 C	3.8069660	2.1824610 *	1.1046728 *	2.1940912 *
4 C	2.4569612 *	3.4433278	2.2057182 *	1.1082597 *
5 C	1.5137653 *	3.9359682	3.4756617	2.1768992 *

6 C	2.6099780 *	3.5283117	4.0547440	3.5096645
7 C	3.8903438	2.1916957 *	3.4921072	3.9375132
8 C	5.1328389	2.6418216 *	4.6564761	5.3773744
9 C	5.4383110	4.0419457	5.9271323	6.2633822
10 C	4.6300215	4.8649157	6.2684258	6.0155148
11 C	3.2219393	4.6951039	5.5243656	4.8259511
12 N	3.0062172	6.0324694	6.4825470	5.2408889
13 C	4.1697657	7.1580619	7.7699901	6.5217541
14 C	4.8579312	8.5391456	8.9352396	7.3989979
15 C	4.6899952	9.1223029	9.1383666	7.2865725
16 C	5.9020288	10.5203778	10.4520964	8.4824028
17 C	7.0907286	11.3805917	11.5408824	9.6957949
18 C	7.2496352	10.9716493	11.4374121	9.8344587
19 C	6.2688582	9.6202527	10.2226417	8.7902405
20 O	3.5815449	8.4302264	8.1269751	6.1101669
21 N	0.0000000	5.4423553	4.6620007	2.6078293 *
22 H	5.4423553	0.0000000	2.5417041 *	4.3600762
23 H	4.6620007	2.5417041 *	0.0000000	2.5275236 *
24 H	2.6078293 *	4.3600762	2.5275236 *	0.0000000
25 H	6.0616099	2.3351843 *	4.7376489	5.9364533
26 H	6.5251132	4.7338891	6.8412498	7.3424707
27 H	5.3405259	5.9360461	7.3621929	6.9845671
28 H	4.9953658	7.2221576	8.1540859	7.1791459
29 H	6.1110070	11.0471254	10.7391397	8.6078061
30 H	8.0429038	12.4665957	12.5593876	10.6371939
31 H	8.3027633	11.8021215	12.3994406	10.8732780
32 H	6.7435639	9.4879175	10.3530539	9.1556132
33 H	4.0707840	9.1581180	8.6387372	6.4668970
34 H	1.0445626 *	5.8438525	5.0627209	3.0131740
35 H	1.0415627 *	5.7962168	4.5735794	2.2046885 *

H H H H

1 CO	6.5430123	6.3119851	4.5451452	3.8746352
2 C	2.6428566 *	4.6529510	5.3858222	6.4647321
3 C	4.0418393	5.9243494	6.2838990	7.0521846
4 C	4.8505577	6.2473513	6.0268524	6.4180845
5 C	4.6493061	5.4765472	4.8284087	5.0476498
6 C	3.5191306	4.0276068	3.5108786	4.1179490
7 C	2.1890714 *	3.4832777	3.9433065	5.0667697
8 C	1.1042337 *	2.1866200 *	3.4220747	4.9783158
9 C	2.1844150 *	1.1042677 *	2.1713739 *	3.9411442
10 C	3.4516823	2.1974558 *	1.1031130 *	2.5986982 *
11 C	3.9717918	3.4815642	2.1886553 *	2.6861629 *
12 N	5.4340023	4.6777250	2.6968758 *	2.1049858 *
13 C	6.2556859	4.9884602	2.6130772 *	1.1079656 *

14 C	7.7198984	6.3860473	3.9346497	2.1634900 *
15 C	8.6154458	7.5579081	5.1710572	3.5216804
16 C	10.0076313	8.8521448	6.4132637	4.6569294
17 C	10.6183741	9.1668207	6.6833996	4.8461518
18 C	9.9508039	8.2593372	5.8022373	3.9917100
19 C	8.5405494	6.8582185	4.3984811	2.5769903 *
20 O	8.2729876	7.6347075	5.4622641	4.1479791
21 N	6.0616099	6.5251132	5.3405259	4.9953658
22 H	2.3351843 *	4.7338891	5.9360461	7.2221576
23 H	4.7376489	6.8412498	7.3621929	8.1540859
24 H	5.9364533	7.3424707	6.9845671	7.1791459
25 H	0.0000000	2.5384543 *	4.3426977	6.0041585
26 H	2.5384543 *	0.0000000	2.4872104 *	4.3914232
27 H	4.3426977	2.4872104 *	0.0000000	1.9908225 *
28 H	6.0041585	4.3914232	1.9908225 *	0.0000000
29 H	10.7289565	9.7453825	7.3497900	5.6473624
30 H	11.7234529	10.2487142	7.7652124	5.9230609
31 H	10.6324045	8.7663972	6.3777259	4.6552409
32 H	8.1765251	6.2697668	3.9113515	2.2713756 *
33 H	9.1465050	8.5981935	6.4431735	5.1151451
34 H	6.4202986	6.8085215	5.5701837	4.9982821
35 H	6.7206832	7.4010078	6.3058644	5.9830473

H H H H

1 CO	4.6216445	6.4437664	6.6919639	5.2874859
2 C	9.9984766	11.4939528	10.9599688	8.7240882
3 C	9.8163540	11.5538556	11.3214837	9.2538169
4 C	8.5408148	10.3995252	10.3898822	8.5031277
5 C	7.3520120	9.0868233	8.9912248	7.1014564
6 C	7.5494217	8.9513014	8.4604587	6.3222399
7 C	8.9965974	10.3043255	9.6157680	7.3287916
8 C	9.6268412	10.6370353	9.6134665	7.1868958
9 C	9.0318992	9.7608421	8.5115262	6.0374883
10 C	7.6197978	8.3433558	7.1920827	4.7651903
11 C	6.7625122	7.8558535	7.1253719	4.9024173
12 N	5.3007561	6.4473420	5.9521172	3.9910581
13 C	4.7970550	5.4701892	4.6808844	2.6589254 *
14 C	3.4997467	4.0048892	3.5102797	2.1998555 *
15 C	2.1890917 *	3.4467398	3.9282557	3.4396458
16 C	1.1067809 *	2.1951117 *	3.4678950	3.9347125
17 C	2.1995767 *	1.1055716 *	2.1962874 *	3.4496376
18 C	3.4678131	2.2029168 *	1.1061102 *	2.1776553 *
19 C	3.9373361	3.4619228	2.1954751 *	1.1038753 *
20 O	2.6654081 *	4.6434666	5.3870661	4.6866569
21 N	6.1110070	8.0429038	8.3027633	6.7435639

22 H	11.0471254	12.4665957	11.8021215	9.4879175
23 H	10.7391397	12.5593876	12.3994406	10.3530539
24 H	8.6078061	10.6371939	10.8732780	9.1556132
25 H	10.7289565	11.7234529	10.6324045	8.1765251
26 H	9.7453825	10.2487142	8.7663972	6.2697668
27 H	7.3497900	7.7652124	6.3777259	3.9113515
28 H	5.6473624	5.9230609	4.6552409	2.2713756 *
29 H	0.0000000	2.5262976 *	4.3833501	5.0408851
30 H	2.5262976 *	0.0000000	2.5407324 *	4.3670019
31 H	4.3833501	2.5407324 *	0.0000000	2.5113056 *
32 H	5.0408851	4.3670019	2.5113056 *	0.0000000
33 H	2.2650112 *	4.6026591	5.7921290	5.4549256
34 H	6.0387248	7.8898661	8.1622576	6.6670414
35 H	6.4403180	8.5690563	9.0618061	7.6475213

H H H

1 CO	2.6603209 *	2.4994456 *	2.5786639 *
2 C	8.0831826	4.7624511	4.7112676
3 C	7.7662406	4.2443765	3.9036481
4 C	6.4562879	2.9441474 *	2.4806117 *
5 C	5.3635689	2.1059337 *	2.0866664 *
6 C	5.7827916	3.0566254	3.4109777
7 C	7.2383441	4.3044521	4.5344605
8 C	8.0706583	5.4918039	5.8679468
9 C	7.7316500	5.7449501	6.3044651
10 C	6.4158132	4.9085071	5.5726143
11 C	5.3045077	3.5449031	4.1758403
12 N	3.9588616	3.2541632	3.9542397
13 C	4.0413365	4.2351327	5.1043002
14 C	3.3279874	4.8509414	5.6623958
15 C	2.0377861 *	4.6917794	5.2919661
16 C	2.4832140 *	5.8298909	6.3958535
17 C	3.9037641	6.9679928	7.6781815
18 C	4.7073059	7.1310633	7.9827063
19 C	4.4691299	6.1930853	7.0957829
20 O	0.9909360 *	3.7239278	4.0133220
21 N	4.0707840	1.0445626 *	1.0415627 *
22 H	9.1581180	5.8438525	5.7962168
23 H	8.6387372	5.0627209	4.5735794
24 H	6.4668970	3.0131740	2.2046885 *
25 H	9.1465050	6.4202986	6.7206832
26 H	8.5981935	6.8085215	7.4010078
27 H	6.4431735	5.5701837	6.3058644
28 H	5.1151451	4.9982821	5.9830473
29 H	2.2650112 *	6.0387248	6.4403180

30 H	4.6026591	7.8898661	8.5690563
31 H	5.7921290	8.1622576	9.0618061
32 H	5.4549256	6.6670414	7.6475213
33 H	0.0000000	4.2023730	4.2823290
34 H	4.2023730	0.0000000	1.6745944 *
35 H	4.2823290	1.6745944 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 2734.3 SECONDS (45.6 MIN)
WALL CLOCK TIME: STEP = 0.79 , TOTAL = 2527.0 SECONDS (42.1 MIN)
CPU UTILIZATION: STEP = 98.50% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.02 , TOTAL = 2735.3 SECONDS (45.6 MIN)
WALL CLOCK TIME: STEP = 1.01 , TOTAL = 2528.0 SECONDS (42.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.631623356	-284.631623356	0.015035168	0.001065283	195860697
11514192					
2 1	-284.631683710	-0.000060354	0.002071349	0.000086454	154479608
15027268					
3 2	-284.631682290	0.000001419	0.001034011	0.000226014	140571949
16105896					
4 3	-284.631684927	-0.000002637	0.000629351	0.000062711	135410395
16515497					
5 4	-284.631684740	0.000000187	0.000392523	0.000114628	127089650
17172649					
6 5	-284.631684999	-0.000000259	0.000120716	0.000018371	122439457
17527700					
7 6	-284.631685012	-0.000000013	0.000099591	0.000016864	114223458
18088711					
8 7	-284.631685047	-0.000000035	0.000198916	0.000015136	107115864
18669329					

9 8	-284.631685068	-0.000000021	0.000271142	0.000014653	136933176
16480945					
10 9	-284.631685088	-0.000000020	0.000202590	0.000015550	156373267
15046434					
11 10	-284.631685104	-0.000000015	0.000265972	0.000014398	156500132
14944946					
-----DISABLING FDIFF OPTION-----					
12 11	-284.631685137	-0.000000034	0.000150722	0.000011113	195856331
11514518					
13 12	-284.631685146	-0.000000009	0.000256270	0.000009710	195856362
11514518					
14 13	-284.631685154	-0.000000008	0.000094732	0.000006670	195856392
11514518					
15 14	-284.631685156	-0.000000002	0.000047096	0.000006688	195856420
11514515					
16 15	-284.631685158	-0.000000002	0.000038622	0.000005610	195856374
11514516					
17 16	-284.631685159	-0.000000001	0.000065574	0.000004235	195856417
11514515					
18 17	-284.631685161	-0.000000002	0.000080466	0.000002460	195856444
11514514					
19 18	-284.631685162	-0.000000001	0.000044640	0.000002824	195856432
11514513					
20 19	-284.631685162	-0.000000001	0.000019696	0.000002938	195856426
11514515					
21 20	-284.631685163	0.000000000	0.000041971	0.000002534	195856486
11514513					
22 21	-284.631685163	-0.000000001	0.000033014	0.000001697	195856495
11514513					
23 22	-284.631685163	0.000000000	0.000015003	0.000001348	195856504
11514512					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 77.0 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 24.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.1 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6316851634 AFTER 23 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5925834214
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000491732

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 80.27 , TOTAL = 2815.6 SECONDS (46.9 MIN)
WALL CLOCK TIME: STEP = 73.60 , TOTAL = 2601.6 SECONDS (43.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.89 , TOTAL = 2819.5 SECONDS (47.0 MIN)
WALL CLOCK TIME: STEP = 3.87 , TOTAL = 2605.5 SECONDS (43.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.89 , TOTAL = 2822.4 SECONDS (47.0 MIN)
WALL CLOCK TIME: STEP = 2.73 , TOTAL = 2608.2 SECONDS (43.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 24 ENERGY= -284.6316852

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0001451	-0.0003275	0.0003924
2 C	6.0	0.0001993	-0.0005889	-0.0000569
3 C	6.0	0.0007714	-0.0009217	-0.0004062
4 C	6.0	0.0004467	0.0005754	-0.0004003
5 C	6.0	0.0002965	0.0006857	0.0000403
6 C	6.0	0.0006586	-0.0000148	-0.0005874

7 C	6.0	-0.0004432	-0.0000263	-0.0003011
8 C	6.0	0.0010631	-0.0005690	-0.0002695
9 C	6.0	-0.0002802	0.0007841	-0.0000575
10 C	6.0	0.0003048	0.0007370	-0.0000922
11 C	6.0	0.0003336	0.0009008	-0.0003286
12 N	7.0	0.0007568	-0.0000960	-0.0000995
13 C	6.0	0.0006242	0.0002606	0.0003646
14 C	6.0	0.0007027	-0.0004709	0.0005575
15 C	6.0	0.0003587	0.0008586	-0.0002299
16 C	6.0	0.0003096	0.0013347	0.0004294
17 C	6.0	-0.0012260	-0.0001598	0.0003328
18 C	6.0	-0.0014109	-0.0002721	0.0005318
19 C	6.0	-0.0002621	-0.0010624	0.0005431
20 O	8.0	0.0002149	0.0000714	-0.0013025
21 N	7.0	-0.0002116	-0.0007030	0.0007646
22 H	1.0	-0.0000384	0.0007729	0.0002427
23 H	1.0	0.0005651	-0.0000871	0.0000872
24 H	1.0	-0.0004603	-0.0002215	-0.0002013
25 H	1.0	0.0002232	-0.0011673	0.0001721
26 H	1.0	0.0000481	0.0001123	0.0001351
27 H	1.0	-0.0001656	-0.0002200	-0.0004935
28 H	1.0	-0.0008590	0.0005401	-0.0003215
29 H	1.0	0.0004718	0.0002000	-0.0014554
30 H	1.0	-0.0003341	0.0000602	-0.0012066
31 H	1.0	-0.0018407	-0.0000221	0.0008668
32 H	1.0	-0.0009122	-0.0015673	0.0001948
33 H	1.0	-0.0003189	0.0005896	0.0001482
34 H	1.0	0.0000702	0.0007869	-0.0002236
35 H	1.0	0.0001987	-0.0007729	0.0022299

MAXIMUM GRADIENT = 0.0022299 RMS GRADIENT = 0.0006505
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001221880
 PREDICTED ENERGY CHANGE WAS -0.0001655545 RATIO= 0.738
 GDIIS STEP HAS LENGTH = 0.306311
 RADIUS OF STEP TAKEN= 0.05261 CURRENT TRUST RADIUS= 0.05261

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 2822.4 SECONDS (47.0 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2608.2 SECONDS (43.5
 MIN)
 CPU UTILIZATION: STEP = 95.58%, TOTAL = 100.00%

1NSERCH= 25

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1126768553	-1.6781179616	1.0433149010
C	6.0	5.0023261221	0.6716292757	0.4287950428
C	6.0	5.2288958931	-0.6885947404	0.1868753447
C	6.0	4.0940557660	-1.5504754665	0.0596693736
C	6.0	2.7780724507	-1.0636338049	0.1882471580
C	6.0	2.4778344801	0.3357999385	0.4704318829
C	6.0	3.6644096160	1.2007175448	0.5687355638
C	6.0	3.5328869485	2.6147802727	0.8181274417
C	6.0	2.2736594469	3.2068831016	0.9822041906
C	6.0	1.1060410744	2.3845108082	0.9234745434
C	6.0	1.1713231350	0.9937781347	0.6667661292
N	7.0	-0.0686447553	0.2116929177	0.6961632018
C	6.0	-1.2819887251	0.7503149447	0.5374338269
C	6.0	-2.5914527842	0.0799437174	0.5953135305
C	6.0	-2.8644516457	-1.3246109777	0.7110866090
C	6.0	-4.1596563907	-1.8706097561	0.6451965418
C	6.0	-5.2825497278	-0.9988629768	0.5208718048
C	6.0	-5.0792328221	0.4090475221	0.4750223541
C	6.0	-3.7596403570	0.9272077430	0.4884488983
O	8.0	-1.7527568109	-2.2543608367	0.9017215921
N	7.0	1.7003617842	-2.1020714866	-0.0422113999
H	1.0	5.8491926130	1.3769002240	0.5206316115
H	1.0	6.2512874446	-1.0935961681	0.0843860806
H	1.0	4.2553313391	-2.6236523508	-0.1665305949
H	1.0	4.4563840565	3.2166968272	0.8888650414
H	1.0	2.1739762837	4.2877938189	1.1863151809
H	1.0	0.1338042353	2.8657638292	1.1235634238
H	1.0	-1.3555119200	1.8304551595	0.3014477700
H	1.0	-4.3129749993	-2.9663401330	0.6741952984
H	1.0	-6.3012522766	-1.4238043024	0.4497210174
H	1.0	-5.9471016224	1.0914417092	0.4129099985
H	1.0	-3.6134701772	2.0187605409	0.4127165589
H	1.0	-2.0829176199	-3.1818094439	1.0129139473
H	1.0	1.4177114179	-2.0906152096	-1.0477567203
H	1.0	2.1093686716	-3.0418574148	0.1438198558

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4596352	5.2809414	4.1030756
2 C	5.4596352	0.0000000	1.4000244 *	2.4287771 *

3 C	5.2809414	1.4000244 *	0.0000000	1.4306928 *
4 C	4.1030756	2.4287771 *	1.4306928 *	0.0000000
5 C	2.8658446 *	2.8313081 *	2.4793531 *	1.4090277 *
6 C	3.1588021	2.5470715 *	2.9492588 *	2.5177236 *
7 C	4.5964905	1.4455235 *	2.4825260 *	2.8306902 *
8 C	5.4934071	2.4671171 *	3.7665916	4.2707756
9 C	5.3419861	3.7655538	4.9538589	5.1766180
10 C	4.1840276	4.2848230	5.1946596	5.0158258
11 C	2.8985427 *	3.8518819	4.4186616	3.9222645
12 N	1.9299681 *	5.0988011	5.3975762	4.5649137
13 C	2.8457502 *	6.2857463	6.6771978	5.8671756
14 C	3.2563481	7.6186152	7.8686293	6.9022609
15 C	3.0163947	8.1210132	8.1352067	6.9925807
16 C	4.2951581	9.5106116	9.4737602	8.2806457
17 C	5.4628568	10.4200621	10.5213264	9.4041328
18 C	5.6245126	10.0850839	10.3704081	9.3894341
19 C	4.7000467	8.7658962	9.1375898	8.2464119
20 O	1.9575360 *	7.3767353	7.1906956	5.9489263
21 N	1.9694790 *	4.3379986	3.8080113	2.4585379 *
22 H	6.5202720	1.1059041 *	2.1822994 *	3.4442009
23 H	6.2404928	2.1896444 *	1.1044522 *	2.2052207 *
24 H	4.4180706	3.4309321	2.1948056 *	1.1085508 *
25 H	6.5460567	2.6433097 *	4.0423837	4.8522963
26 H	6.3135971	4.6529609	5.9241756	6.2483137
27 H	4.5446395	5.3851123	6.2825798	6.0264942
28 H	3.8750523	6.4638378	7.0507564	6.4177049
29 H	4.6240848	10.0034933	9.8220622	8.5475424
30 H	6.4463568	11.4961804	11.5565539	10.4033944
31 H	6.6924425	10.9574843	11.3191228	10.3889050
32 H	5.2866565	8.7204912	9.2503089	8.5011790
33 H	2.6613244 *	8.0864618	7.7692391	6.4594834
34 H	2.4991698 *	4.7602166	4.2444204	2.9463473 *
35 H	2.5798556 *	4.7159725	3.9078318	2.4840057 *

C C C C

1 CO	2.8658446 *	3.1588021	4.5964905	5.4934071
2 C	2.8313081 *	2.5470715 *	1.4455235 *	2.4671171 *
3 C	2.4793531 *	2.9492588 *	2.4825260 *	3.7665916
4 C	1.4090277 *	2.5177236 *	2.8306902 *	4.2707756
5 C	0.0000000	1.4588303 *	2.4612298 *	3.8075221
6 C	1.4588303 *	0.0000000	1.4716340 *	2.5353065 *
7 C	2.4612298 *	1.4716340 *	0.0000000	1.4418973 *
8 C	3.8075221	2.5353065 *	1.4418973 *	0.0000000
9 C	4.3728840	2.9234768 *	2.4758519 *	1.4011284 *
10 C	3.9020443	2.5068468 *	2.8412068 *	2.4400211 *

11 C	2.6539721 *	1.4759588 *	2.5035803 *	2.8683692 *
12 N	3.1604170	2.5594753 *	3.8639491	4.3313664
13 C	4.4605424	3.7831974	4.9669607	5.1708846
14 C	5.5050226	5.0772760	6.3555216	6.6319363
15 C	5.6727020	5.5995446	7.0016839	7.5137342
16 C	6.9994353	6.9967901	8.4056473	8.9063939
17 C	8.0677422	7.8744798	9.2134970	9.5319831
18 C	7.9992672	7.5574237	8.7799093	8.8967177
19 C	6.8407061	6.2654753	7.4295203	7.4924991
20 O	4.7387013	4.9792415	6.4338277	7.1870406
21 N	1.5142405 *	2.6096904 *	3.8909068	5.1329350
22 H	3.9368090	3.5288051	2.1924030 *	2.6431274 *
23 H	3.4748967	4.0535357	3.4914763	4.6561930
24 H	2.1775718 *	3.5104949	3.9389859	5.3789082
25 H	4.6506801	3.5198454	2.1894928 *	1.1046059 *
26 H	5.4771206	4.0277878	3.4832221	2.1865897 *
27 H	4.8277465	3.5102387	3.9427639	3.4219946
28 H	5.0472849	4.1178993	5.0663226	4.9778075
29 H	7.3579475	7.5538561	9.0007865	9.6294949
30 H	9.0902271	8.9537143	10.3061485	10.6374895
31 H	8.9901883	8.4589510	9.6133954	9.6101480
32 H	7.0995323	6.3197848	7.3253717	7.1826191
33 H	5.3661875	5.7851813	7.2412435	8.0731441
34 H	2.1054640 *	3.0522529	4.3004153	5.4860038
35 H	2.0886616 *	3.4133578	4.5385183	5.8718519

C C C N

1 CO	5.3419861	4.1840276	2.8985427 *	1.9299681 *
2 C	3.7655538	4.2848230	3.8518819	5.0988011
3 C	4.9538589	5.1946596	4.4186616	5.3975762
4 C	5.1766180	5.0158258	3.9222645	4.5649137
5 C	4.3728840	3.9020443	2.6539721 *	3.1604170
6 C	2.9234768 *	2.5068468 *	1.4759588 *	2.5594753 *
7 C	2.4758519 *	2.8412068 *	2.5035803 *	3.8639491
8 C	1.4011284 *	2.4400211 *	2.8683692 *	4.3313664
9 C	0.0000000	1.4293628 *	2.4924847 *	3.8130529
10 C	1.4293628 *	0.0000000	1.4157324 *	2.4804626 *
11 C	2.4924847 *	1.4157324 *	0.0000000	1.4663021 *
12 N	3.8130529	2.4804626 *	1.4663021 *	0.0000000
13 C	4.3445577	2.9192996 *	2.4687528 *	1.3369788 *
14 C	5.7962705	4.3692310	3.8728131	2.5282581 *
15 C	6.8562474	5.4376011	4.6545000	3.1901393
16 C	8.2025643	6.7757700	6.0518201	4.5907470
17 C	8.6601054	7.2404005	6.7560624	5.3554624
18 C	7.8835361	6.5085465	6.2807743	5.0193471

19	C	6.4684945	5.0978265	4.9346357	3.7654422
20	O	6.7855501	5.4490668	4.3767402	2.9933107 *
21	N	5.4371956	4.6276546	3.2197540	3.0046775
22	H	4.0430587	4.8657012	4.6958067	6.0340135
23	H	5.9263584	6.2669656	5.5228919	6.4822522
24	H	6.2643243	6.0156329	4.8261054	5.2421553
25	H	2.1847415 *	3.4523223	3.9726969	5.4353536
26	H	1.1045207 *	2.1981940 *	3.4822096	4.6780548
27	H	2.1714799 *	1.1031249 *	2.1884788 *	2.6958763 *
28	H	3.9406685	2.5986801 *	2.6867046 *	2.1052835 *
29	H	9.0325693	7.6196772	6.7646225	5.3023312
30	H	9.7599137	8.3424038	7.8569203	6.4483317
31	H	8.5076495	7.1888473	7.1236193	5.9506676
32	H	6.0327644	4.7611378	4.8999364	3.9889375
33	H	7.7327938	6.4157134	5.3052269	3.9589752
34	H	5.7373231	4.8999637	3.5374819	3.2482509
35	H	6.3068723	5.5731499	4.1760935	3.9540379

C C C C

1	CO	2.8457502 *	3.2563481	3.0163947	4.2951581
2	C	6.2857463	7.6186152	8.1210132	9.5106116
3	C	6.6771978	7.8686293	8.1352067	9.4737602
4	C	5.8671756	6.9022609	6.9925807	8.2806457
5	C	4.4605424	5.5050226	5.6727020	6.9994353
6	C	3.7831974	5.0772760	5.5995446	6.9967901
7	C	4.9669607	6.3555216	7.0016839	8.4056473
8	C	5.1708846	6.6319363	7.5137342	8.9063939
9	C	4.3445577	5.7962705	6.8562474	8.2025643
10	C	2.9192996 *	4.3692310	5.4376011	6.7757700
11	C	2.4687528 *	3.8728131	4.6545000	6.0518201
12	N	1.3369788 *	2.5282581 *	3.1901393	4.5907470
13	C	0.0000000	1.4722241 *	2.6152747 *	3.8938195
14	C	1.4722241 *	0.0000000	1.4355158 *	2.5032798 *
15	C	2.6152747 *	1.4355158 *	0.0000000	1.4071288 *
16	C	3.8938195	2.5032798 *	1.4071288 *	0.0000000
17	C	4.3662783	2.9002359 *	2.4473438 *	1.4269858 *
18	C	3.8130593	2.5123353 *	2.8225084 *	2.4640246 *
19	C	2.4844412 *	1.4470448 *	2.4334375 *	2.8306122 *
20	O	3.0630711	2.4992548 *	1.4617257 *	2.4507622 *
21	N	4.1673147	4.8566759	4.6914203	5.9047368
22	H	7.1586758	8.5400333	9.1248031	10.5232550
23	H	7.7688809	8.9348921	9.1401762	10.4549515
24	H	6.5223565	7.4005602	7.2903381	8.4875198
25	H	6.2558345	7.7199350	8.6168276	10.0088069
26	H	4.9878350	6.3847161	7.5571612	8.8506297

27 H	2.6121144 *	3.9327939	5.1690344	6.4106063
28 H	1.1080605 *	2.1629141 *	3.5212420	4.6561004
29 H	4.7978231	3.4999581	2.1897158 *	1.1067848 *
30 H	5.4706028	4.0056295	3.4481517	2.1964241 *
31 H	4.6792256	3.5095268	3.9279703	3.4673717
32 H	2.6571252 *	2.1992889 *	3.4392131	3.9344082
33 H	4.0409369	3.3274663	2.0374203 *	2.4834059 *
34 H	4.2275400	4.8460709	4.6922503	5.8327973
35 H	5.1026276	5.6610256	5.2924111	6.3971771

C C C O

1 CO	5.4628568	5.6245126	4.7000467	1.9575360 *
2 C	10.4200621	10.0850839	8.7658962	7.3767353
3 C	10.5213264	10.3704081	9.1375898	7.1906956
4 C	9.4041328	9.3894341	8.2464119	5.9489263
5 C	8.0677422	7.9992672	6.8407061	4.7387013
6 C	7.8744798	7.5574237	6.2654753	4.9792415
7 C	9.2134970	8.7799093	7.4295203	6.4338277
8 C	9.5319831	8.8967177	7.4924991	7.1870406
9 C	8.6601054	7.8835361	6.4684945	6.7855501
10 C	7.2404005	6.5085465	5.0978265	5.4490668
11 C	6.7560624	6.2807743	4.9346357	4.3767402
12 N	5.3554624	5.0193471	3.7654422	2.9933107 *
13 C	4.3662783	3.8130593	2.4844412 *	3.0630711
14 C	2.9002359 *	2.5123353 *	1.4470448 *	2.4992548 *
15 C	2.4473438 *	2.8225084 *	2.4334375 *	1.4617257 *
16 C	1.4269858 *	2.4640246 *	2.8306122 *	2.4507622 *
17 C	0.0000000	1.4232540 *	2.4556165 *	3.7657349
18 C	1.4232540 *	0.0000000	1.4177428 *	4.2826696
19 C	2.4556165 *	1.4177428 *	0.0000000	3.7842773
20 O	3.7657349	4.2826696	3.7842773	0.0000000
21 N	7.0919098	7.2481827	6.2665586	3.5830475
22 H	11.3824399	10.9712944	9.6194038	8.4333221
23 H	11.5424821	11.4363991	10.2208410	8.1289690
24 H	9.6996720	9.8357992	8.7907552	6.1134820
25 H	10.6185307	9.9489773	8.5384513	8.2756309
26 H	9.1646787	8.2558859	6.8548058	7.6354446
27 H	6.6809781	5.7992944	4.3954842	5.4611357
28 H	4.8450814	3.9895645	2.5750066 *	4.1477529
29 H	2.1987609 *	3.4669962	3.9370542	2.6670958 *
30 H	1.1060707 *	2.2030246 *	3.4624484	4.6457443
31 H	2.1960552 *	1.1057649 *	2.1949182 *	5.3875653
32 H	3.4501559	2.1779619 *	1.1038970 *	4.6862508
33 H	3.9044854	4.7075987	4.4688349	0.9907224 *
34 H	6.9674972	7.1258301	6.1864493	3.7254727

35 H	7.6783105	7.9808791	7.0934839	4.0137986
	N	H	H	H
1 CO	1.9694790 *	6.5202720	6.2404928	4.4180706
2 C	4.3379986	1.1059041 *	2.1896444 *	3.4309321
3 C	3.8080113	2.1822994 *	1.1044522 *	2.1948056 *
4 C	2.4585379 *	3.4442009	2.2052207 *	1.1085508 *
5 C	1.5142405 *	3.9368090	3.4748967	2.1775718 *
6 C	2.6096904 *	3.5288051	4.0535357	3.5104949
7 C	3.8909068	2.1924030 *	3.4914763	3.9389859
8 C	5.1329350	2.6431274 *	4.6561930	5.3789082
9 C	5.4371956	4.0430587	5.9263584	6.2643243
10 C	4.6276546	4.8657012	6.2669656	6.0156329
11 C	3.2197540	4.6958067	5.5228919	4.8261054
12 N	3.0046775	6.0340135	6.4822522	5.2421553
13 C	4.1673147	7.1586758	7.7688809	6.5223565
14 C	4.8566759	8.5400333	8.9348921	7.4005602
15 C	4.6914203	9.1248031	9.1401762	7.2903381
16 C	5.9047368	10.5232550	10.4549515	8.4875198
17 C	7.0919098	11.3824399	11.5424821	9.6996720
18 C	7.2481827	10.9712944	11.4363991	9.8357992
19 C	6.2665586	9.6194038	10.2208410	8.7907552
20 O	3.5830475	8.4333221	8.1289690	6.1134820
21 N	0.0000000	5.4436048	4.6630434	2.6106266 *
22 H	5.4436048	0.0000000	2.5407367 *	4.3608493
23 H	4.6630434	2.5407367 *	0.0000000	2.5274240 *
24 H	2.6106266 *	4.3608493	2.5274240 *	0.0000000
25 H	6.0623311	2.3367420 *	4.7378782	5.9383466
26 H	6.5241066	4.7353618	6.8409117	7.3437265
27 H	5.3378386	5.9368262	7.3607080	6.9846273
28 H	4.9921169	7.2222933	8.1523364	7.1791113
29 H	6.1172231	11.0524644	10.7451704	8.6162711
30 H	8.0453634	12.4692536	12.5621957	10.6424085
31 H	8.2999614	11.8002393	12.3968954	10.8732384
32 H	6.7398091	9.4850207	10.3492999	9.1545378
33 H	4.0733680	9.1620166	8.6418616	6.4711690
34 H	1.0445783 *	5.8413638	5.0635216	3.0187373
35 H	1.0416774 *	5.8011800	4.5776353	2.2082501 *

H H H H

1 CO	6.5460567	6.3135971	4.5446395	3.8750523
2 C	2.6433097 *	4.6529609	5.3851123	6.4638378
3 C	4.0423837	5.9241756	6.2825798	7.0507564
4 C	4.8522963	6.2483137	6.0264942	6.4177049

5 C	4.6506801	5.4771206	4.8277465	5.0472849
6 C	3.5198454	4.0277878	3.5102387	4.1178993
7 C	2.1894928 *	3.4832221	3.9427639	5.0663226
8 C	1.1046059 *	2.1865897 *	3.4219946	4.9778075
9 C	2.1847415 *	1.1045207 *	2.1714799 *	3.9406685
10 C	3.4523223	2.1981940 *	1.1031249 *	2.5986801 *
11 C	3.9726969	3.4822096	2.1884788 *	2.6867046 *
12 N	5.4353536	4.6780548	2.6958763 *	2.1052835 *
13 C	6.2558345	4.9878350	2.6121144 *	1.1080605 *
14 C	7.7199350	6.3847161	3.9327939	2.1629141 *
15 C	8.6168276	7.5571612	5.1690344	3.5212420
16 C	10.0088069	8.8506297	6.4106063	4.6561004
17 C	10.6185307	9.1646787	6.6809781	4.8450814
18 C	9.9489773	8.2558859	5.7992944	3.9895645
19 C	8.5384513	6.8548058	4.3954842	2.5750066 *
20 O	8.2756309	7.6354446	5.4611357	4.1477529
21 N	6.0623311	6.5241066	5.3378386	4.9921169
22 H	2.3367420 *	4.7353618	5.9368262	7.2222933
23 H	4.7378782	6.8409117	7.3607080	8.1523364
24 H	5.9383466	7.3437265	6.9846273	7.1791113
25 H	0.0000000	2.5387222 *	4.3431479	6.0037372
26 H	2.5387222 *	0.0000000	2.4876513 *	4.3907620
27 H	4.3431479	2.4876513 *	0.0000000	1.9914318 *
28 H	6.0037372	4.3907620	1.9914318 *	0.0000000
29 H	10.7320868	9.7450122	7.3477353	5.6475458
30 H	11.7240709	10.2466786	7.7630156	5.9222071
31 H	10.6290054	8.7616624	6.3742186	4.6520168
32 H	8.1721672	6.2643039	3.9070172	2.2685271 *
33 H	9.1497944	8.5991969	6.4419905	5.1144990
34 H	6.4149510	6.8005232	5.5613615	4.9885783
35 H	6.7255539	7.4036989	6.3057705	5.9807754

H H H H

1 CO	4.6240848	6.4463568	6.6924425	5.2866565
2 C	10.0034933	11.4961804	10.9574843	8.7204912
3 C	9.8220622	11.5565539	11.3191228	9.2503089
4 C	8.5475424	10.4033944	10.3889050	8.5011790
5 C	7.3579475	9.0902271	8.9901883	7.0995323
6 C	7.5538561	8.9537143	8.4589510	6.3197848
7 C	9.0007865	10.3061485	9.6133954	7.3253717
8 C	9.6294949	10.6374895	9.6101480	7.1826191
9 C	9.0325693	9.7599137	8.5076495	6.0327644
10 C	7.6196772	8.3424038	7.1888473	4.7611378
11 C	6.7646225	7.8569203	7.1236193	4.8999364
12 N	5.3023312	6.4483317	5.9506676	3.9889375

13 C	4.7978231	5.4706028	4.6792256	2.6571252 *
14 C	3.4999581	4.0056295	3.5095268	2.1992889 *
15 C	2.1897158 *	3.4481517	3.9279703	3.4392131
16 C	1.1067848 *	2.1964241 *	3.4673717	3.9344082
17 C	2.1987609 *	1.1060707 *	2.1960552 *	3.4501559
18 C	3.4669962	2.2030246 *	1.1057649 *	2.1779619 *
19 C	3.9370542	3.4624484	2.1949182 *	1.1038970 *
20 O	2.6670958 *	4.6457443	5.3875653	4.6862508
21 N	6.1172231	8.0453634	8.2999614	6.7398091
22 H	11.0524644	12.4692536	11.8002393	9.4850207
23 H	10.7451704	12.5621957	12.3968954	10.3492999
24 H	8.6162711	10.6424085	10.8732384	9.1545378
25 H	10.7320868	11.7240709	10.6290054	8.1721672
26 H	9.7450122	10.2466786	8.7616624	6.2643039
27 H	7.3477353	7.7630156	6.3742186	3.9070172
28 H	5.6475458	5.9222071	4.6520168	2.2685271 *
29 H	0.0000000	2.5264703 *	4.3822635	5.0407248
30 H	2.5264703 *	0.0000000	2.5403229 *	4.3676990
31 H	4.3822635	2.5403229 *	0.0000000	2.5111264 *
32 H	5.0407248	4.3676990	2.5111264 *	0.0000000
33 H	2.2659023 *	4.6045755	5.7924605	5.4542420
34 H	6.0475433	7.8911011	8.1547228	6.6582835
35 H	6.4446489	8.5703102	9.0588788	7.6441510

H H H

1 CO	2.6613244 *	2.4991698 *	2.5798556 *
2 C	8.0864618	4.7602166	4.7159725
3 C	7.7692391	4.2444204	3.9078318
4 C	6.4594834	2.9463473 *	2.4840057 *
5 C	5.3661875	2.1054640 *	2.0886616 *
6 C	5.7851813	3.0522529	3.4133578
7 C	7.2412435	4.3004153	4.5385183
8 C	8.0731441	5.4860038	5.8718519
9 C	7.7327938	5.7373231	6.3068723
10 C	6.4157134	4.8999637	5.5731499
11 C	5.3052269	3.5374819	4.1760935
12 N	3.9589752	3.2482509	3.9540379
13 C	4.0409369	4.2275400	5.1026276
14 C	3.3274663	4.8460709	5.6610256
15 C	2.0374203 *	4.6922503	5.2924111
16 C	2.4834059 *	5.8327973	6.3971771
17 C	3.9044854	6.9674972	7.6783105
18 C	4.7075987	7.1258301	7.9808791
19 C	4.4688349	6.1864493	7.0934839
20 O	0.9907224 *	3.7254727	4.0137986

21 N	4.0733680	1.0445783 *	1.0416774 *
22 H	9.1620166	5.8413638	5.8011800
23 H	8.6418616	5.0635216	4.5776353
24 H	6.4711690	3.0187373	2.2082501 *
25 H	9.1497944	6.4149510	6.7255539
26 H	8.5991969	6.8005232	7.4036989
27 H	6.4419905	5.5613615	6.3057705
28 H	5.1144990	4.9885783	5.9807754
29 H	2.2659023 *	6.0475433	6.4446489
30 H	4.6045755	7.8911011	8.5703102
31 H	5.7924605	8.1547228	9.0588788
32 H	5.4542420	6.6582835	7.6441510
33 H	0.0000000	4.2061232	4.2837105
34 H	4.2061232	0.0000000	1.6742480 *
35 H	4.2837105	1.6742480 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.75 , TOTAL = 2823.2 SECONDS (47.1 MIN)
WALL CLOCK TIME: STEP = 0.75 , TOTAL = 2609.0 SECONDS (43.5 MIN)

CPU UTILIZATION: STEP = 99.82%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.76 , TOTAL = 2823.9 SECONDS (47.1 MIN)
WALL CLOCK TIME: STEP = 0.76 , TOTAL = 2609.8 SECONDS (43.5 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.631749695	-284.631749695	0.015970094	0.001015690	195837733
11515433					
2 1	-284.631808637	-0.000058942	0.001590042	0.000074874	154105362
15057931					
3 2	-284.631808102	0.000000535	0.000875857	0.000198984	138429025
16294109					

4 3	-284.631809576	-0.000001474	0.000591682	0.000064340	132723510
16743815					
5 4	-284.631809442	0.000000134	0.000475026	0.000098577	127006190
17191582					
6 5	-284.631809643	-0.000000201	0.000155686	0.000017956	122214665
17551614					
7 6	-284.631809642	0.000000001	0.000114435	0.000020821	114187153
18092005					
8 7	-284.631809669	-0.000000027	0.000204974	0.000015092	106935465
18679834					
9 8	-284.631809694	-0.000000025	0.000311094	0.000014330	137232715
16466028					
10 9	-284.631809713	-0.000000019	0.000180517	0.000014286	157699719
14925665					
11 10	-284.631809728	-0.000000015	0.000254675	0.000012595	156996287
14909742					
-----DISABLING FDIFF OPTION-----					
12 11	-284.631809790	-0.000000063	0.000134211	0.000012146	195832944
11515684					
13 12	-284.631809798	-0.000000008	0.000218641	0.000008618	195832862
11515690					
14 13	-284.631809804	-0.000000006	0.000066913	0.000006085	195832761
11515695					
15 14	-284.631809807	-0.000000003	0.000062665	0.000006321	195832737
11515697					
16 15	-284.631809808	-0.000000001	0.000036383	0.000005304	195832793
11515691					
17 16	-284.631809809	-0.000000001	0.000072826	0.000003890	195832831
11515689					
18 17	-284.631809811	-0.000000002	0.000087141	0.000002537	195832817
11515691					
19 18	-284.631809812	-0.000000001	0.000026570	0.000003435	195832762
11515694					
20 19	-284.631809813	-0.000000001	0.000020141	0.000003155	195832770
11515694					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 66.0 SECONDS (3.3 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 21.6 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.1
 TIME TO SOLVE SCF EQUATIONS= 1.8 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6318098125 AFTER 20 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.5917094850

INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000467292

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 69.06 , TOTAL = 2893.0 SECONDS (48.2 MIN)
WALL CLOCK TIME: STEP = 63.93 , TOTAL = 2673.7 SECONDS (44.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.60 , TOTAL = 2896.6 SECONDS (48.3 MIN)
WALL CLOCK TIME: STEP = 3.59 , TOTAL = 2677.3 SECONDS (44.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.89 , TOTAL = 2899.5 SECONDS (48.3 MIN)
WALL CLOCK TIME: STEP = 2.72 , TOTAL = 2680.0 SECONDS (44.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 25 ENERGY= -284.6318098

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0001454	-0.0002789	0.0004358
2 C	6.0	0.0000162	-0.0003882	-0.0000514

3 C	6.0	0.0008430	-0.0007953	-0.0004009
4 C	6.0	0.0005793	0.0005092	-0.0003709
5 C	6.0	0.0004211	0.0006579	0.0001898
6 C	6.0	0.0005230	0.0002524	-0.0004796
7 C	6.0	-0.0003101	0.0000103	-0.0003094
8 C	6.0	0.0008243	-0.0005836	-0.0002161
9 C	6.0	-0.0000129	0.0007272	-0.0000539
10 C	6.0	0.0001450	0.0003459	-0.0002024
11 C	6.0	0.0005914	0.0007676	-0.0003358
12 N	7.0	0.0004225	-0.0000337	-0.0000535
13 C	6.0	0.0005926	0.0001425	0.0002994
14 C	6.0	0.0006469	-0.0004682	0.0004902
15 C	6.0	0.0002905	0.0010329	-0.0000635
16 C	6.0	0.0004667	0.0015170	0.0003777
17 C	6.0	-0.0011548	-0.0002898	0.0003218
18 C	6.0	-0.0015028	-0.0002169	0.0005147
19 C	6.0	-0.0001020	-0.0011142	0.0005595
20 O	8.0	0.0003838	-0.0002442	-0.0014219
21 N	7.0	-0.0003047	-0.0007792	0.0007531
22 H	1.0	0.0001505	0.0008219	0.0002356
23 H	1.0	0.0004005	-0.0000422	0.0000808
24 H	1.0	-0.0004319	-0.0004191	-0.0002979
25 H	1.0	0.0004346	-0.0010098	0.0001292
26 H	1.0	0.0000786	0.0002921	0.0001346
27 H	1.0	-0.0001650	-0.0002179	-0.0004668
28 H	1.0	-0.0009620	0.0005942	-0.0003376
29 H	1.0	0.0003195	0.0002239	-0.0013116
30 H	1.0	-0.0007018	0.0000271	-0.0012554
31 H	1.0	-0.0016371	-0.0001535	0.0007512
32 H	1.0	-0.0008389	-0.0015394	0.0003546
33 H	1.0	-0.0003381	0.0008087	0.0001097
34 H	1.0	0.0001142	0.0008096	-0.0002176
35 H	1.0	0.0000725	-0.0009665	0.0021087

MAXIMUM GRADIENT = 0.0021087 RMS GRADIENT = 0.0006406
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001246491
 PREDICTED ENERGY CHANGE WAS -0.0001553581 RATIO= 0.802
 GDIIS STEP HAS LENGTH = 0.347055
 RADIUS OF STEP TAKEN= 0.07440 CURRENT TRUST RADIUS= 0.07440

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 0.02 , TOTAL = 2899.5 SECONDS (48.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2680.0 SECONDS (44.7
 MIN)
 CPU UTILIZATION: STEP = 93.35% , TOTAL = 100.00%

INSERCH= 26

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1129503669	-1.6819070985	1.0432564362
C	6.0	5.0025806822	0.6736582384	0.4295453035
C	6.0	5.2292975526	-0.6865003825	0.1884885512
C	6.0	4.0959906885	-1.5511319623	0.0618490770
C	6.0	2.7796639114	-1.0649648899	0.1910972192
C	6.0	2.4791204309	0.3345536450	0.4741209358
C	6.0	3.6646567738	1.2016458729	0.5709763710
C	6.0	3.5317928411	2.6160017018	0.8182880883
C	6.0	2.2715907803	3.2058784322	0.9830466318
C	6.0	1.1052152725	2.3812101968	0.9261763947
C	6.0	1.1718413429	0.9904173159	0.6701004726
N	7.0	-0.0682809105	0.2083940905	0.6989806304
C	6.0	-1.2811039431	0.7470814605	0.5371950318
C	6.0	-2.5907059351	0.0777645768	0.5954112687
C	6.0	-2.8656078317	-1.3260877748	0.7150602891
C	6.0	-4.1619982655	-1.8699910421	0.6530093707
C	6.0	-5.2832997248	-0.9966490763	0.5213381073
C	6.0	-5.0764134497	0.4104226224	0.4684902231
C	6.0	-3.7567573362	0.9271694990	0.4857541154
O	8.0	-1.7538968405	-2.2570194222	0.9022235348
N	7.0	1.7001288848	-2.1006409859	-0.0464465176
H	1.0	5.8503469682	1.3786453228	0.5189811271
H	1.0	6.2517170948	-1.0903955511	0.0842924318
H	1.0	4.2590974759	-2.6235818223	-0.1668932497
H	1.0	4.4543329099	3.2202807702	0.8855654913
H	1.0	2.1705536402	4.2872367792	1.1851546594
H	1.0	0.1327570591	2.8612058692	1.1274518244
H	1.0	-1.3543244362	1.8266605067	0.2988784403
H	1.0	-4.3193396276	-2.9646306338	0.6920885274
H	1.0	-6.3034052808	-1.4193355404	0.4509080209
H	1.0	-5.9423222267	1.0942621288	0.3984382640
H	1.0	-3.6077792557	2.0184515604	0.4122312764
H	1.0	-2.0849653229	-3.1842960886	1.0106677147
H	1.0	1.4162715554	-2.0790163612	-1.0514496805
H	1.0	2.1062911555	-3.0436869578	0.1286106174

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C	
1	CO	0.0000000	5.4620339	5.2819003	4.1042506
2	C	5.4620339	0.0000000	1.3998358 *	2.4303904 *
3	C	5.2819003	1.3998358 *	0.0000000	1.4310869 *
4	C	4.1042506	2.4303904 *	1.4310869 *	0.0000000
5	C	2.8667323 *	2.8321417 *	2.4786987 *	1.4091770 *
6	C	3.1605047	2.5465330 *	2.9474754 *	2.5179451 *
7	C	4.5991896	1.4452730 *	2.4818328 *	2.8324981 *
8	C	5.4964638	2.4671919 *	3.7662567	4.2726481
9	C	5.3435757	3.7652103	4.9527734	5.1774693
10	C	4.1841629	4.2839040	5.1925992	5.0154874
11	C	2.8985881 *	3.8513331	4.4166677	3.9217460
12	N	1.9299247 *	5.0992846	5.3968302	4.5654164
13	C	2.8459570 *	6.2850356	6.6754836	5.8669315
14	C	3.2568032	7.6184383	7.8677914	6.9028910
15	C	3.0176363	8.1233548	8.1371889	6.9957976
16	C	4.2968423	9.5136531	9.4769651	8.2852594
17	C	5.4645670	10.4210215	10.5224371	9.4068948
18	C	5.6247397	10.0825063	10.3677056	9.3886128
19	C	4.7002901	8.7631861	9.1346308	8.2454427
20	O	1.9585104 *	7.3798567	7.1931184	5.9519485
21	N	1.9702605 *	4.3392963	3.8092020	2.4604556 *
22	H	6.5237693	1.1062157 *	2.1816862 *	3.4453346
23	H	6.2413103	2.1889329 *	1.1042327 *	2.2045267 *
24	H	4.4206051	3.4322439	2.1954200 *	1.1086368 *
25	H	6.5501080	2.6445825 *	4.0434423	4.8552340
26	H	6.3154212	4.6528779	5.9234550	6.2494538
27	H	4.5439362	5.3840153	6.2803341	6.0258987
28	H	3.8751827	6.4619448	7.0478537	6.4165099
29	H	4.6275148	10.0102084	9.8295454	8.5564575
30	H	6.4489875	11.4981041	11.5589423	10.4075056
31	H	6.6924758	10.9530258	11.3146048	10.3864878
32	H	5.2853265	8.7147614	9.2444985	8.4978095
33	H	2.6625304 *	8.0904155	7.7726060	6.4631029
34	H	2.4988268 *	4.7573287	4.2444923	2.9494051 *
35	H	2.5815555 *	4.7220451	3.9131934	2.4881884 *

	C	C	C	C	
1	CO	2.8667323 *	3.1605047	4.5991896	5.4964638
2	C	2.8321417 *	2.5465330 *	1.4452730 *	2.4671919 *
3	C	2.4786987 *	2.9474754 *	2.4818328 *	3.7662567
4	C	1.4091770 *	2.5179451 *	2.8324981 *	4.2726481
5	C	0.0000000	1.4591371 *	2.4627312 *	3.8090132
6	C	1.4591371 *	0.0000000	1.4719804 *	2.5360551 *

7 C	2.4627312 *	1.4719804 *	0.0000000	1.4419495 *
8 C	3.8090132	2.5360551 *	1.4419495 *	0.0000000
9 C	4.3732625	2.9234534 *	2.4753551 *	1.4011457 *
10 C	3.9013129	2.5061470 *	2.8404718 *	2.4402962 *
11 C	2.6531365 *	1.4756503 *	2.5037116 *	2.8694695 *
12 N	3.1607243	2.5604163 *	3.8649396	4.3325904
13 C	4.4601717	3.7833114	4.9667212	5.1706723
14 C	5.5054675	5.0777743	6.3555699	6.6315393
15 C	5.6755454	5.6019552	7.0038956	7.5151488
16 C	7.0034351	6.9997483	8.4082229	8.9076299
17 C	8.0700129	7.8758807	9.2141679	9.5312791
18 C	7.9982290	7.5559169	8.7774054	8.8931520
19 C	6.8396071	6.2639844	7.4269770	7.4890384
20 O	4.7412939	4.9817625	6.4368326	7.1897076
21 N	1.5147435 *	2.6092128 *	3.8917450	5.1331742
22 H	3.9379986	3.5294912	2.1934616 *	2.6450574 *
23 H	3.4737886	4.0515345	3.4904436	4.6555470
24 H	2.1785701 *	3.5113791	3.9408347	5.3807797
25 H	4.6529703	3.5211038	2.1903063 *	1.1048799 *
26 H	5.4777028	4.0279631	3.4828767	2.1864560 *
27 H	4.8267683	3.5094492	3.9418422	3.4218638
28 H	5.0460850	4.1173283	5.0650620	4.9766442
29 H	7.3658383	7.5598403	9.0064825	9.6332583
30 H	9.0936916	8.9559714	10.3075808	10.6372006
31 H	8.9876746	8.4559790	9.6091283	9.6047291
32 H	7.0961812	6.3158286	7.3198837	7.1760322
33 H	5.3691599	5.7880104	7.2448582	8.0764124
34 H	2.1050088 *	3.0466922	4.2953751	5.4785531
35 H	2.0910946 *	3.4162682	4.5439016	5.8770559

C C C N

1 CO	5.3435757	4.1841629	2.8985881 *	1.9299247 *
2 C	3.7652103	4.2839040	3.8513331	5.0992846
3 C	4.9527734	5.1925992	4.4166677	5.3968302
4 C	5.1774693	5.0154874	3.9217460	4.5654164
5 C	4.3732625	3.9013129	2.6531365 *	3.1607243
6 C	2.9234534 *	2.5061470 *	1.4756503 *	2.5604163 *
7 C	2.4753551 *	2.8404718 *	2.5037116 *	3.8649396
8 C	1.4011457 *	2.4402962 *	2.8694695 *	4.3325904
9 C	0.0000000	1.4295957 *	2.4931210 *	3.8132146
10 C	1.4295957 *	0.0000000	1.4157396 *	2.4798873 *
11 C	2.4931210 *	1.4157396 *	0.0000000	1.4663893 *
12 N	3.8132146	2.4798873 *	1.4663893 *	0.0000000
13 C	4.3435131	2.9182534 *	2.4685657 *	1.3368988 *
14 C	5.7945912	4.3675051	3.8723734	2.5279277 *

15	C	6.8557526	5.4365489	4.6550202	3.1906004
16	C	8.2014903	6.7742801	6.0524436	4.5913310
17	C	8.6574120	7.2378831	6.7556946	5.3553811
18	C	7.8786108	6.5043073	6.2783540	5.0175027
19	C	6.4638066	5.0938182	4.9324506	3.7639025
20	O	6.7863345	5.4486943	4.3771761	2.9934717 *
21	N	5.4355840	4.6245981	3.2167015	3.0024287
22	H	4.0449516	4.8669517	4.6970175	6.0358963
23	H	5.9251274	6.2647662	5.5206966	6.4812862
24	H	6.2653932	6.0157890	4.8262510	5.2436656
25	H	2.1849653 *	3.4528651	3.9740995	5.4369395
26	H	1.1047136 *	2.1988526 *	3.4830627	4.6782158
27	H	2.1712351 *	1.1029880 *	2.1883136 *	2.6947011 *
28	H	3.9392372	2.5981462 *	2.6867493 *	2.1054159 *
29	H	9.0332830	7.6196199	6.7672710	5.3046804
30	H	9.7573733	8.3401251	7.8571156	6.4488619
31	H	8.5011209	7.1834899	7.1201059	5.9480626
32	H	6.0251809	4.7547924	4.8957251	3.9857975
33	H	7.7339947	6.4155476	5.3057523	3.9591049
34	H	5.7272034	4.8889040	3.5277336	3.2403933
35	H	6.3098694	5.5738473	4.1761711	3.9534942

C C C C

1	CO	2.8459570 *	3.2568032	3.0176363	4.2968423
2	C	6.2850356	7.6184383	8.1233548	9.5136531
3	C	6.6754836	7.8677914	8.1371889	9.4769651
4	C	5.8669315	6.9028910	6.9957976	8.2852594
5	C	4.4601717	5.5054675	5.6755454	7.0034351
6	C	3.7833114	5.0777743	5.6019552	6.9997483
7	C	4.9667212	6.3555699	7.0038956	8.4082229
8	C	5.1706723	6.6315393	7.5151488	8.9076299
9	C	4.3435131	5.7945912	6.8557526	8.2014903
10	C	2.9182534 *	4.3675051	5.4365489	6.7742801
11	C	2.4685657 *	3.8723734	4.6550202	6.0524436
12	N	1.3368988 *	2.5279277 *	3.1906004	4.5913310
13	C	0.0000000	1.4718803 *	2.6154004 *	3.8938456
14	C	1.4718803 *	0.0000000	1.4355098 *	2.5032038 *
15	C	2.6154004 *	1.4355098 *	0.0000000	1.4072346 *
16	C	3.8938456	2.5032038 *	1.4072346 *	0.0000000
17	C	4.3655949	2.8999850 *	2.4477116 *	1.4273684 *
18	C	3.8108311	2.5110779 *	2.8220430 *	2.4638362 *
19	C	2.4827279 *	1.4467858 *	2.4339057 *	2.8313074 *
20	O	3.0629073	2.4991198 *	1.4620414 *	2.4517037 *
21	N	4.1638816	4.8547601	4.6931628	5.9082123
22	H	7.1593852	8.5410483	9.1280828	10.5270442

23 H	7.7669064	8.9338841	9.1421569	10.4583304
24 H	6.5231084	7.4025798	7.2953930	8.4944095
25 H	6.2556625	7.7195965	8.6185887	10.0103003
26 H	4.9866313	6.3825580	7.5560124	8.8484940
27 H	2.6109247 *	3.9303770	5.1665934	6.4073585
28 H	1.1079923 *	2.1622229 *	3.5209383	4.6554993
29 H	4.7991327	3.5005270	2.1905905 *	1.1065800 *
30 H	5.4703125	4.0057866	3.4491916	2.1976258 *
31 H	4.6761890	3.5079050	3.9274056	3.4671540
32 H	2.6543202 *	2.1986948 *	3.4392539	3.9351136
33 H	4.0405568	3.3270484	2.0370873 *	2.4838243 *
34 H	4.2173991	4.8393929	4.6927551	5.8366057
35 H	5.1001286	5.6588996	5.2928111	6.3987505

C C C O

1 CO	5.4645670	5.6247397	4.7002901	1.9585104 *
2 C	10.4210215	10.0825063	8.7631861	7.3798567
3 C	10.5224371	10.3677056	9.1346308	7.1931184
4 C	9.4068948	9.3886128	8.2454427	5.9519485
5 C	8.0700129	7.9982290	6.8396071	4.7412939
6 C	7.8758807	7.5559169	6.2639844	4.9817625
7 C	9.2141679	8.7774054	7.4269770	6.4368326
8 C	9.5312791	8.8931520	7.4890384	7.1897076
9 C	8.6574120	7.8786108	6.4638066	6.7863345
10 C	7.2378831	6.5043073	5.0938182	5.4486943
11 C	6.7556946	6.2783540	4.9324506	4.3771761
12 N	5.3553811	5.0175027	3.7639025	2.9934717 *
13 C	4.3655949	3.8108311	2.4827279 *	3.0629073
14 C	2.8999850 *	2.5110779 *	1.4467858 *	2.4991198 *
15 C	2.4477116 *	2.8220430 *	2.4339057 *	1.4620414 *
16 C	1.4273684 *	2.4638362 *	2.8313074 *	2.4517037 *
17 C	0.0000000	1.4231815 *	2.4561506 *	3.7670004
18 C	1.4231815 *	0.0000000	1.4173276 *	4.2828131
19 C	2.4561506 *	1.4173276 *	0.0000000	3.7847003
20 O	3.7670004	4.2828131	3.7847003	0.0000000
21 N	7.0929157	7.2451450	6.2632644	3.5853484
22 H	11.3842047	10.9696900	9.6177642	8.4373845
23 H	11.5436740	11.4335736	10.2176955	8.1314130
24 H	9.7045307	9.8366996	8.7913430	6.1182906
25 H	10.6177516	9.9450682	8.5346477	8.2790828
26 H	9.1607877	8.2499593	6.8492502	7.6360101
27 H	6.6771318	5.7944824	4.3909674	5.4595257
28 H	4.8432853	3.9860312	2.5720984 *	4.1473034
29 H	2.1980278 *	3.4661422	3.9376619	2.6695256 *
30 H	1.1064536 *	2.2031416 *	3.4630501	4.6479487

31 H	2.1957515 *	1.1055957 *	2.1936814 *	5.3877449
32 H	3.4511020	2.1784877 *	1.1038553 *	4.6857896
33 H	3.9057120	4.7079423	4.4692921	0.9905597 *
34 H	6.9663072	7.1177582	6.1774086	3.7280681
35 H	7.6779328	7.9773201	7.0901756	4.0147695

N H H H

1 CO	1.9702605 *	6.5237693	6.2413103	4.4206051
2 C	4.3392963	1.1062157 *	2.1889329 *	3.4322439
3 C	3.8092020	2.1816862 *	1.1042327 *	2.1954200 *
4 C	2.4604556 *	3.4453346	2.2045267 *	1.1086368 *
5 C	1.5147435 *	3.9379986	3.4737886	2.1785701 *
6 C	2.6092128 *	3.5294912	4.0515345	3.5113791
7 C	3.8917450	2.1934616 *	3.4904436	3.9408347
8 C	5.1331742	2.6450574 *	4.6555470	5.3807797
9 C	5.4355840	4.0449516	5.9251274	6.2653932
10 C	4.6245981	4.8669517	6.2647662	6.0157890
11 C	3.2167015	4.6970175	5.5206966	4.8262510
12 N	3.0024287	6.0358963	6.4812862	5.2436656
13 C	4.1638816	7.1593852	7.7669064	6.5231084
14 C	4.8547601	8.5410483	8.9338841	7.4025798
15 C	4.6931628	9.1280828	9.1421569	7.2953930
16 C	5.9082123	10.5270442	10.4583304	8.4944095
17 C	7.0929157	11.3842047	11.5436740	9.7045307
18 C	7.2451450	10.9696900	11.4335736	9.8366996
19 C	6.2632644	9.6177642	10.2176955	8.7913430
20 O	3.5853484	8.4373845	8.1314130	6.1182906
21 N	0.0000000	5.4451310	4.6641874	2.6146309 *
22 H	5.4451310	0.0000000	2.5389398 *	4.3612293
23 H	4.6641874	2.5389398 *	0.0000000	2.5267147 *
24 H	2.6146309 *	4.3612293	2.5267147 *	0.0000000
25 H	6.0635381	2.3398420 *	4.7386241	5.9410871
26 H	6.5225090	4.7375701	6.8400820	7.3450298
27 H	5.3342868	5.9379337	7.3583291	6.9846196
28 H	4.9872469	7.2219425	8.1490571	7.1785866
29 H	6.1258398	11.0596807	10.7531118	8.6280790
30 H	8.0478629	12.4718493	12.5647804	10.6488662
31 H	8.2953232	11.7967136	12.3921754	10.8724849
32 H	6.7343298	9.4803428	10.3432172	9.1526831
33 H	4.0766085	9.1668627	8.6453956	6.4767417
34 H	1.0445449 *	5.8380392	5.0644659	3.0266567
35 H	1.0416086 *	5.8075267	4.5827795	2.2132297 *

H H H H

1 CO	6.5501080	6.3154212	4.5439362	3.8751827
2 C	2.6445825 *	4.6528779	5.3840153	6.4619448
3 C	4.0434423	5.9234550	6.2803341	7.0478537
4 C	4.8552340	6.2494538	6.0258987	6.4165099
5 C	4.6529703	5.4777028	4.8267683	5.0460850
6 C	3.5211038	4.0279631	3.5094492	4.1173283
7 C	2.1903063 *	3.4828767	3.9418422	5.0650620
8 C	1.1048799 *	2.1864560 *	3.4218638	4.9766442
9 C	2.1849653 *	1.1047136 *	2.1712351 *	3.9392372
10 C	3.4528651	2.1988526 *	1.1029880 *	2.5981462 *
11 C	3.9740995	3.4830627	2.1883136 *	2.6867493 *
12 N	5.4369395	4.6782158	2.6947011 *	2.1054159 *
13 C	6.2556625	4.9866313	2.6109247 *	1.1079923 *
14 C	7.7195965	6.3825580	3.9303770	2.1622229 *
15 C	8.6185887	7.5560124	5.1665934	3.5209383
16 C	10.0103003	8.8484940	6.4073585	4.6554993
17 C	10.6177516	9.1607877	6.6771318	4.8432853
18 C	9.9450682	8.2499593	5.7944824	3.9860312
19 C	8.5346477	6.8492502	4.3909674	2.5720984 *
20 O	8.2790828	7.6360101	5.4595257	4.1473034
21 N	6.0635381	6.5225090	5.3342868	4.9872469
22 H	2.3398420 *	4.7375701	5.9379337	7.2219425
23 H	4.7386241	6.8400820	7.3583291	8.1490571
24 H	5.9410871	7.3450298	6.9846196	7.1785866
25 H	0.0000000	2.5384634 *	4.3432087	6.0022395
26 H	2.5384634 *	0.0000000	2.4878723 *	4.3891556
27 H	4.3432087	2.4878723 *	0.0000000	1.9920415 *
28 H	6.0022395	4.3891556	1.9920415 *	0.0000000
29 H	10.7362886	9.7443014	7.3451397	5.6482210
30 H	11.7236469	10.2426591	7.7591837	5.9205578
31 H	10.6229792	8.7540142	6.3686843	4.6471543
32 H	8.1649306	6.2557116	3.9004342	2.2644406 *
33 H	9.1540525	8.6002146	6.4404988	5.1137233
34 H	6.4081506	6.7897363	5.5498484	4.9753291
35 H	6.7322784	7.4069466	6.3055753	5.9770508

H H H H

1 CO	4.6275148	6.4489875	6.6924758	5.2853265
2 C	10.0102084	11.4981041	10.9530258	8.7147614
3 C	9.8295454	11.5589423	11.3146048	9.2444985
4 C	8.5564575	10.4075056	10.3864878	8.4978095
5 C	7.3658383	9.0936916	8.9876746	7.0961812
6 C	7.5598403	8.9559714	8.4559790	6.3158286
7 C	9.0064825	10.3075808	9.6091283	7.3198837
8 C	9.6332583	10.6372006	9.6047291	7.1760322

9 C	9.0332830	9.7573733	8.5011209	6.0251809
10 C	7.6196199	8.3401251	7.1834899	4.7547924
11 C	6.7672710	7.8571156	7.1201059	4.8957251
12 N	5.3046804	6.4488619	5.9480626	3.9857975
13 C	4.7991327	5.4703125	4.6761890	2.6543202 *
14 C	3.5005270	4.0057866	3.5079050	2.1986948 *
15 C	2.1905905 *	3.4491916	3.9274056	3.4392539
16 C	1.1065800 *	2.1976258 *	3.4671540	3.9351136
17 C	2.1980278 *	1.1064536 *	2.1957515 *	3.4511020
18 C	3.4661422	2.2031416 *	1.1055957 *	2.1784877 *
19 C	3.9376619	3.4630501	2.1936814 *	1.1038553 *
20 O	2.6695256 *	4.6479487	5.3877449	4.6857896
21 N	6.1258398	8.0478629	8.2953232	6.7343298
22 H	11.0596807	12.4718493	11.7967136	9.4803428
23 H	10.7531118	12.5647804	12.3921754	10.3432172
24 H	8.6280790	10.6488662	10.8724849	9.1526831
25 H	10.7362886	11.7236469	10.6229792	8.1649306
26 H	9.7443014	10.2426591	8.7540142	6.2557116
27 H	7.3451397	7.7591837	6.3686843	3.9004342
28 H	5.6482210	5.9205578	4.6471543	2.2644406 *
29 H	0.0000000	2.5263851 *	4.3812000	5.0414032
30 H	2.5263851 *	0.0000000	2.5399424 *	4.3687842
31 H	4.3812000	2.5399424 *	0.0000000	2.5108579 *
32 H	5.0414032	4.3687842	2.5108579 *	0.0000000
33 H	2.2676362 *	4.6069135	5.7931069	5.4539593
34 H	6.0598246	7.8921270	8.1437567	6.6462540
35 H	6.4507742	8.5711952	9.0540382	7.6391287

H H H

1 CO	2.6625304 *	2.4988268 *	2.5815555 *
2 C	8.0904155	4.7573287	4.7220451
3 C	7.7726060	4.2444923	3.9131934
4 C	6.4631029	2.9494051 *	2.4881884 *
5 C	5.3691599	2.1050088 *	2.0910946 *
6 C	5.7880104	3.0466922	3.4162682
7 C	7.2448582	4.2953751	4.5439016
8 C	8.0764124	5.4785531	5.8770559
9 C	7.7339947	5.7272034	6.3098694
10 C	6.4155476	4.8889040	5.5738473
11 C	5.3057523	3.5277336	4.1761711
12 N	3.9591049	3.2403933	3.9534942
13 C	4.0405568	4.2173991	5.1001286
14 C	3.3270484	4.8393929	5.6588996
15 C	2.0370873 *	4.6927551	5.2928111
16 C	2.4838243 *	5.8366057	6.3987505

17	C	3.9057120	6.9663072	7.6779328
18	C	4.7079423	7.1177582	7.9773201
19	C	4.4692921	6.1774086	7.0901756
20	O	0.9905597 *	3.7280681	4.0147695
21	N	4.0766085	1.0445449 *	1.0416086 *
22	H	9.1668627	5.8380392	5.8075267
23	H	8.6453956	5.0644659	4.5827795
24	H	6.4767417	3.0266567	2.2132297 *
25	H	9.1540525	6.4081506	6.7322784
26	H	8.6002146	6.7897363	7.4069466
27	H	6.4404988	5.5498484	6.3055753
28	H	5.1137233	4.9753291	5.9770508
29	H	2.2676362 *	6.0598246	6.4507742
30	H	4.6069135	7.8921270	8.5711952
31	H	5.7931069	8.1437567	9.0540382
32	H	5.4539593	6.6462540	7.6391287
33	H	0.0000000	4.2110131	4.2853736
34	H	4.2110131	0.0000000	1.6730985 *
35	H	4.2853736	1.6730985 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 2900.3 SECONDS (48.3 MIN)
WALL CLOCK TIME: STEP = 0.79 , TOTAL = 2680.8 SECONDS (44.7 MIN)
CPU UTILIZATION: STEP = 98.85% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.10 , TOTAL = 2901.4 SECONDS (48.4 MIN)
WALL CLOCK TIME: STEP = 1.10 , TOTAL = 2681.9 SECONDS (44.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.631869642 -284.631869642 0.022914751 0.001384775 195816093
11515903

2 1	-284.631983888	-0.000114246	0.001714366	0.000089170	156657322
14843648					
3 2	-284.631983291	0.000000597	0.001264507	0.000233424	141127910
16074178					
4 3	-284.631985632	-0.000002340	0.000541433	0.000080254	135505718
16516454					
5 4	-284.631985478	0.000000154	0.000509052	0.000121955	129160234
17028225					
6 5	-284.631985771	-0.000000293	0.000189605	0.000024820	124201709
17401194					
7 6	-284.631985781	-0.000000010	0.000157564	0.000022750	118238687
17805660					
8 7	-284.631985815	-0.000000033	0.000327235	0.000022374	110673915
18411003					
9 8	-284.631985862	-0.000000047	0.000473446	0.000021215	140953252
16181763					
10 9	-284.631985904	-0.000000042	0.000272848	0.000023129	160881945
14681634					
11 10	-284.631985937	-0.000000033	0.000379025	0.000017130	160185442
14648924					

-----DISABLING FDIFF OPTION-----

12 11	-284.631986006	-0.000000069	0.000170947	0.000019059	195812216
11516178					
13 12	-284.631986023	-0.000000017	0.000241253	0.000011036	195812003
11516184					
14 13	-284.631986033	-0.000000010	0.000116872	0.000007710	195812206
11516173					
15 14	-284.631986038	-0.000000005	0.000051185	0.000008969	195812247
11516174					
16 15	-284.631986041	-0.000000002	0.000053254	0.000007646	195812180
11516181					
17 16	-284.631986043	-0.000000002	0.000085415	0.000005476	195812079
11516173					
18 17	-284.631986046	-0.000000003	0.000158677	0.000004595	195812069
11516177					
19 18	-284.631986049	-0.000000002	0.000027991	0.000004869	195812055
11516178					
20 19	-284.631986050	-0.000000001	0.000028870	0.000004410	195812045
11516177					
21 20	-284.631986051	-0.000000001	0.000054080	0.000003557	195812006
11516180					
22 21	-284.631986052	-0.000000001	0.000049359	0.000002248	195812030
11516177					
23 22	-284.631986052	0.000000000	0.000033087	0.000001632	195812042
11516175					

24 23 -284.631986052 0.000000000 0.000010896 0.000001194 195812032
11516177

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 80.3 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 25.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6319860524 AFTER 24 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5910839853
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000438630

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 83.42 , TOTAL = 2984.8 SECONDS (49.7 MIN)
WALL CLOCK TIME: STEP = 76.68 , TOTAL = 2758.6 SECONDS (46.0
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.73 , TOTAL = 2988.5 SECONDS (49.8 MIN)
WALL CLOCK TIME: STEP = 3.71 , TOTAL = 2762.3 SECONDS (46.0
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.74 , TOTAL = 2991.3 SECONDS (49.9 MIN)

WALL CLOCK TIME: STEP = 2.64 , TOTAL = 2764.9 SECONDS (46.1 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 26 ENERGY= -284.6319861

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0001559	-0.0001589	0.0004691
2 C	6.0	-0.0001700	-0.0003563	-0.0001008
3 C	6.0	0.0008397	-0.0002805	-0.0003241
4 C	6.0	0.0007217	0.0001170	-0.0003555
5 C	6.0	0.0004513	0.0007294	0.0004064
6 C	6.0	0.0004801	0.0003863	-0.0003427
7 C	6.0	-0.0001865	0.0001176	-0.0002867
8 C	6.0	0.0008853	-0.0005784	-0.0001656
9 C	6.0	0.0000489	0.0006973	-0.0000222
10 C	6.0	-0.0000172	0.0001418	-0.0002852
11 C	6.0	0.0006748	0.0003699	-0.0003576
12 N	7.0	0.0001623	0.0000476	0.0000148
13 C	6.0	0.0004542	0.0001939	0.0001640
14 C	6.0	0.0005742	-0.0004783	0.0004059
15 C	6.0	0.0002306	0.0010777	0.0001275
16 C	6.0	0.0007148	0.0012925	0.0003143
17 C	6.0	-0.0013347	-0.0001958	0.0002387
18 C	6.0	-0.0010543	-0.0004091	0.0005132
19 C	6.0	-0.0002577	-0.0008824	0.0005551
20 O	8.0	0.0004934	-0.0004898	-0.0015540
21 N	7.0	-0.0003213	-0.0009383	0.0007559
22 H	1.0	0.0004070	0.0008590	0.0002196
23 H	1.0	0.0002208	0.0000014	0.0000550
24 H	1.0	-0.0003798	-0.0004859	-0.0003877
25 H	1.0	0.0005570	-0.0008241	0.0000656
26 H	1.0	0.0001390	0.0004323	0.0001101
27 H	1.0	-0.0000673	-0.0002537	-0.0004521
28 H	1.0	-0.0010522	0.0005610	-0.0003311
29 H	1.0	0.0001504	0.0003784	-0.0010997
30 H	1.0	-0.0009840	-0.0000188	-0.0012642
31 H	1.0	-0.0014762	-0.0001799	0.0005823
32 H	1.0	-0.0007137	-0.0015316	0.0005913
33 H	1.0	-0.0003668	0.0009786	0.0000587
34 H	1.0	0.0001876	0.0007538	-0.0001617
35 H	1.0	-0.0001674	-0.0010738	0.0018434

MAXIMUM GRADIENT = 0.0018434 RMS GRADIENT = 0.0006179
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0001762399
PREDICTED ENERGY CHANGE WAS -0.0002017263 RATIO= 0.874
GDIIS STEP HAS LENGTH = 0.371640
RADIUS OF STEP TAKEN= 0.10521 CURRENT TRUST RADIUS= 0.10521

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 2991.3 SECONDS (49.9 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2765.0 SECONDS (46.1
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

1NSERCH= 27

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1132039797	-1.6871015491	1.0425268765
C	6.0	5.0023625975	0.6764094805	0.4308193971
C	6.0	5.2291870613	-0.6840581931	0.1909271758
C	6.0	4.0977947221	-1.5515801179	0.0651632872
C	6.0	2.7810124906	-1.0669582720	0.1945275901
C	6.0	2.4804557990	0.3325957092	0.4794005922
C	6.0	3.6648111369	1.2025816383	0.5743909699
C	6.0	3.5297138911	2.6177246716	0.8185724721
C	6.0	2.2683720885	3.2041757413	0.9842798593
C	6.0	1.1037720044	2.3767378974	0.9303744906
C	6.0	1.1720406094	0.9858848765	0.6750099168
N	7.0	-0.0676722073	0.2036594505	0.7026133352
C	6.0	-1.2796139623	0.7424695317	0.5369307975
C	6.0	-2.5898009283	0.0746570492	0.5950893486
C	6.0	-2.8671034119	-1.3284540718	0.7197543808
C	6.0	-4.1652413929	-1.8695922037	0.6635245313
C	6.0	-5.2829733118	-0.9934275677	0.5218704174
C	6.0	-5.0716915026	0.4128502158	0.4588508592
C	6.0	-3.7518949518	0.9275528731	0.4813884231
O	8.0	-1.7556493491	-2.2603899098	0.9042071456
N	7.0	1.6995481986	-2.0982491007	-0.0529066227
H	1.0	5.8513408089	1.3803822186	0.5165007430
H	1.0	6.2516435984	-1.0859645945	0.0841412759
H	1.0	4.2643163306	-2.6231820117	-0.1668967191
H	1.0	4.4503883126	3.2257455130	0.8809958724
H	1.0	2.1653415652	4.2859644296	1.1835025390

H	1.0	0.1311755759	2.8551826799	1.1331933736
H	1.0	-1.3518195731	1.8212663741	0.2958420482
H	1.0	-4.3278939807	-2.9629816703	0.7174354464
H	1.0	-6.3048109891	-1.4129358383	0.4540570844
H	1.0	-5.9344776243	1.0984509638	0.3782048212
H	1.0	-3.5991344481	2.0189976191	0.4109596218
H	1.0	-2.0869767572	-3.1881802366	1.0079668126
H	1.0	1.4139277021	-2.0637054468	-1.0570200181
H	1.0	2.1023429176	-3.0454231494	0.1066888551

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4648186	5.2824806	4.1049445
2 C	5.4648186	0.0000000	1.3999535 *	2.4322593 *
3 C	5.2824806	1.3999535 *	0.0000000	1.4312440 *
4 C	4.1049445	2.4322593 *	1.4312440 *	0.0000000
5 C	2.8672082 *	2.8336480 *	2.4779395 *	1.4090809 *
6 C	3.1623044	2.5456987 *	2.9448813 *	2.5174384 *
7 C	4.6025356	1.4444770 *	2.4806705 *	2.8341127 *
8 C	5.5003840	2.4673369 *	3.7661542	4.2747449
9 C	5.3453471	3.7643890	4.9511814	5.1777192
10 C	4.1843272	4.2824853	5.1898270	5.0144237
11 C	2.8984582 *	3.8505546	4.4140099	3.9205457
12 N	1.9295685 *	5.0992762	5.3950518	4.5649012
13 C	2.8457661 *	6.2832200	6.6722703	5.8653007
14 C	3.2573347	7.6177449	7.8661025	6.9028548
15 C	3.0191128	8.1259742	8.1390923	6.9991486
16 C	4.2990744	9.5174177	9.4807239	8.2907740
17 C	5.4654365	10.4204021	10.5219175	9.4084496
18 C	5.6243770	10.0775401	10.3625813	9.3858113
19 C	4.7000302	8.7580052	9.1291562	8.2423887
20 O	1.9596950 *	7.3837397	7.1959384	5.9556035
21 N	1.9711684 *	4.3406571	3.8102154	2.4625949 *
22 H	6.5278154	1.1062020 *	2.1805934 *	3.4460169
23 H	6.2418194	2.1878874 *	1.1037886 *	2.2036840 *
24 H	4.4238768	3.4335522	2.1952710 *	1.1090139 *
25 H	6.5554044	2.6469697 *	4.0458976	4.8592947
26 H	6.3173301	4.6523228	5.9222867	6.2499587
27 H	4.5432246	5.3822713	6.2772456	6.0244762
28 H	3.8745939	6.4579058	7.0425355	6.4130805
29 H	4.6321599	10.0190321	9.8391311	8.5679486
30 H	6.4507658	11.4986120	11.5600005	10.4107957
31 H	6.6914183	10.9451067	11.3066273	10.3810957

32 H	5.2835125	8.7056699	9.2354851	8.4918384
33 H	2.6636867 *	8.0948678	7.7758880	6.4667408
34 H	2.4983614 *	4.7538154	4.2446440	2.9537620 *
35 H	2.5840867 *	4.7293988	3.9192212	2.4930141 *

C C C C

1 CO	2.8672082 *	3.1623044	4.6025356	5.5003840
2 C	2.8336480 *	2.5456987 *	1.4444770 *	2.4673369 *
3 C	2.4779395 *	2.9448813 *	2.4806705 *	3.7661542
4 C	1.4090809 *	2.5174384 *	2.8341127 *	4.2747449
5 C	0.0000000	1.4595336 *	2.4649965 *	3.8114137
6 C	1.4595336 *	0.0000000	1.4726154 *	2.5372809 *
7 C	2.4649965 *	1.4726154 *	0.0000000	1.4423958 *
8 C	3.8114137	2.5372809 *	1.4423958 *	0.0000000
9 C	4.3736820	2.9233293 *	2.4747585 *	1.4008451 *
10 C	3.9004679	2.5054247 *	2.8397691 *	2.4404443 *
11 C	2.6521348 *	1.4754660 *	2.5041938 *	2.8709118 *
12 N	3.1603204	2.5611335 *	3.8659693	4.3338602
13 C	4.4586944	3.7827808	4.9659285	5.1696749
14 C	5.5053948	5.0781315	6.3555342	6.6306560
15 C	5.6785083	5.6047521	7.0066526	7.5167389
16 C	7.0081825	7.0034866	8.4116538	8.9091183
17 C	8.0709620	7.8759744	9.2134717	9.5284788
18 C	7.9952899	7.5526017	8.7728846	8.8867905
19 C	6.8366105	6.2606848	7.4223864	7.4827937
20 O	4.7443888	4.9848392	6.4406787	7.1929410
21 N	1.5147110 *	2.6080978 *	3.8924599	5.1331658
22 H	3.9395505	3.5301698	2.1945105 *	2.6480588 *
23 H	3.4724381	4.0485060	3.4884797	4.6546326
24 H	2.1800574 *	3.5123326	3.9427632	5.3831118
25 H	4.6567542	3.5230993	2.1918782 *	1.1050916 *
26 H	5.4782208	4.0279251	3.4823376	2.1857973 *
27 H	4.8255485	3.5085620	3.9408033	3.4213207
28 H	5.0430553	4.1153577	5.0623062	4.9736266
29 H	7.3759670	7.5677683	9.0141952	9.6382837
30 H	9.0961115	8.9570327	10.3077048	10.6347062
31 H	8.9823439	8.4503183	9.6018580	9.5954696
32 H	7.0905741	6.3095208	7.3115081	7.1655496
33 H	5.3720187	5.7910867	7.2491270	8.0803228
34 H	2.1044708 *	3.0397911	4.2891269	5.4690206
35 H	2.0934735 *	3.4194875	4.5503403	5.8834862

C C C N

1 CO	5.3453471	4.1843272	2.8984582 *	1.9295685 *
------	-----------	-----------	-------------	-------------

2 C	3.7643890	4.2824853	3.8505546	5.0992762
3 C	4.9511814	5.1898270	4.4140099	5.3950518
4 C	5.1777192	5.0144237	3.9205457	4.5649012
5 C	4.3736820	3.9004679	2.6521348 *	3.1603204
6 C	2.9233293 *	2.5054247 *	1.4754660 *	2.5611335 *
7 C	2.4747585 *	2.8397691 *	2.5041938 *	3.8659693
8 C	1.4008451 *	2.4404443 *	2.8709118 *	4.3338602
9 C	0.0000000	1.4296337 *	2.4936730 *	3.8130745
10 C	1.4296337 *	0.0000000	1.4157485 *	2.4791988 *
11 C	2.4936730 *	1.4157485 *	0.0000000	1.4661263 *
12 N	3.8130745	2.4791988 *	1.4661263 *	0.0000000
13 C	4.3414656	2.9165321 *	2.4675751 *	1.3366263 *
14 C	5.7919946	4.3651430	3.8714565	2.5277137 *
15 C	6.8547659	5.4351320	4.6554110	3.1913133
16 C	8.1998407	6.7723726	6.0531364	4.5923821
17 C	8.6519659	7.2329390	6.7533943	5.3539752
18 C	7.8704579	6.4973486	6.2736978	5.0143185
19 C	6.4559683	5.0871630	4.9280862	3.7611779
20 O	6.7867988	5.4479289	4.3774650	2.9935675 *
21 N	5.4327733	4.6203138	3.2124771	2.9987766 *
22 H	4.0475554	4.8686164	4.6985746	6.0377172
23 H	5.9230065	6.2615494	5.5176129	6.4791504
24 H	6.2663466	6.0159990	4.8266282	5.2453031
25 H	2.1845658 *	3.4529832	3.9757980	5.4385380
26 H	1.1047949 *	2.1991248 *	3.4836384	4.6779075
27 H	2.1706175 *	1.1027188 *	2.1880600 *	2.6936063 *
28 H	3.9360097	2.5963648 *	2.6854238 *	2.1050296 *
29 H	9.0341443	7.6197732	6.7708661	5.3082318
30 H	9.7518369	8.3352029	7.8553466	6.4480277
31 H	8.4904739	7.1746684	7.1136043	5.9435089
32 H	6.0133997	4.7450078	4.8888808	3.9814244
33 H	7.7351044	6.4152328	5.3061167	3.9592181
34 H	5.7138037	4.8747790	3.5154570	3.2299213
35 H	6.3130989	5.5745343	4.1761101	3.9522942

C C C C

1 CO	2.8457661 *	3.2573347	3.0191128	4.2990744
2 C	6.2832200	7.6177449	8.1259742	9.5174177
3 C	6.6722703	7.8661025	8.1390923	9.4807239
4 C	5.8653007	6.9028548	6.9991486	8.2907740
5 C	4.4586944	5.5053948	5.6785083	7.0081825
6 C	3.7827808	5.0781315	5.6047521	7.0034866
7 C	4.9659285	6.3555342	7.0066526	8.4116538
8 C	5.1696749	6.6306560	7.5167389	8.9091183
9 C	4.3414656	5.7919946	6.8547659	8.1998407

10	C	2.9165321 *	4.3651430	5.4351320	6.7723726
11	C	2.4675751 *	3.8714565	4.6554110	6.0531364
12	N	1.3366263 *	2.5277137 *	3.1913133	4.5923821
13	C	0.0000000	1.4717153 *	2.6157736 *	3.8943213
14	C	1.4717153 *	0.0000000	1.4356737 *	2.5033580 *
15	C	2.6157736 *	1.4356737 *	0.0000000	1.4075349 *
16	C	3.8943213	2.5033580 *	1.4075349 *	0.0000000
17	C	4.3635366	2.8981620 *	2.4470039 *	1.4272544 *
18	C	3.8071771	2.5085287 *	2.8214216 *	2.4643633 *
19	C	2.4798214 *	1.4459674 *	2.4350034 *	2.8333813 *
20	O	3.0624608	2.4987611 *	1.4621414 *	2.4529135 *
21	N	4.1584850	4.8517972	4.6950928	5.9128094
22	H	7.1594599	8.5418949	9.1318331	10.5316603
23	H	7.7632487	8.9319232	9.1440884	10.4623731
24	H	6.5236605	7.4052604	7.3020284	8.5038192
25	H	6.2544357	7.7185080	8.6204651	10.0119347
26	H	4.9841880	6.3790846	7.5539566	8.8451984
27	H	2.6094852 *	3.9274154	5.1636639	6.4033808
28	H	1.1077635 *	2.1616639 *	3.5208700	4.6554237
29	H	4.8015582	3.5018831	2.1921667 *	1.1067352 *
30	H	5.4685689	4.0042630	3.4489949	2.1977647 *
31	H	4.6711532	3.5045763	3.9262334	3.4671147
32	H	2.6505788 *	2.1984354 *	3.4404442	3.9376893
33	H	4.0402620	3.3270719	2.0372151 *	2.4852563 *
34	H	4.2036251	4.8303108	4.6930533	5.8416677
35	H	5.0961624	5.6559393	5.2933193	6.4011919

C C C O

1	CO	5.4654365	5.6243770	4.7000302	1.9596950 *
2	C	10.4204021	10.0775401	8.7580052	7.3837397
3	C	10.5219175	10.3625813	9.1291562	7.1959384
4	C	9.4084496	9.3858113	8.2423887	5.9556035
5	C	8.0709620	7.9952899	6.8366105	4.7443888
6	C	7.8759744	7.5526017	6.2606848	4.9848392
7	C	9.2134717	8.7728846	7.4223864	6.4406787
8	C	9.5284788	8.8867905	7.4827937	7.1929410
9	C	8.6519659	7.8704579	6.4559683	6.7867988
10	C	7.2329390	6.4973486	5.0871630	5.4479289
11	C	6.7533943	6.2736978	4.9280862	4.3774650
12	N	5.3539752	5.0143185	3.7611779	2.9935675 *
13	C	4.3635366	3.8071771	2.4798214 *	3.0624608
14	C	2.8981620 *	2.5085287 *	1.4459674 *	2.4987611 *
15	C	2.4470039 *	2.8214216 *	2.4350034 *	1.4621414 *
16	C	1.4272544 *	2.4643633 *	2.8333813 *	2.4529135 *
17	C	0.0000000	1.4234566 *	2.4568284 *	3.7674115

18 C	1.4234566 *	0.0000000	1.4167885 *	4.2826032
19 C	2.4568284 *	1.4167885 *	0.0000000	3.7850695
20 O	3.7674115	4.2826032	3.7850695	0.0000000
21 N	7.0927150	7.2399726	6.2577297	3.5889757
22 H	11.3845489	10.9659508	9.6139703	8.4422649
23 H	11.5432906	11.4282444	10.2118971	8.1344037
24 H	9.7098527	9.8371792	8.7913386	6.1252648
25 H	10.6145523	9.9378363	8.5275334	8.2833039
26 H	9.1535311	8.2401930	6.8399986	7.6358975
27 H	6.6707215	5.7870158	4.3839301	5.4572544
28 H	4.8402025	3.9809113	2.5677837 *	4.1464569
29 H	2.1976273 *	3.4664595	3.9400193	2.6730060 *
30 H	1.1066788 *	2.2032025 *	3.4635263	4.6492672
31 H	2.1956897 *	1.1049670 *	2.1916934 *	5.3871232
32 H	3.4528713	2.1795475 *	1.1043313 *	4.6856043
33 H	3.9073806	4.7092962	4.4708496	0.9906255 *
34 H	6.9632516	7.1059446	6.1644181	3.7324677
35 H	7.6763245	7.9718531	7.0849869	4.0170159

N H H H

1 CO	1.9711684 *	6.5278154	6.2418194	4.4238768
2 C	4.3406571	1.1062020 *	2.1878874 *	3.4335522
3 C	3.8102154	2.1805934 *	1.1037886 *	2.1952710 *
4 C	2.4625949 *	3.4460169	2.2036840 *	1.1090139 *
5 C	1.5147110 *	3.9395505	3.4724381	2.1800574 *
6 C	2.6080978 *	3.5301698	4.0485060	3.5123326
7 C	3.8924599	2.1945105 *	3.4884797	3.9427632
8 C	5.1331658	2.6480588 *	4.6546326	5.3831118
9 C	5.4327733	4.0475554	5.9230065	6.2663466
10 C	4.6203138	4.8686164	6.2615494	6.0159990
11 C	3.2124771	4.6985746	5.5176129	4.8266282
12 N	2.9987766 *	6.0377172	6.4791504	5.2453031
13 C	4.1584850	7.1594599	7.7632487	6.5236605
14 C	4.8517972	8.5418949	8.9319232	7.4052604
15 C	4.6950928	9.1318331	9.1440884	7.3020284
16 C	5.9128094	10.5316603	10.4623731	8.5038192
17 C	7.0927150	11.3845489	11.5432906	9.7098527
18 C	7.2399726	10.9659508	11.4282444	9.8371792
19 C	6.2577297	9.6139703	10.2118971	8.7913386
20 O	3.5889757	8.4422649	8.1344037	6.1252648
21 N	0.0000000	5.4463274	4.6653054	2.6204167 *
22 H	5.4463274	0.0000000	2.5357531 *	4.3605281
23 H	4.6653054	2.5357531 *	0.0000000	2.5249806 *
24 H	2.6204167 *	4.3605281	2.5249806 *	0.0000000
25 H	6.0649991	2.3453977 *	4.7402892	5.9449689

26 H	6.5194979	4.7406634	6.8384268	7.3461267
27 H	5.3294570	5.9393296	7.3548135	6.9846665
28 H	4.9794651	7.2200131	8.1430622	7.1769235
29 H	6.1376908	11.0689659	10.7634042	8.6442805
30 H	8.0496231	12.4731131	12.5661569	10.6563001
31 H	8.2875267	11.7900012	12.3838482	10.8702845
32 H	6.7262865	9.4726159	10.3337035	9.1497327
33 H	4.0805850	9.1722510	8.6490088	6.4837066
34 H	1.0445171 *	5.8333817	5.0657400	3.0380995
35 H	1.0415628 *	5.8146955	4.5887561	2.2197445 *

H H H H

1 CO	6.5554044	6.3173301	4.5432246	3.8745939
2 C	2.6469697 *	4.6523228	5.3822713	6.4579058
3 C	4.0458976	5.9222867	6.2772456	7.0425355
4 C	4.8592947	6.2499587	6.0244762	6.4130805
5 C	4.6567542	5.4782208	4.8255485	5.0430553
6 C	3.5230993	4.0279251	3.5085620	4.1153577
7 C	2.1918782 *	3.4823376	3.9408033	5.0623062
8 C	1.1050916 *	2.1857973 *	3.4213207	4.9736266
9 C	2.1845658 *	1.1047949 *	2.1706175 *	3.9360097
10 C	3.4529832	2.1991248 *	1.1027188 *	2.5963648 *
11 C	3.9757980	3.4836384	2.1880600 *	2.6854238 *
12 N	5.4385380	4.6779075	2.6936063 *	2.1050296 *
13 C	6.2544357	4.9841880	2.6094852 *	1.1077635 *
14 C	7.7185080	6.3790846	3.9274154	2.1616639 *
15 C	8.6204651	7.5539566	5.1636639	3.5208700
16 C	10.0119347	8.8451984	6.4033808	4.6554237
17 C	10.6145523	9.1535311	6.6707215	4.8402025
18 C	9.9378363	8.2401930	5.7870158	3.9809113
19 C	8.5275334	6.8399986	4.3839301	2.5677837 *
20 O	8.2833039	7.6358975	5.4572544	4.1464569
21 N	6.0649991	6.5194979	5.3294570	4.9794651
22 H	2.3453977 *	4.7406634	5.9393296	7.2200131
23 H	4.7402892	6.8384268	7.3548135	8.1430622
24 H	5.9449689	7.3461267	6.9846665	7.1769235
25 H	0.0000000	2.5371269 *	4.3424094	5.9983817
26 H	2.5371269 *	0.0000000	2.4874683 *	4.3855559
27 H	4.3424094	2.4874683 *	0.0000000	1.9923390 *
28 H	5.9983817	4.3855559	1.9923390 *	0.0000000
29 H	10.7417567	9.7430255	7.3421518	5.6501141
30 H	11.7206635	10.2348932	7.7524180	5.9175350
31 H	10.6124277	8.7416141	6.3598949	4.6400432
32 H	8.1530357	6.2422067	3.8905064	2.2589320 *
33 H	9.1592416	8.6009222	6.4387978	5.1129378

34 H	6.3995539	6.7751658	5.5351557	4.9570757
35 H	6.7409513	7.4103131	6.3052646	5.9709031

H H H H

1 CO	4.6321599	6.4507658	6.6914183	5.2835125
2 C	10.0190321	11.4986120	10.9451067	8.7056699
3 C	9.8391311	11.5600005	11.3066273	9.2354851
4 C	8.5679486	10.4107957	10.3810957	8.4918384
5 C	7.3759670	9.0961115	8.9823439	7.0905741
6 C	7.5677683	8.9570327	8.4503183	6.3095208
7 C	9.0141952	10.3077048	9.6018580	7.3115081
8 C	9.6382837	10.6347062	9.5954696	7.1655496
9 C	9.0341443	9.7518369	8.4904739	6.0133997
10 C	7.6197732	8.3352029	7.1746684	4.7450078
11 C	6.7708661	7.8553466	7.1136043	4.8888808
12 N	5.3082318	6.4480277	5.9435089	3.9814244
13 C	4.8015582	5.4685689	4.6711532	2.6505788 *
14 C	3.5018831	4.0042630	3.5045763	2.1984354 *
15 C	2.1921667 *	3.4489949	3.9262334	3.4404442
16 C	1.1067352 *	2.1977647 *	3.4671147	3.9376893
17 C	2.1976273 *	1.1066788 *	2.1956897 *	3.4528713
18 C	3.4664595	2.2032025 *	1.1049670 *	2.1795475 *
19 C	3.9400193	3.4635263	2.1916934 *	1.1043313 *
20 O	2.6730060 *	4.6492672	5.3871232	4.6856043
21 N	6.1376908	8.0496231	8.2875267	6.7262865
22 H	11.0689659	12.4731131	11.7900012	9.4726159
23 H	10.7634042	12.5661569	12.3838482	10.3337035
24 H	8.6442805	10.6563001	10.8702845	9.1497327
25 H	10.7417567	11.7206635	10.6124277	8.1530357
26 H	9.7430255	10.2348932	8.7416141	6.2422067
27 H	7.3421518	7.7524180	6.3598949	3.8905064
28 H	5.6501141	5.9175350	4.6400432	2.2589320 *
29 H	0.0000000	2.5259080 *	4.3808017	5.0443172
30 H	2.5259080 *	0.0000000	2.5396779 *	4.3704359
31 H	4.3808017	2.5396779 *	0.0000000	2.5104396 *
32 H	5.0443172	4.3704359	2.5104396 *	0.0000000
33 H	2.2708661 *	4.6096024	5.7943999	5.4550655
34 H	6.0766690	7.8921342	8.1276174	6.6297979
35 H	6.4597024	8.5712261	9.0463196	7.6320235

H H H

1 CO	2.6636867 *	2.4983614 *	2.5840867 *
2 C	8.0948678	4.7538154	4.7293988
3 C	7.7758880	4.2446440	3.9192212

4 C	6.4667408	2.9537620 *	2.4930141 *
5 C	5.3720187	2.1044708 *	2.0934735 *
6 C	5.7910867	3.0397911	3.4194875
7 C	7.2491270	4.2891269	4.5503403
8 C	8.0803228	5.4690206	5.8834862
9 C	7.7351044	5.7138037	6.3130989
10 C	6.4152328	4.8747790	5.5745343
11 C	5.3061167	3.5154570	4.1761101
12 N	3.9592181	3.2299213	3.9522942
13 C	4.0402620	4.2036251	5.0961624
14 C	3.3270719	4.8303108	5.6559393
15 C	2.0372151 *	4.6930533	5.2933193
16 C	2.4852563 *	5.8416677	6.4011919
17 C	3.9073806	6.9632516	7.6763245
18 C	4.7092962	7.1059446	7.9718531
19 C	4.4708496	6.1644181	7.0849869
20 O	0.9906255 *	3.7324677	4.0170159
21 N	4.0805850	1.0445171 *	1.0415628 *
22 H	9.1722510	5.8333817	5.8146955
23 H	8.6490088	5.0657400	4.5887561
24 H	6.4837066	3.0380995	2.2197445 *
25 H	9.1592416	6.3995539	6.7409513
26 H	8.6009222	6.7751658	7.4103131
27 H	6.4387978	5.5351557	6.3052646
28 H	5.1129378	4.9570757	5.9709031
29 H	2.2708661 *	6.0766690	6.4597024
30 H	4.6096024	7.8921342	8.5712261
31 H	5.7943999	8.1276174	9.0463196
32 H	5.4550655	6.6297979	7.6320235
33 H	0.0000000	4.2172202	4.2875495
34 H	4.2172202	0.0000000	1.6708990 *
35 H	4.2875495	1.6708990 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 2992.1 SECONDS (49.9 MIN)
WALL CLOCK TIME: STEP = 0.78 , TOTAL = 2765.7 SECONDS (46.1 MIN)
CPU UTILIZATION: STEP = 99.37% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.16 , TOTAL = 2993.2 SECONDS (49.9 MIN)

WALL CLOCK TIME: STEP = 1.14 , TOTAL = 2766.9 SECONDS (46.1 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.632001352	-284.632001352	0.029027808	0.001873581	195822627 11513797
2	1	-284.632223198	-0.000221846	0.002518458	0.000100956	159166678 14632324
3	2	-284.632222990	0.000000208	0.002240943	0.000216904	143708337 15873539
4	3	-284.632226454	-0.000003464	0.000525775	0.000079912	138267161 16292398
5	4	-284.632226407	0.000000047	0.000470110	0.000122361	131438551 16849613
6	5	-284.632226712	-0.000000305	0.000378158	0.000032751	124938006 17352760
7	6	-284.632226745	-0.000000033	0.000224479	0.000033212	123918960 17409804
8	7	-284.632226841	-0.000000096	0.000469992	0.000033011	116076883 17998441
9	8	-284.632226930	-0.000000089	0.000719281	0.000030718	144208582 15921284
10	9	-284.632227025	-0.000000094	0.000541278	0.000033936	164769011 14365117
11	10	-284.632227107	-0.000000082	0.000507028	0.000023784	164484933 14315669
12	11	-284.632227150	-0.000000043	0.000215781	0.000026927	164161896 14321058
13	12	-284.632227187	-0.000000037	0.000207336	0.000014390	160328579 14631574
14	13	-284.632227205	-0.000000019	0.000191303	0.000008474	159309725 14696019
15	14	-284.632227213	-0.000000008	0.000067606	0.000011328	156130801 14979830
16	15	-284.632227217	-0.000000004	0.000057332	0.000010339	152729686 15180717
17	16	-284.632227221	-0.000000004	0.000129745	0.000008510	150387506 15431361

-----DISABLING FDIFF OPTION-----

18 17	-284.632227253	-0.000000032	0.000226523	0.000008154	195820935
11513966					
19 18	-284.632227259	-0.000000007	0.000102810	0.000005835	195820872
11513958					
20 19	-284.632227261	-0.000000002	0.000048069	0.000005139	195820879
11513965					
21 20	-284.632227264	-0.000000002	0.000056009	0.000004476	195820875
11513965					
22 21	-284.632227265	-0.000000002	0.000055897	0.000003162	195820912
11513961					
23 22	-284.632227266	-0.000000001	0.000027623	0.000002354	195820824
11513965					
24 23	-284.632227267	0.000000000	0.000019165	0.000001496	195820834
11513963					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 79.2 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 25.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.8, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 3.5 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6322272665 AFTER 24 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5911971599
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000403115

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 83.69 , TOTAL = 3076.9 SECONDS (51.3 MIN)
WALL CLOCK TIME: STEP = 77.13 , TOTAL = 2844.0 SECONDS (47.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.70 , TOTAL = 3080.6 SECONDS (51.3 MIN)
WALL CLOCK TIME: STEP = 3.75 , TOTAL = 2847.8 SECONDS (47.5 MIN)

CPU UTILIZATION: STEP = 98.73%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.80 , TOTAL = 3083.4 SECONDS (51.4 MIN)
WALL CLOCK TIME: STEP = 2.64 , TOTAL = 2850.4 SECONDS (47.5 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 27 ENERGY= -284.6322273

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0001552	0.0000593	0.0004547
2 C	6.0	-0.0005090	0.0002386	-0.0000707
3 C	6.0	0.0008859	-0.0001905	-0.0003150
4 C	6.0	0.0006298	0.0002122	-0.0001658
5 C	6.0	0.0004951	0.0003942	0.0005645
6 C	6.0	0.0004509	0.0003936	-0.0001325
7 C	6.0	0.0003319	-0.0000673	-0.0002826
8 C	6.0	0.0008179	-0.0002111	-0.0000642
9 C	6.0	0.0001933	0.0004984	-0.0000207
10 C	6.0	-0.0000887	0.0000865	-0.0003367
11 C	6.0	0.0004674	-0.0000949	-0.0003338
12 N	7.0	-0.0001255	0.0001444	0.0000428
13 C	6.0	0.0004910	0.0003972	0.0000074
14 C	6.0	-0.0000754	-0.0004019	0.0002975
15 C	6.0	0.0002788	0.0010346	0.0002469
16 C	6.0	0.0004902	0.0011944	0.0001814
17 C	6.0	-0.0010903	-0.0004743	0.0001350
18 C	6.0	-0.0007761	-0.0002221	0.0004409
19 C	6.0	-0.0000901	-0.0009198	0.0006041
20 O	8.0	0.0005061	-0.0004928	-0.0016544
21 N	7.0	-0.0002540	-0.0007775	0.0008497
22 H	1.0	0.0005577	0.0006882	0.0001565
23 H	1.0	-0.0000782	0.0001616	0.0000169

24 H	1.0	-0.0001874	-0.0007005	-0.0005259
25 H	1.0	0.0005904	-0.0005731	-0.0000164
26 H	1.0	0.0002122	0.0004950	0.0000565
27 H	1.0	0.0001182	-0.0003207	-0.0004565
28 H	1.0	-0.0010956	0.0004440	-0.0003090
29 H	1.0	-0.0000454	0.0002764	-0.0007770
30 H	1.0	-0.0011362	-0.0000689	-0.0011974
31 H	1.0	-0.0010111	-0.0003238	0.0003807
32 H	1.0	-0.0005486	-0.0011465	0.0008958
33 H	1.0	-0.0003945	0.0009207	-0.0000045
34 H	1.0	0.0002789	0.0005515	-0.0000794
35 H	1.0	-0.0004447	-0.0012052	0.0014113

MAXIMUM GRADIENT = 0.0016544 RMS GRADIENT = 0.0005606
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0002412141
 PREDICTED ENERGY CHANGE WAS -0.0002521766 RATIO= 0.957
 GDIIS STEP HAS LENGTH = 0.351452
 RADIUS OF STEP TAKEN= 0.21042 CURRENT TRUST RADIUS= 0.21042

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 3083.4 SECONDS (51.4 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2850.4 SECONDS (47.5
 MIN)
 CPU UTILIZATION: STEP = 93.40% , TOTAL = 100.00%

INSERCH= 28

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1134007802	-1.6976271710	1.0401499699
C	6.0	5.0018052230	0.6806127614	0.4335367912
C	6.0	5.2278380571	-0.6793696205	0.1961257547
C	6.0	4.1004303627	-1.5524697185	0.0717014590
C	6.0	2.7823242373	-1.0704057034	0.2004112423
C	6.0	2.4823458533	0.3284872594	0.4897048314
C	6.0	3.6639214387	1.2043695792	0.5815072031
C	6.0	3.5245393519	2.6205019487	0.8191043641
C	6.0	2.2615565075	3.2005533026	0.9867922059
C	6.0	1.1003721780	2.3676886547	0.9392476338
C	6.0	1.1724065730	0.9776642851	0.6850426575
N	7.0	-0.0661856536	0.1939124051	0.7094873109
C	6.0	-1.2768368983	0.7326418940	0.5366888035
C	6.0	-2.5868435508	0.0684040450	0.5939869513

C	6.0	-2.8701485864	-1.3335496243	0.7280640093
C	6.0	-4.1709581256	-1.8695043836	0.6840016070
C	6.0	-5.2808770258	-0.9861438646	0.5229384139
C	6.0	-5.0614273122	0.4178398168	0.4392317627
C	6.0	-3.7416250804	0.9291682667	0.4717868662
O	8.0	-1.7591989006	-2.2668908633	0.9099917469
N	7.0	1.6980629197	-2.0930635765	-0.0667798287
H	1.0	5.8522537802	1.3831843879	0.5114791060
H	1.0	6.2511119692	-1.0775747843	0.0838984107
H	1.0	4.2742397323	-2.6215433842	-0.1659719051
H	1.0	4.4412952935	3.2368664544	0.8721067456
H	1.0	2.1543990553	4.2826304610	1.1802590069
H	1.0	0.1276327247	2.8438762899	1.1451132411
H	1.0	-1.3454528806	1.8105070569	0.2905554087
H	1.0	-4.3441732585	-2.9602825355	0.7678277156
H	1.0	-6.3054643640	-1.4000393242	0.4621936454
H	1.0	-5.9178878550	1.1072922518	0.3382291828
H	1.0	-3.5812300935	2.0209593589	0.4069487927
H	1.0	-2.0897635421	-3.1962226619	1.0033263532
H	1.0	1.4086855844	-2.0341094504	-1.0685757729
H	1.0	2.0954485056	-3.0472588134	0.0627753130

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4699637	5.2826787	4.1055290
2 C	5.4699637	0.0000000	1.3989306 *	2.4351712 *
3 C	5.2826787	1.3989306 *	0.0000000	1.4313746 *
4 C	4.1055290	2.4351712 *	1.4313746 *	0.0000000
5 C	2.8673542 *	2.8366369 *	2.4765834 *	1.4093813 *
6 C	3.1654431	2.5445673 *	2.9393352 *	2.5161326 *
7 C	4.6084851	1.4443509 *	2.4784728 *	2.8373588 *
8 C	5.5073557	2.4686326 *	3.7654324	4.2783121
9 C	5.3487935	3.7636624	4.9475026	5.1778447
10 C	4.1846250	4.2805547	5.1838951	5.0120482
11 C	2.8990997 *	3.8491283	4.4080977	3.9180466
12 N	1.9286034 *	5.0987800	5.3900694	4.5625991
13 C	2.8447217 *	6.2797049	6.6648748	5.8611391
14 C	3.2571839	7.6149940	7.8604521	6.9006990
15 C	3.0218400	8.1308827	8.1417626	7.0048347
16 C	4.3025707	9.5239392	9.4864015	8.3000777
17 C	5.4655237	10.4172753	10.5182703	9.4092119
18 C	5.6227350	10.0666643	10.3504566	9.3785305
19 C	4.6993952	8.7470462	9.1167238	8.2350731

20 O	1.9615381 *	7.3909379	7.2005912	5.9622465
21 N	1.9730225 *	4.3426156	3.8114253	2.4663309 *
22 H	6.5349313	1.1058683 *	2.1779513 *	3.4467890
23 H	6.2426261	2.1850029 *	1.1037445 *	2.2025225 *
24 H	4.4295521	3.4340934	2.1937419 *	1.1088809 *
25 H	6.5656787	2.6534785 *	4.0512350	4.8677077
26 H	6.3205052	4.6518649	5.9191207	6.2501465
27 H	4.5427385	5.3799264	6.2710393	6.0218927
28 H	3.8726156	6.4486270	7.0296911	6.4043075
29 H	4.6409508	10.0356954	9.8566124	8.5894039
30 H	6.4516991	11.4971422	11.5588590	10.4143346
31 H	6.6885505	10.9284416	11.2889132	10.3688028
32 H	5.2800688	8.6871014	9.2160677	8.4787790
33 H	2.6647847 *	8.1021516	7.7803223	6.4721209
34 H	2.4975403 *	4.7472695	4.2450813	2.9627182 *
35 H	2.5894555 *	4.7414555	3.9289370	2.5008851 *

C C C C

1 CO	2.8673542 *	3.1654431	4.6084851	5.5073557
2 C	2.8366369 *	2.5445673 *	1.4443509 *	2.4686326 *
3 C	2.4765834 *	2.9393352 *	2.4784728 *	3.7654324
4 C	1.4093813 *	2.5161326 *	2.8373588 *	4.2783121
5 C	0.0000000	1.4596504 *	2.4692206 *	3.8152934
6 C	1.4596504 *	0.0000000	1.4736751 *	2.5392918 *
7 C	2.4692206 *	1.4736751 *	0.0000000	1.4426748 *
8 C	3.8152934	2.5392918 *	1.4426748 *	0.0000000
9 C	4.3738638	2.9231160 *	2.4729805 *	1.3998944 *
10 C	3.8981194	2.5040532 *	2.8377939 *	2.4402736 *
11 C	2.6497723 *	1.4749673 *	2.5039491 *	2.8721798 *
12 N	3.1577947	2.5615284 *	3.8666654	4.3351654
13 C	4.4543072	3.7811378	4.9634291	5.1669128
14 C	5.5027041	5.0769281	6.3531596	6.6266796
15 C	5.6831427	5.6096683	7.0111756	7.5189658
16 C	7.0157362	7.0096628	8.4169201	8.9106168
17 C	8.0700891	7.8738167	9.2092996	9.5200297
18 C	7.9872616	7.5444712	8.7618823	8.8721388
19 C	6.8288986	6.2529156	7.4114704	7.4684928
20 O	4.7497909	4.9903237	6.4473084	7.1981080
21 N	1.5142136 *	2.6055102 *	3.8933201	5.1321055
22 H	3.9422500	3.5311669	2.1967424 *	2.6540238 *
23 H	3.4707514	4.0429305	3.4854612	4.6530095
24 H	2.1831346 *	3.5133284	3.9457348	5.3862292
25 H	4.6643277	3.5273763	2.1954047 *	1.1059638 *
26 H	5.4780825	4.0273642	3.4803522	2.1841219 *
27 H	4.8230128	3.5073375	3.9383971	3.4198176

28 H	5.0345137	4.1095117	5.0542939	4.9651062
29 H	7.3946307	7.5825274	9.0282126	9.6469904
30 H	9.0975321	8.9562363	10.3046511	10.6264345
31 H	8.9696741	8.4376186	9.5853888	9.5749922
32 H	7.0777129	6.2958926	7.2931139	7.1429184
33 H	5.3759659	5.7958236	7.2558965	8.0863230
34 H	2.1037909 *	3.0270197	4.2774536	5.4502826
35 H	2.0973054 *	3.4245613	4.5613084	5.8938821

C C C N

1 CO	5.3487935	4.1846250	2.8990997 *	1.9286034 *
2 C	3.7636624	4.2805547	3.8491283	5.0987800
3 C	4.9475026	5.1838951	4.4080977	5.3900694
4 C	5.1778447	5.0120482	3.9180466	4.5625991
5 C	4.3738638	3.8981194	2.6497723 *	3.1577947
6 C	2.9231160 *	2.5040532 *	1.4749673 *	2.5615284 *
7 C	2.4729805 *	2.8377939 *	2.5039491 *	3.8666654
8 C	1.3998944 *	2.4402736 *	2.8721798 *	4.3351654
9 C	0.0000000	1.4297808 *	2.4936993 *	3.8125019
10 C	1.4297808 *	0.0000000	1.4149123 *	2.4776905 *
11 C	2.4936993 *	1.4149123 *	0.0000000	1.4659384 *
12 N	3.8125019	2.4776905 *	1.4659384 *	0.0000000
13 C	4.3374425	2.9131692 *	2.4659356 *	1.3363253 *
14 C	5.7854678	4.3590681	3.8687216	2.5264222 *
15 C	6.8526949	5.4322001	4.6568029	3.1930696
16 C	8.1959997	6.7680040	6.0545782	4.5942894
17 C	8.6389755	7.2209312	6.7474209	5.3497981
18 C	7.8529873	6.4822604	6.2637458	5.0075564
19 C	6.4391467	5.0727505	4.9188959	3.7557899
20 O	6.7871436	5.4458544	4.3785901	2.9936681 *
21 N	5.4267779	4.6116847	3.2048278	2.9908900 *
22 H	4.0523893	4.8716130	4.7005894	6.0399918
23 H	5.9189653	6.2555242	5.5116813	6.4742791
24 H	6.2671021	6.0155949	4.8269960	5.2471433
25 H	2.1830558 *	3.4527880	3.9780172	5.4409006
26 H	1.1044470 *	2.1991047 *	3.4831523	4.6765626
27 H	2.1693120 *	1.1024325 *	2.1876848 *	2.6925163 *
28 H	3.9277845	2.5910062 *	2.6812056 *	2.1036651 *
29 H	9.0354585	7.6196940	6.7784166	5.3154047
30 H	9.7383008	8.3228462	7.8499484	6.4444112
31 H	8.4679210	7.1558225	7.0999548	5.9341818
32 H	5.9888075	4.7245067	4.8747166	3.9730552
33 H	7.7364722	6.4139053	5.3070133	3.9590687
34 H	5.6880243	4.8479107	3.4931056	3.2094914
35 H	6.3179550	5.5749472	4.1760303	3.9491885

	C	C	C	C
1 CO	2.8447217 *	3.2571839	3.0218400	4.3025707
2 C	6.2797049	7.6149940	8.1308827	9.5239392
3 C	6.6648748	7.8604521	8.1417626	9.4864015
4 C	5.8611391	6.9006990	7.0048347	8.3000777
5 C	4.4543072	5.5027041	5.6831427	7.0157362
6 C	3.7811378	5.0769281	5.6096683	7.0096628
7 C	4.9634291	6.3531596	7.0111756	8.4169201
8 C	5.1669128	6.6266796	7.5189658	8.9106168
9 C	4.3374425	5.7854678	6.8526949	8.1959997
10 C	2.9131692 *	4.3590681	5.4322001	6.7680040
11 C	2.4659356 *	3.8687216	4.6568029	6.0545782
12 N	1.3363253 *	2.5264222 *	3.1930696	4.5942894
13 C	0.0000000	1.4699022 *	2.6161831 *	3.8947149
14 C	1.4699022 *	0.0000000	1.4365627 *	2.5045979 *
15 C	2.6161831 *	1.4365627 *	0.0000000	1.4075846 *
16 C	3.8947149	2.5045979 *	1.4075846 *	0.0000000
17 C	4.3573789	2.8939481 *	2.4442543 *	1.4276509 *
18 C	3.7989107	2.5039208 *	2.8200162 *	2.4667369 *
19 C	2.4734623 *	1.4454647 *	2.4382456 *	2.8393539 *
20 O	3.0609190	2.4976903 *	1.4623381 *	2.4547037 *
21 N	4.1471454	4.8444792	4.6986375	5.9210691
22 H	7.1587551	8.5413008	9.1382633	10.5391900
23 H	7.7557667	8.9265288	9.1475607	10.4693276
24 H	6.5237062	7.4086313	7.3144045	8.5211140
25 H	6.2514544	7.7143529	8.6236108	10.0140559
26 H	4.9789539	6.3704631	7.5493071	8.8377134
27 H	2.6076859 *	3.9211437	5.1586345	6.3958162
28 H	1.1077378 *	2.1605658 *	3.5215342	4.6562607
29 H	4.8062114	3.5059051	2.1955842 *	1.1076224 *
30 H	5.4626892	4.0002295	3.4462302	2.1967506 *
31 H	4.6603759	3.4986507	3.9240789	3.4688096
32 H	2.6432598 *	2.1991499 *	3.4440503	3.9446477
33 H	4.0391307	3.3275268	2.0382152 *	2.4886785 *
34 H	4.1765797	4.8113336	4.6933059	5.8507304
35 H	5.0876863	5.6491946	5.2949563	6.4063156

	C	C	C	O
1 CO	5.4655237	5.6227350	4.6993952	1.9615381 *
2 C	10.4172753	10.0666643	8.7470462	7.3909379
3 C	10.5182703	10.3504566	9.1167238	7.2005912
4 C	9.4092119	9.3785305	8.2350731	5.9622465
5 C	8.0700891	7.9872616	6.8288986	4.7497909

6 C	7.8738167	7.5444712	6.2529156	4.9903237
7 C	9.2092996	8.7618823	7.4114704	6.4473084
8 C	9.5200297	8.8721388	7.4684928	7.1981080
9 C	8.6389755	7.8529873	6.4391467	6.7871436
10 C	7.2209312	6.4822604	5.0727505	5.4458544
11 C	6.7474209	6.2637458	4.9188959	4.3785901
12 N	5.3497981	5.0075564	3.7557899	2.9936681 *
13 C	4.3573789	3.7989107	2.4734623 *	3.0609190
14 C	2.8939481 *	2.5039208 *	1.4454647 *	2.4976903 *
15 C	2.4442543 *	2.8200162 *	2.4382456 *	1.4623381 *
16 C	1.4276509 *	2.4667369 *	2.8393539 *	2.4547037 *
17 C	0.0000000	1.4234940 *	2.4577090 *	3.7672722
18 C	1.4234940 *	0.0000000	1.4157664 *	4.2818345
19 C	2.4577090 *	1.4157664 *	0.0000000	3.7864008
20 O	3.7672722	4.2818345	3.7864008	0.0000000
21 N	7.0907434	7.2285124	6.2461304	3.5967983
22 H	11.3824624	10.9565298	9.6046977	8.4508031
23 H	11.5407056	11.4164825	10.1996210	8.1401464
24 H	9.7185074	9.8366052	8.7902434	6.1388808
25 H	10.6054877	9.9214933	8.5115165	8.2908931
26 H	9.1364864	8.2191166	6.8198784	7.6344956
27 H	6.6564355	5.7715046	4.3692827	5.4530135
28 H	4.8335103	3.9711576	2.5595398 *	4.1448837
29 H	2.1987743 *	3.4690257	3.9469649	2.6801297 *
30 H	1.1066972 *	2.2029163 *	3.4638955	4.6497833
31 H	2.1959907 *	1.1041154 *	2.1876210 *	5.3857885
32 H	3.4561428	2.1822049 *	1.1054132 *	4.6859908
33 H	3.9113203	4.7127949	4.4754923	0.9907784 *
34 H	6.9556737	7.0815182	6.1383574	3.7422465
35 H	7.6726868	7.9604962	7.0746513	4.0230656

N H H H

1 CO	1.9730225 *	6.5349313	6.2426261	4.4295521
2 C	4.3426156	1.1058683 *	2.1850029 *	3.4340934
3 C	3.8114253	2.1779513 *	1.1037445 *	2.1937419 *
4 C	2.4663309 *	3.4467890	2.2025225 *	1.1088809 *
5 C	1.5142136 *	3.9422500	3.4707514	2.1831346 *
6 C	2.6055102 *	3.5311669	4.0429305	3.5133284
7 C	3.8933201	2.1967424 *	3.4854612	3.9457348
8 C	5.1321055	2.6540238 *	4.6530095	5.3862292
9 C	5.4267779	4.0523893	5.9189653	6.2671021
10 C	4.6116847	4.8716130	6.2555242	6.0155949
11 C	3.2048278	4.7005894	5.5116813	4.8269960
12 N	2.9908900 *	6.0399918	6.4742791	5.2471433
13 C	4.1471454	7.1587551	7.7557667	6.5237062

14 C	4.8444792	8.5413008	8.9265288	7.4086313
15 C	4.6986375	9.1382633	9.1475607	7.3144045
16 C	5.9210691	10.5391900	10.4693276	8.5211140
17 C	7.0907434	11.3824624	11.5407056	9.7185074
18 C	7.2285124	10.9565298	11.4164825	9.8366052
19 C	6.2461304	9.6046977	10.1996210	8.7902434
20 O	3.5967983	8.4508031	8.1401464	6.1388808
21 N	0.0000000	5.4475669	4.6673523	2.6316947 *
22 H	5.4475669	0.0000000	2.5292783 *	4.3573975
23 H	4.6673523	2.5292783 *	0.0000000	2.5207733 *
24 H	2.6316947 *	4.3573975	2.5207733 *	0.0000000
25 H	6.0675354	2.3573276 *	4.7445877	5.9520148
26 H	6.5125128	4.7463864	6.8349736	7.3466781
27 H	5.3205555	5.9419188	7.3485341	6.9845620
28 H	4.9627150	7.2137641	8.1296692	7.1716409
29 H	6.1609461	11.0859616	10.7829688	8.6754693
30 H	8.0508723	12.4723243	12.5664116	10.6684958
31 H	8.2709743	11.7746493	12.3661993	10.8645248
32 H	6.7097346	9.4555963	10.3140790	9.1427280
33 H	4.0877520	9.1808781	8.6547225	6.4960028
34 H	1.0444185 *	5.8240681	5.0687522	3.0612372
35 H	1.0417238 *	5.8261263	4.5988738	2.2317460 *

H H H H

1 CO	6.5656787	6.3205052	4.5427385	3.8726156
2 C	2.6534785 *	4.6518649	5.3799264	6.4486270
3 C	4.0512350	5.9191207	6.2710393	7.0296911
4 C	4.8677077	6.2501465	6.0218927	6.4043075
5 C	4.6643277	5.4780825	4.8230128	5.0345137
6 C	3.5273763	4.0273642	3.5073375	4.1095117
7 C	2.1954047 *	3.4803522	3.9383971	5.0542939
8 C	1.1059638 *	2.1841219 *	3.4198176	4.9651062
9 C	2.1830558 *	1.1044470 *	2.1693120 *	3.9277845
10 C	3.4527880	2.1991047 *	1.1024325 *	2.5910062 *
11 C	3.9780172	3.4831523	2.1876848 *	2.6812056 *
12 N	5.4409006	4.6765626	2.6925163 *	2.1036651 *
13 C	6.2514544	4.9789539	2.6076859 *	1.1077378 *
14 C	7.7143529	6.3704631	3.9211437	2.1605658 *
15 C	8.6236108	7.5493071	5.1586345	3.5215342
16 C	10.0140559	8.8377134	6.3958162	4.6562607
17 C	10.6054877	9.1364864	6.6564355	4.8335103
18 C	9.9214933	8.2191166	5.7715046	3.9711576
19 C	8.5115165	6.8198784	4.3692827	2.5595398 *
20 O	8.2908931	7.6344956	5.4530135	4.1448837
21 N	6.0675354	6.5125128	5.3205555	4.9627150

22 H	2.3573276 *	4.7463864	5.9419188	7.2137641
23 H	4.7445877	6.8349736	7.3485341	8.1296692
24 H	5.9520148	7.3466781	6.9845620	7.1716409
25 H	0.0000000	2.5334709 *	4.3401220	5.9882516
26 H	2.5334709 *	0.0000000	2.4857656 *	4.3762918
27 H	4.3401220	2.4857656 *	0.0000000	1.9920096 *
28 H	5.9882516	4.3762918	1.9920096 *	0.0000000
29 H	10.7517435	9.7396781	7.3367331	5.6551345
30 H	11.7116082	10.2165377	7.7370496	5.9109036
31 H	10.5892770	8.7151364	6.3415381	4.6264398
32 H	8.1274667	6.2137434	3.8701088	2.2486746 *
33 H	9.1682378	8.6010154	6.4358174	5.1116908
34 H	6.3832717	6.7464472	5.5078363	4.9207309
35 H	6.7563485	7.4148177	6.3046988	5.9573128

H H H H

1 CO	4.6409508	6.4516991	6.6885505	5.2800688
2 C	10.0356954	11.4971422	10.9284416	8.6871014
3 C	9.8566124	11.5588590	11.2889132	9.2160677
4 C	8.5894039	10.4143346	10.3688028	8.4787790
5 C	7.3946307	9.0975321	8.9696741	7.0777129
6 C	7.5825274	8.9562363	8.4376186	6.2958926
7 C	9.0282126	10.3046511	9.5853888	7.2931139
8 C	9.6469904	10.6264345	9.5749922	7.1429184
9 C	9.0354585	9.7383008	8.4679210	5.9888075
10 C	7.6196940	8.3228462	7.1558225	4.7245067
11 C	6.7784166	7.8499484	7.0999548	4.8747166
12 N	5.3154047	6.4444112	5.9341818	3.9730552
13 C	4.8062114	5.4626892	4.6603759	2.6432598 *
14 C	3.5059051	4.0002295	3.4986507	2.1991499 *
15 C	2.1955842 *	3.4462302	3.9240789	3.4440503
16 C	1.1076224 *	2.1967506 *	3.4688096	3.9446477
17 C	2.1987743 *	1.1066972 *	2.1959907 *	3.4561428
18 C	3.4690257	2.2029163 *	1.1041154 *	2.1822049 *
19 C	3.9469649	3.4638955	2.1876210 *	1.1054132 *
20 O	2.6801297 *	4.6497833	5.3857885	4.6859908
21 N	6.1609461	8.0508723	8.2709743	6.7097346
22 H	11.0859616	12.4723243	11.7746493	9.4555963
23 H	10.7829688	12.5664116	12.3661993	10.3140790
24 H	8.6754693	10.6684958	10.8645248	9.1427280
25 H	10.7517435	11.7116082	10.5892770	8.1274667
26 H	9.7396781	10.2165377	8.7151364	6.2137434
27 H	7.3367331	7.7370496	6.3415381	3.8701088
28 H	5.6551345	5.9109036	4.6264398	2.2486746 *
29 H	0.0000000	2.5247641 *	4.3824990	5.0522358

30 H	2.5247641 *	0.0000000	2.5401367 *	4.3735268
31 H	4.3824990	2.5401367 *	0.0000000	2.5098764 *
32 H	5.0522358	4.3735268	2.5098764 *	0.0000000
33 H	2.2789231 *	4.6142424	5.7980282	5.4588577
34 H	6.1094647	7.8900830	8.0948245	6.5969701
35 H	6.4786875	8.5701928	9.0304889	7.6177405

H H H

1 CO	2.6647847 *	2.4975403 *	2.5894555 *
2 C	8.1021516	4.7472695	4.7414555
3 C	7.7803223	4.2450813	3.9289370
4 C	6.4721209	2.9627182 *	2.5008851 *
5 C	5.3759659	2.1037909 *	2.0973054 *
6 C	5.7958236	3.0270197	3.4245613
7 C	7.2558965	4.2774536	4.5613084
8 C	8.0863230	5.4502826	5.8938821
9 C	7.7364722	5.6880243	6.3179550
10 C	6.4139053	4.8479107	5.5749472
11 C	5.3070133	3.4931056	4.1760303
12 N	3.9590687	3.2094914	3.9491885
13 C	4.0391307	4.1765797	5.0876863
14 C	3.3275268	4.8113336	5.6491946
15 C	2.0382152 *	4.6933059	5.2949563
16 C	2.4886785 *	5.8507304	6.4063156
17 C	3.9113203	6.9556737	7.6726868
18 C	4.7127949	7.0815182	7.9604962
19 C	4.4754923	6.1383574	7.0746513
20 O	0.9907784 *	3.7422465	4.0230656
21 N	4.0877520	1.0444185 *	1.0417238 *
22 H	9.1808781	5.8240681	5.8261263
23 H	8.6547225	5.0687522	4.5988738
24 H	6.4960028	3.0612372	2.2317460 *
25 H	9.1682378	6.3832717	6.7563485
26 H	8.6010154	6.7464472	7.4148177
27 H	6.4358174	5.5078363	6.3046988
28 H	5.1116908	4.9207309	5.9573128
29 H	2.2789231 *	6.1094647	6.4786875
30 H	4.6142424	7.8900830	8.5701928
31 H	5.7980282	8.0948245	9.0304889
32 H	5.4588577	6.5969701	7.6177405
33 H	0.0000000	4.2287624	4.2921820
34 H	4.2287624	0.0000000	1.6667544 *
35 H	4.2921820	1.6667544 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.76 , TOTAL = 3084.2 SECONDS (51.4 MIN)
WALL CLOCK TIME: STEP = 0.76 , TOTAL = 2851.2 SECONDS (47.5 MIN)
CPU UTILIZATION: STEP = 99.83% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 3085.0 SECONDS (51.4 MIN)
WALL CLOCK TIME: STEP = 0.78 , TOTAL = 2852.0 SECONDS (47.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

		NONZERO BLOCKS				
ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD	
-----START SECOND ORDER SCF-----						
1	0	-284.631693275	-284.631693275	0.049112953	0.003584068	195875194
11506773						
2	1	-284.632560675	-0.000867400	0.007626612	0.000209540	165092596
14142041						
3	2	-284.632561523	-0.000000848	0.004481923	0.000411040	151192498
15280054						
4	3	-284.632573046	-0.000011523	0.002517182	0.000185507	144992644
15773713						
5	4	-284.632572964	0.000000082	0.001258979	0.000249305	140533068
16139917						
6	5	-284.632574327	-0.000001363	0.001298803	0.000070744	133568594
16699688						
7	6	-284.632574537	-0.000000210	0.000475363	0.000072348	154864134
14994589						
8	7	-284.632574961	-0.000000423	0.001106603	0.000074019	147065725
15640598						
9	8	-284.632575397	-0.000000437	0.001585506	0.000069962	171141903
13731009						
-----DISABLING FDIFF OPTION-----						
10	9	-284.632575899	-0.000000502	0.001399504	0.000069517	195872214
11506768						
11	10	-284.632576319	-0.000000420	0.000997669	0.000061657	195872736
11506716						

12 11	-284.632576529	-0.000000210	0.000489754	0.000058414	195872521
11506697					
13 12	-284.632576677	-0.000000148	0.000468776	0.000028209	195871982
11506724					
14 13	-284.632576760	-0.000000083	0.000347916	0.000016793	195871793
11506716					
15 14	-284.632576799	-0.000000038	0.000173926	0.000022522	195871950
11506712					
16 15	-284.632576815	-0.000000016	0.000138064	0.000021351	195871769
11506720					
17 16	-284.632576833	-0.000000018	0.000374605	0.000018523	195871857
11506711					
18 17	-284.632576870	-0.000000037	0.000433165	0.000012290	195871492
11506716					
19 18	-284.632576897	-0.000000027	0.000269199	0.000011933	195871284
11506722					
20 19	-284.632576909	-0.000000012	0.000081181	0.000010495	195871222
11506725					
21 20	-284.632576918	-0.000000009	0.000088215	0.000006291	195871253
11506721					
22 21	-284.632576923	-0.000000005	0.000070805	0.000005363	195871237
11506726					
23 22	-284.632576926	-0.000000003	0.000048563	0.000003736	195871282
11506723					
24 23	-284.632576927	-0.000000001	0.000038255	0.000002500	195871411
11506719					
25 24	-284.632576928	-0.000000001	0.000017688	0.000001517	195871360
11506722					
26 25	-284.632576928	0.000000000	0.000016113	0.000001056	195871396
11506719					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 88.5 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 28.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.3
TIME TO SOLVE SCF EQUATIONS= 2.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6325769277 AFTER 26 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5920831528
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000355062

SPIN SZ = 1.500

S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 91.89 , TOTAL = 3176.9 SECONDS (52.9 MIN)
WALL CLOCK TIME: STEP = 84.31 , TOTAL = 2936.3 SECONDS (48.9 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.78 , TOTAL = 3180.6 SECONDS (53.0 MIN)
WALL CLOCK TIME: STEP = 3.74 , TOTAL = 2940.0 SECONDS (49.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84 , TOTAL = 3183.5 SECONDS (53.1 MIN)
WALL CLOCK TIME: STEP = 2.68 , TOTAL = 2942.7 SECONDS (49.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 28 ENERGY= -284.6325769

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000217	0.0004853	0.0004049
2 C	6.0	0.0001146	-0.0000512	-0.0002674
3 C	6.0	0.0000382	0.0009993	-0.0000666
4 C	6.0	0.0009658	-0.0002393	0.0000653
5 C	6.0	-0.0001088	0.0002483	0.0009377
6 C	6.0	0.0004337	-0.0002684	0.0002031
7 C	6.0	0.0002900	0.0004030	-0.0000296

8 C	6.0	0.0001154	-0.0000329	0.0000226
9 C	6.0	0.0008402	0.0003661	-0.0000305
10 C	6.0	-0.0001615	-0.0007440	-0.0005132
11 C	6.0	0.0004663	-0.0000151	-0.0001229
12 N	7.0	-0.0005722	0.0002223	0.0000097
13 C	6.0	-0.0004444	0.0001700	-0.0001516
14 C	6.0	0.0001597	-0.0001963	0.0001678
15 C	6.0	-0.0002719	0.0006861	0.0002293
16 C	6.0	0.0005245	0.0006873	-0.0000109
17 C	6.0	-0.0007236	-0.0001704	-0.0001541
18 C	6.0	-0.0002203	-0.0004150	0.0002698
19 C	6.0	-0.0003516	-0.0004276	0.0006496
20 O	8.0	0.0004126	-0.0003737	-0.0016870
21 N	7.0	-0.0000313	-0.0001425	0.0009113
22 H	1.0	0.0006303	0.0002972	0.0000026
23 H	1.0	-0.0001357	0.0003361	-0.0001327
24 H	1.0	0.0001975	-0.0005638	-0.0006322
25 H	1.0	0.0008251	0.0001894	-0.0001382
26 H	1.0	0.0003367	0.0002813	-0.0000985
27 H	1.0	0.0003656	-0.0002978	-0.0004451
28 H	1.0	-0.0010118	0.0005045	-0.0003468
29 H	1.0	-0.0004049	-0.0003439	-0.0000947
30 H	1.0	-0.0010855	-0.0001969	-0.0009684
31 H	1.0	-0.0002165	-0.0003655	0.0000040
32 H	1.0	-0.0002151	-0.0002889	0.0014713
33 H	1.0	-0.0003538	0.0007317	-0.0001609
34 H	1.0	0.0004080	0.0000927	0.0000933
35 H	1.0	-0.0008370	-0.0015673	0.0006089

MAXIMUM GRADIENT = 0.0016870 RMS GRADIENT = 0.0005076
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0003496612
 PREDICTED ENERGY CHANGE WAS -0.0003552738 RATIO= 0.984
 GDIIS STEP HAS LENGTH = 0.201684
 RADIUS OF STEP TAKEN= 0.20168 CURRENT TRUST RADIUS= 0.42084

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 3183.5 SECONDS (53.1 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 2942.7 SECONDS (49.0 MIN)
 CPU UTILIZATION: STEP = 93.23% , TOTAL = 100.00%

INSERCH= 29

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1135529680	-1.7082476852	1.0365672718
C	6.0	4.9994560261	0.6839604973	0.4367530105
C	6.0	5.2265048122	-0.6765526693	0.2013175002
C	6.0	4.1004735288	-1.5534168331	0.0775397969
C	6.0	2.7833343821	-1.0729697841	0.2040549684
C	6.0	2.4827197515	0.3259285429	0.4989779893
C	6.0	3.6619590654	1.2049398849	0.5883104139
C	6.0	3.5195010238	2.6222759067	0.8195604996
C	6.0	2.2530969699	3.1966658038	0.9893690211
C	6.0	1.0964456209	2.3607043900	0.9487940273
C	6.0	1.1723228814	0.9693969111	0.6945308772
N	7.0	-0.0636906082	0.1843371842	0.7157294512
C	6.0	-1.2730736670	0.7231122845	0.5367435547
C	6.0	-2.5836231959	0.0625756332	0.5921197717
C	6.0	-2.8720771862	-1.3392035718	0.7348680727
C	6.0	-4.1756704157	-1.8706347516	0.7028456914
C	6.0	-5.2774412242	-0.9786320635	0.5242616453
C	6.0	-5.0499090780	0.4230709935	0.4201973494
C	6.0	-3.7308636455	0.9319549056	0.4610268649
O	8.0	-1.7624751196	-2.2727327451	0.9186354873
N	7.0	1.6958008563	-2.0889145626	-0.0817746166
H	1.0	5.8518074170	1.3853040829	0.5067758956
H	1.0	6.2497813218	-1.0705738622	0.0839540819
H	1.0	4.2824603464	-2.6188664280	-0.1635631627
H	1.0	4.4304018799	3.2469326537	0.8640866383
H	1.0	2.1430045548	4.2790693558	1.1775035978
H	1.0	0.1234591106	2.8340605811	1.1572807660
H	1.0	-1.3373520731	1.7996133239	0.2869134176
H	1.0	-4.3580904791	-2.9567919423	0.8149296586
H	1.0	-6.3032365826	-1.3874219361	0.4726383558
H	1.0	-5.9016140364	1.1165583586	0.3009849098
H	1.0	-3.5634172325	2.0227610855	0.4001578647
H	1.0	-2.0908978913	-3.2044595985	1.0001524648
H	1.0	1.4027754302	-2.0070501254	-1.0802421009
H	1.0	2.0905714882	-3.0456488203	0.0208859645

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.000000	5.4730691	5.2824533	4.1035645
2 C	5.4730691	0.000000	1.3992774 *	2.4378394 *
3 C	5.2824533	1.3992774 *	0.000000	1.4325356 *

4 C	4.1035645	2.4378394 *	1.4325356 *	0.0000000
5 C	2.8678193 *	2.8376306 *	2.4751234 *	1.4077255 *
6 C	3.1685685	2.5428371 *	2.9363118 *	2.5152885 *
7 C	4.6128930	1.4433597 *	2.4774142 *	2.8393156 *
8 C	5.5137110	2.4685775 *	3.7654158	4.2807165
9 C	5.3514533	3.7631849	4.9461097	5.1775977
10 C	4.1869026	4.2786851	5.1808340	5.0103505
11 C	2.8996143 *	3.8464102	4.4032716	3.9139920
12 N	1.9277525 *	5.0953808	5.3844144	4.5571195
13 C	2.8432496 *	6.2734488	6.6570334	5.8539271
14 C	3.2570091	7.6100820	7.8547525	6.8958954
15 C	3.0234423	8.1328409	8.1431451	7.0067418
16 C	4.3052499	9.5278385	9.4909568	8.3057928
17 C	5.4642121	10.4108832	10.5132501	9.4061269
18 C	5.6199441	10.0527646	10.3373963	9.3676796
19 C	4.6990909	8.7338750	9.1043503	8.2252038
20 O	1.9626596 *	7.3958068	7.2047329	5.9664918
21 N	1.9746150 *	4.3441736	3.8132372	2.4687223 *
22 H	6.5405126	1.1060239 *	2.1761345 *	3.4478246
23 H	6.2423872	2.1831563 *	1.1027791 *	2.2028850 *
24 H	4.4327563	3.4326561	2.1901919 *	1.1074442 *
25 H	6.5740966	2.6599366 *	4.0579280	4.8755373
26 H	6.3234881	4.6511111	5.9176940	6.2497600
27 H	4.5439228	5.3774935	6.2673237	6.0193390
28 H	3.8693921	6.4360135	7.0159063	6.3919164
29 H	4.6479653	10.0479736	9.8711944	8.6058417
30 H	6.4495064	11.4909866	11.5548209	10.4125329
31 H	6.6860186	10.9104951	11.2720987	10.3547308
32 H	5.2768886	8.6669790	9.1972040	8.4633535
33 H	2.6645037 *	8.1061920	7.7828551	6.4738116
34 H	2.4964494 *	4.7411943	4.2465898	2.9704911 *
35 H	2.5940032 *	4.7481091	3.9343678	2.5039313 *

C C C C

1 CO	2.8678193 *	3.1685685	4.6128930	5.5137110
2 C	2.8376306 *	2.5428371 *	1.4433597 *	2.4685775 *
3 C	2.4751234 *	2.9363118 *	2.4774142 *	3.7654158
4 C	1.4077255 *	2.5152885 *	2.8393156 *	4.2807165
5 C	0.0000000	1.4609125 *	2.4715392 *	3.8178042
6 C	1.4609125 *	0.0000000	1.4735150 *	2.5398622 *
7 C	2.4715392 *	1.4735150 *	0.0000000	1.4431259 *
8 C	3.8178042	2.5398622 *	1.4431259 *	0.0000000
9 C	4.3735178	2.9213597 *	2.4723900 *	1.4009061 *
10 C	3.8974797	2.5028790 *	2.8368291 *	2.4405570 *
11 C	2.6471091 *	1.4728993 *	2.5030085 *	2.8734799 *

12 N	3.1540740	2.5595380 *	3.8650137	4.3351572
13 C	4.4487120	3.7769254	4.9587665	5.1629042
14 C	5.4994810	5.0740379	6.3491975	6.6220782
15 C	5.6865036	5.6126784	7.0133997	7.5201572
16 C	7.0223080	7.0143148	8.4202561	8.9115393
17 C	8.0676846	7.8690925	9.2024435	9.5099912
18 C	7.9777540	7.5336671	8.7484986	8.8561156
19 C	6.8205963	6.2431824	7.3989560	7.4534233
20 O	4.7554643	4.9950808	6.4519615	7.2020967
21 N	1.5154443 *	2.6053756 *	3.8941327	5.1316277
22 H	3.9433840	3.5317261	2.1987758 *	2.6584933 *
23 H	3.4685277	4.0389623	3.4826947	4.6510952
24 H	2.1845636 *	3.5142345	3.9461159	5.3868555
25 H	4.6701210	3.5297358	2.1991570 *	1.1054045 *
26 H	5.4774034	4.0253106	3.4791728	2.1835362 *
27 H	4.8216659	3.5057381	3.9368443	3.4193579
28 H	5.0238089	4.0999594	5.0435690	4.9547461
29 H	7.4109313	7.5942586	9.0383938	9.6531066
30 H	9.0959765	8.9514967	10.2975164	10.6152817
31 H	8.9572182	8.4238560	9.5682965	9.5547640
32 H	7.0642241	6.2805078	7.2739464	7.1206073
33 H	5.3791412	5.7993788	7.2600125	8.0907377
34 H	2.1042500 *	3.0171187	4.2667151	5.4332713
35 H	2.0987934 *	3.4278107	4.5671363	5.8995840

C C C N

1 CO	5.3514533	4.1869026	2.8996143 *	1.9277525 *
2 C	3.7631849	4.2786851	3.8464102	5.0953808
3 C	4.9461097	5.1808340	4.4032716	5.3844144
4 C	5.1775977	5.0103505	3.9139920	4.5571195
5 C	4.3735178	3.8974797	2.6471091 *	3.1540740
6 C	2.9213597 *	2.5028790 *	1.4728993 *	2.5595380 *
7 C	2.4723900 *	2.8368291 *	2.5030085 *	3.8650137
8 C	1.4009061 *	2.4405570 *	2.8734799 *	4.3351572
9 C	0.0000000	1.4276975 *	2.4931364 *	3.8100534
10 C	1.4276975 *	0.0000000	1.4163840 *	2.4772584 *
11 C	2.4931364 *	1.4163840 *	0.0000000	1.4644103 *
12 N	3.8100534	2.4772584 *	1.4644103 *	0.0000000
13 C	4.3309602	2.9096589 *	2.4628271 *	1.3360097 *
14 C	5.7770399	4.3533342	3.8652223	2.5258989 *
15 C	6.8488168	5.4299407	4.6570844	3.1950865
16 C	8.1907680	6.7646086	6.0553184	4.5968961
17 C	8.6231342	7.2081779	6.7396784	5.3453113
18 C	7.8326676	6.4661823	6.2521917	5.0006707
19 C	6.4199568	5.0578806	4.9088862	3.7512616

20 O	6.7855835	5.4445456	4.3788888	2.9940328 *
21 N	5.4217421	4.6065613	3.1984291	2.9832024 *
22 H	4.0576649	4.8744489	4.7016812	6.0397930
23 H	5.9162992	6.2512789	5.5058940	6.4679108
24 H	6.2664171	6.0153266	4.8254445	5.2459636
25 H	2.1814855 *	3.4507739	3.9788185	5.4404382
26 H	1.1041342 *	2.1972068 *	3.4827313	4.6743524
27 H	2.1668028 *	1.1019236 *	2.1888863 *	2.6927730 *
28 H	3.9161874	2.5838499 *	2.6746737 *	2.1012410 *
29 H	9.0334529	7.6187697	6.7834303	5.3215038
30 H	9.7206849	8.3084579	7.8414170	6.4390569
31 H	8.4439346	7.1372540	7.0864038	5.9264154
32 H	5.9629741	4.7042033	4.8603977	3.9657880
33 H	7.7359430	6.4134894	5.3068910	3.9590920
34 H	5.6643620	4.8257751	3.4730627	3.1903315
35 H	6.3190874	5.5747605	4.1734363	3.9441681

C C C C

1 CO	2.8432496 *	3.2570091	3.0234423	4.3052499
2 C	6.2734488	7.6100820	8.1328409	9.5278385
3 C	6.6570334	7.8547525	8.1431451	9.4909568
4 C	5.8539271	6.8958954	7.0067418	8.3057928
5 C	4.4487120	5.4994810	5.6865036	7.0223080
6 C	3.7769254	5.0740379	5.6126784	7.0143148
7 C	4.9587665	6.3491975	7.0133997	8.4202561
8 C	5.1629042	6.6220782	7.5201572	8.9115393
9 C	4.3309602	5.7770399	6.8488168	8.1907680
10 C	2.9096589 *	4.3533342	5.4299407	6.7646086
11 C	2.4628271 *	3.8652223	4.6570844	6.0553184
12 N	1.3360097 *	2.5258989 *	3.1950865	4.5968961
13 C	0.0000000	1.4686440 *	2.6171000 *	3.8961752
14 C	1.4686440 *	0.0000000	1.4382516 *	2.5068261 *
15 C	2.6171000 *	1.4382516 *	0.0000000	1.4081193 *
16 C	3.8961752	2.5068261 *	1.4081193 *	0.0000000
17 C	4.3509826	2.8888361 *	2.4413404 *	1.4287967 *
18 C	3.7905268	2.4984156 *	2.8191454 *	2.4708843 *
19 C	2.4678087 *	1.4453949 *	2.4434942 *	2.8479533 *
20 O	3.0594841	2.4969105 *	1.4616648 *	2.4559641 *
21 N	4.1357316	4.8369943	4.7004767	5.9276850
22 H	7.1556500	8.5389334	9.1422716	10.5446618
23 H	7.7469785	8.9202744	9.1489974	10.4744054
24 H	6.5209822	7.4097430	7.3233956	8.5352499
25 H	6.2455149	7.7078300	8.6241257	10.0139890
26 H	4.9724234	6.3610143	7.5440017	8.8300518
27 H	2.6060455 *	3.9152050	5.1543966	6.3893023

28 H	1.1069785 *	2.1595468 *	3.5225298	4.6583014
29 H	4.8100324	3.5092676	2.1980076 *	1.1070580 *
30 H	5.4553646	3.9940321	3.4415032	2.1938614 *
31 H	4.6512114	3.4935229	3.9239157	3.4732832
32 H	2.6369331 *	2.1998120 *	3.4485922	3.9528477
33 H	4.0384905	3.3290822	2.0395580 *	2.4927408 *
34 H	4.1507346	4.7928613	4.6920154	5.8580773
35 H	5.0777729	5.6422924	5.2961880	6.4118262

C C C O

1 CO	5.4642121	5.6199441	4.6990909	1.9626596 *
2 C	10.4108832	10.0527646	8.7338750	7.3958068
3 C	10.5132501	10.3373963	9.1043503	7.2047329
4 C	9.4061269	9.3676796	8.2252038	5.9664918
5 C	8.0676846	7.9777540	6.8205963	4.7554643
6 C	7.8690925	7.5336671	6.2431824	4.9950808
7 C	9.2024435	8.7484986	7.3989560	6.4519615
8 C	9.5099912	8.8561156	7.4534233	7.2020967
9 C	8.6231342	7.8326676	6.4199568	6.7855835
10 C	7.2081779	6.4661823	5.0578806	5.4445456
11 C	6.7396784	6.2521917	4.9088862	4.3788888
12 N	5.3453113	5.0006707	3.7512616	2.9940328 *
13 C	4.3509826	3.7905268	2.4678087 *	3.0594841
14 C	2.8888361 *	2.4984156 *	1.4453949 *	2.4969105 *
15 C	2.4413404 *	2.8191454 *	2.4434942 *	1.4616648 *
16 C	1.4287967 *	2.4708843 *	2.8479533 *	2.4559641 *
17 C	0.0000000	1.4238580 *	2.4589110 *	3.7663263
18 C	1.4238580 *	0.0000000	1.4143941 *	4.2805397
19 C	2.4589110 *	1.4143941 *	0.0000000	3.7886649
20 O	3.7663263	4.2805397	3.7886649	0.0000000
21 N	7.0870383	7.2157224	6.2344986	3.6047583
22 H	11.3775514	10.9444420	9.5934980	8.4574323
23 H	11.5359951	11.4029399	10.1865391	8.1448224
24 H	9.7239493	9.8329690	8.7870249	6.1507892
25 H	10.5930683	9.9018952	8.4928107	8.2958669
26 H	9.1177390	8.1963554	6.7984441	7.6318998
27 H	6.6413148	5.7549892	4.3541451	5.4491318
28 H	4.8269332	3.9617815	2.5518707 *	4.1429223
29 H	2.2006386 *	3.4724487	3.9548720	2.6862448 *
30 H	1.1054548 *	2.2026040 *	3.4636320	4.6477095
31 H	2.1975594 *	1.1047795 *	2.1844563 *	5.3852816
32 H	3.4585605	2.1838196 *	1.1052608 *	4.6865210
33 H	3.9159723	4.7171043	4.4821947	0.9912726 *
34 H	6.9467525	7.0564824	6.1128971	3.7529868
35 H	7.6689997	7.9484545	7.0642878	4.0310447

	N	H	H	H
1 CO	1.9746150 *	6.5405126	6.2423872	4.4327563
2 C	4.3441736	1.1060239 *	2.1831563 *	3.4326561
3 C	3.8132372	2.1761345 *	1.1027791 *	2.1901919 *
4 C	2.4687223 *	3.4478246	2.2028850 *	1.1074442 *
5 C	1.5154443 *	3.9433840	3.4685277	2.1845636 *
6 C	2.6053756 *	3.5317261	4.0389623	3.5142345
7 C	3.8941327	2.1987758 *	3.4826947	3.9461159
8 C	5.1316277	2.6584933 *	4.6510952	5.3868555
9 C	5.4217421	4.0576649	5.9162992	6.2664171
10 C	4.6065613	4.8744489	6.2512789	6.0153266
11 C	3.1984291	4.7016812	5.5058940	4.8254445
12 N	2.9832024 *	6.0397930	6.4679108	5.2459636
13 C	4.1357316	7.1556500	7.7469785	6.5209822
14 C	4.8369943	8.5389334	8.9202744	7.4097430
15 C	4.7004767	9.1422716	9.1489974	7.3233956
16 C	5.9276850	10.5446618	10.4744054	8.5352499
17 C	7.0870383	11.3775514	11.5359951	9.7239493
18 C	7.2157224	10.9444420	11.4029399	9.8329690
19 C	6.2344986	9.5934980	10.1865391	8.7870249
20 O	3.6047583	8.4574323	8.1448224	6.1507892
21 N	0.0000000	5.4487593	4.6693920	2.6416559 *
22 H	5.4487593	0.0000000	2.5235883 *	4.3526528
23 H	4.6693920	2.5235883 *	0.0000000	2.5157159 *
24 H	2.6416559 *	4.3526528	2.5157159 *	0.0000000
25 H	6.0699227	2.3693302 *	4.7496959	5.9569749
26 H	6.5066882	4.7517336	6.8322872	7.3455598
27 H	5.3144333	5.9444113	7.3437064	6.9840055
28 H	4.9453611	7.2044435	8.1144168	7.1629731
29 H	6.1811722	11.0991338	10.7990318	8.7023422
30 H	8.0488549	12.4673281	12.5630302	10.6760567
31 H	8.2548334	11.7582945	12.3485651	10.8574663
32 H	6.6930942	9.4373817	10.2940552	9.1334704
33 H	4.0931766	9.1867251	8.6579338	6.5051402
34 H	1.0437926 *	5.8155463	5.0720614	3.0833755
35 H	1.0400594 *	5.8323519	4.6047720	2.2406565 *

	H	H	H	H
1 CO	6.5740966	6.3234881	4.5439228	3.8693921
2 C	2.6599366 *	4.6511111	5.3774935	6.4360135
3 C	4.0579280	5.9176940	6.2673237	7.0159063
4 C	4.8755373	6.2497600	6.0193390	6.3919164
5 C	4.6701210	5.4774034	4.8216659	5.0238089

6 C	3.5297358	4.0253106	3.5057381	4.0999594
7 C	2.1991570 *	3.4791728	3.9368443	5.0435690
8 C	1.1054045 *	2.1835362 *	3.4193579	4.9547461
9 C	2.1814855 *	1.1041342 *	2.1668028 *	3.9161874
10 C	3.4507739	2.1972068 *	1.1019236 *	2.5838499 *
11 C	3.9788185	3.4827313	2.1888863 *	2.6746737 *
12 N	5.4404382	4.6743524	2.6927730 *	2.1012410 *
13 C	6.2455149	4.9724234	2.6060455 *	1.1069785 *
14 C	7.7078300	6.3610143	3.9152050	2.1595468 *
15 C	8.6241257	7.5440017	5.1543966	3.5225298
16 C	10.0139890	8.8300518	6.3893023	4.6583014
17 C	10.5930683	9.1177390	6.6413148	4.8269332
18 C	9.9018952	8.1963554	5.7549892	3.9617815
19 C	8.4928107	6.7984441	4.3541451	2.5518707 *
20 O	8.2958669	7.6318998	5.4491318	4.1429223
21 N	6.0699227	6.5066882	5.3144333	4.9453611
22 H	2.3693302 *	4.7517336	5.9444113	7.2044435
23 H	4.7496959	6.8322872	7.3437064	8.1144168
24 H	5.9569749	7.3455598	6.9840055	7.1629731
25 H	0.0000000	2.5289766 *	4.3366095	5.9745165
26 H	2.5289766 *	0.0000000	2.4833492 *	4.3650585
27 H	4.3366095	2.4833492 *	0.0000000	1.9903743 *
28 H	5.9745165	4.3650585	1.9903743 *	0.0000000
29 H	10.7576119	9.7341351	7.3304477	5.6592449
30 H	11.6979258	10.1953395	7.7195898	5.9035325
31 H	10.5643803	8.6882478	6.3233348	4.6151110
32 H	8.1003068	6.1853410	3.8502596	2.2400860 *
33 H	9.1742208	8.6000342	6.4336453	5.1105075
34 H	6.3679880	6.7201676	5.4844792	4.8854989
35 H	6.7662675	7.4156598	6.3033251	5.9412116

H H H H

1 CO	4.6479653	6.4495064	6.6860186	5.2768886
2 C	10.0479736	11.4909866	10.9104951	8.6669790
3 C	9.8711944	11.5548209	11.2720987	9.1972040
4 C	8.6058417	10.4125329	10.3547308	8.4633535
5 C	7.4109313	9.0959765	8.9572182	7.0642241
6 C	7.5942586	8.9514967	8.4238560	6.2805078
7 C	9.0383938	10.2975164	9.5682965	7.2739464
8 C	9.6531066	10.6152817	9.5547640	7.1206073
9 C	9.0334529	9.7206849	8.4439346	5.9629741
10 C	7.6187697	8.3084579	7.1372540	4.7042033
11 C	6.7834303	7.8414170	7.0864038	4.8603977
12 N	5.3215038	6.4390569	5.9264154	3.9657880
13 C	4.8100324	5.4553646	4.6512114	2.6369331 *

14 C	3.5092676	3.9940321	3.4935229	2.1998120 *
15 C	2.1980076 *	3.4415032	3.9239157	3.4485922
16 C	1.1070580 *	2.1938614 *	3.4732832	3.9528477
17 C	2.2006386 *	1.1054548 *	2.1975594 *	3.4585605
18 C	3.4724487	2.2026040 *	1.1047795 *	2.1838196 *
19 C	3.9548720	3.4636320	2.1844563 *	1.1052608 *
20 O	2.6862448 *	4.6477095	5.3852816	4.6865210
21 N	6.1811722	8.0488549	8.2548334	6.6930942
22 H	11.0991338	12.4673281	11.7582945	9.4373817
23 H	10.7990318	12.5630302	12.3485651	10.2940552
24 H	8.7023422	10.6760567	10.8574663	9.1334704
25 H	10.7576119	11.6979258	10.5643803	8.1003068
26 H	9.7341351	10.1953395	8.6882478	6.1853410
27 H	7.3304477	7.7195898	6.3233348	3.8502596
28 H	5.6592449	5.9035325	4.6151110	2.2400860 *
29 H	0.0000000	2.5226333 *	4.3862042	5.0595938
30 H	2.5226333 *	0.0000000	2.5417873 *	4.3750671
31 H	4.3862042	2.5417873 *	0.0000000	2.5096221 *
32 H	5.0595938	4.3750671	2.5096221 *	0.0000000
33 H	2.2881890 *	4.6177586	5.8035842	5.4637115
34 H	6.1385065	7.8853027	8.0634250	6.5646045
35 H	6.4979722	8.5679525	9.0154009	7.6026452

H H H

1 CO	2.6645037 *	2.4964494 *	2.5940032 *
2 C	8.1061920	4.7411943	4.7481091
3 C	7.7828551	4.2465898	3.9343678
4 C	6.4738116	2.9704911 *	2.5039313 *
5 C	5.3791412	2.1042500 *	2.0987934 *
6 C	5.7993788	3.0171187	3.4278107
7 C	7.2600125	4.2667151	4.5671363
8 C	8.0907377	5.4332713	5.8995840
9 C	7.7359430	5.6643620	6.3190874
10 C	6.4134894	4.8257751	5.5747605
11 C	5.3068910	3.4730627	4.1734363
12 N	3.9590920	3.1903315	3.9441681
13 C	4.0384905	4.1507346	5.0777729
14 C	3.3290822	4.7928613	5.6422924
15 C	2.0395580 *	4.6920154	5.2961880
16 C	2.4927408 *	5.8580773	6.4118262
17 C	3.9159723	6.9467525	7.6689997
18 C	4.7171043	7.0564824	7.9484545
19 C	4.4821947	6.1128971	7.0642878
20 O	0.9912726 *	3.7529868	4.0310447
21 N	4.0931766	1.0437926 *	1.0400594 *

22 H	9.1867251	5.8155463	5.8323519
23 H	8.6579338	5.0720614	4.6047720
24 H	6.5051402	3.0833755	2.2406565 *
25 H	9.1742208	6.3679880	6.7662675
26 H	8.6000342	6.7201676	7.4156598
27 H	6.4336453	5.4844792	6.3033251
28 H	5.1105075	4.8854989	5.9412116
29 H	2.2881890 *	6.1385065	6.4979722
30 H	4.6177586	7.8853027	8.5679525
31 H	5.8035842	8.0634250	9.0154009
32 H	5.4637115	6.5646045	7.6026452
33 H	0.0000000	4.2388187	4.2975423
34 H	4.2388187	0.0000000	1.6625985 *
35 H	4.2975423	1.6625985 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.82 , TOTAL = 3184.3 SECONDS (53.1 MIN)
WALL CLOCK TIME: STEP = 0.81 , TOTAL = 2943.5 SECONDS (49.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.89 , TOTAL = 3185.2 SECONDS (53.1 MIN)
WALL CLOCK TIME: STEP = 0.89 , TOTAL = 2944.4 SECONDS (49.1 MIN)
CPU UTILIZATION: STEP = 99.69% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.631934426	-284.631934426	0.054228218	0.003055760	195974915
11495252						
2	1	-284.632738533	-0.000804107	0.008612312	0.000259969	165265142
14113075						
3	2	-284.632736202	0.000002331	0.006110376	0.000568459	152373466
15181890						
4	3	-284.632751571	-0.000015369	0.003367330	0.000090160	146131993
15664922						

5 4	-284.632751433	0.000000139	0.000860189	0.000155484	139870263
16195121					
6 5	-284.632752654	-0.000001221	0.000820358	0.000078270	132464172
16767003					
7 6	-284.632752873	-0.000000219	0.000567509	0.000076268	131389649
16865680					
8 7	-284.632753400	-0.000000527	0.001777835	0.000073958	123431888
17539659					
9 8	-284.632754066	-0.000000667	0.001612352	0.000068342	154425797
15141848					
10 9	-284.632754459	-0.000000393	0.000643616	0.000129125	153187347
15258075					
11 10	-284.632754811	-0.000000352	0.000732240	0.000043642	149103085
15512903					
12 11	-284.632755023	-0.000000212	0.000761599	0.000038266	169243780
13900960					
-----DISABLING FDIFF OPTION-----					
13 12	-284.632755178	-0.000000155	0.000839981	0.000037451	195971387
11495436					
14 13	-284.632755217	-0.000000039	0.000189769	0.000020896	195970836
11495449					
15 14	-284.632755256	-0.000000040	0.000157670	0.000018558	195970875
11495448					
16 15	-284.632755268	-0.000000012	0.000134061	0.000015765	195970970
11495438					
17 16	-284.632755289	-0.000000020	0.000577429	0.000013764	195971008
11495434					
18 17	-284.632755333	-0.000000045	0.000475589	0.000011314	195970910
11495442					
19 18	-284.632755351	-0.000000018	0.000197643	0.000015461	195970926
11495440					
20 19	-284.632755366	-0.000000015	0.000164021	0.000009436	195970906
11495435					
21 20	-284.632755375	-0.000000009	0.000062200	0.000006364	195970842
11495438					
22 21	-284.632755379	-0.000000004	0.000056168	0.000004472	195970856
11495440					
23 22	-284.632755381	-0.000000002	0.000027553	0.000003119	195970857
11495439					
24 23	-284.632755381	-0.000000001	0.000023438	0.000002215	195970873
11495438					
25 24	-284.632755382	0.000000000	0.000009307	0.000001257	195970861
11495440					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 84.7 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 26.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6327553818 AFTER 25 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5943009173
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000355116

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 88.13 , TOTAL = 3273.3 SECONDS (54.6 MIN)
WALL CLOCK TIME: STEP = 81.10 , TOTAL = 3025.5 SECONDS (50.4
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 4.01 , TOTAL = 3277.3 SECONDS (54.6 MIN)
WALL CLOCK TIME: STEP = 3.98 , TOTAL = 3029.5 SECONDS (50.5
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.80 , TOTAL = 3280.1 SECONDS (54.7 MIN)
WALL CLOCK TIME: STEP = 2.65 , TOTAL = 3032.1 SECONDS (50.5
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 29 ENERGY= -284.6327554

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0002518	0.0008580	0.0003221
2 C	6.0	-0.0008496	0.0010811	-0.0000368
3 C	6.0	0.0009888	0.0005474	-0.0001233
4 C	6.0	-0.0008206	-0.0012373	0.0001728
5 C	6.0	0.0013975	-0.0002471	0.0010554
6 C	6.0	0.0000298	0.0005881	0.0007932
7 C	6.0	0.0003569	-0.0005755	0.0000396
8 C	6.0	0.0016775	0.0003249	-0.0000274
9 C	6.0	-0.0008359	-0.0001292	-0.0000059
10 C	6.0	0.0005189	0.0008378	-0.0002114
11 C	6.0	0.0006199	-0.0018190	-0.0002471
12 N	7.0	-0.0006194	0.0005489	-0.0000492
13 C	6.0	-0.0009307	0.0004630	-0.0003167
14 C	6.0	0.0000623	0.0001729	0.0000361
15 C	6.0	-0.0001042	-0.0002469	0.0000279
16 C	6.0	0.0002326	-0.0017601	0.0000055
17 C	6.0	-0.0014599	0.0003435	-0.0005413
18 C	6.0	0.0014981	-0.0009095	0.0001582
19 C	6.0	-0.0009148	0.0013417	0.0005686
20 O	8.0	0.0000025	0.0002688	-0.0015053
21 N	7.0	0.0000146	-0.0013108	0.0004484
22 H	1.0	0.0009800	0.0000626	-0.0001902
23 H	1.0	-0.0007062	0.0007828	-0.0002461
24 H	1.0	0.0006627	0.0004569	-0.0004343
25 H	1.0	0.0002012	0.0005071	-0.0002679
26 H	1.0	0.0004207	0.0000593	-0.0002406
27 H	1.0	0.0007135	-0.0003411	-0.0005111
28 H	1.0	-0.0008131	0.0001228	-0.0002676
29 H	1.0	-0.0004548	-0.0000334	0.0004731
30 H	1.0	-0.0001467	-0.0001906	-0.0006145
31 H	1.0	-0.0001851	0.0002425	-0.0003958
32 H	1.0	-0.0000588	-0.0002387	0.0020073
33 H	1.0	-0.0002929	0.0001956	-0.0003448
34 H	1.0	0.0005326	-0.0002771	0.0005720
35 H	1.0	-0.0014653	-0.0004893	-0.0001030

MAXIMUM GRADIENT = 0.0020073 RMS GRADIENT = 0.0006974
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001784540
 PREDICTED ENERGY CHANGE WAS -0.0001647007 RATIO= 1.084

GDIIS STEP HAS LENGTH = 0.097235
RADIUS OF STEP TAKEN= 0.09724 CURRENT TRUST RADIUS= 0.40337

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 3280.2 SECONDS (54.7 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 3032.2 SECONDS (50.5 MIN)
CPU UTILIZATION: STEP = 94.20% , TOTAL = 100.00%

1NSERCH= 30

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1138374332	-1.7140497523	1.0344342557
C	6.0	4.9989499637	0.6847477604	0.4383234868
C	6.0	5.2249007108	-0.6755173748	0.2039361257
C	6.0	4.1014769785	-1.5522953227	0.0801522988
C	6.0	2.7822017438	-1.0737527836	0.2046990148
C	6.0	2.4829140675	0.3241016971	0.5024834646
C	6.0	3.6610631534	1.2055058632	0.5913320487
C	6.0	3.5152001593	2.6228866630	0.8198620229
C	6.0	2.2504540233	3.1947980949	0.9905585893
C	6.0	1.0936253794	2.3561831580	0.9534472123
C	6.0	1.1717589054	0.9670793282	0.6992317854
N	7.0	-0.0622788796	0.1791920931	0.7188531463
C	6.0	-1.2700221441	0.7182023584	0.5370760521
C	6.0	-2.5827327694	0.0595283188	0.5912602954
C	6.0	-2.8729278218	-1.3414529633	0.7384526441
C	6.0	-4.1781153587	-1.8689024741	0.7116793163
C	6.0	-5.2741116494	-0.9757034489	0.5254785669
C	6.0	-5.0459824190	0.4267237515	0.4110665494
C	6.0	-3.7247124825	0.9315437026	0.4553496290
O	8.0	-1.7638491773	-2.2757894342	0.9242913014
N	7.0	1.6947409599	-2.0851969054	-0.0891528755
H	1.0	5.8505919994	1.3861029875	0.5047695676
H	1.0	6.2497510209	-1.0680441837	0.0843080418
H	1.0	4.2857418142	-2.6183029466	-0.1620368611
H	1.0	4.4250700825	3.2511319529	0.8605839124
H	1.0	2.1373068820	4.2772515906	1.1764367866
H	1.0	0.1210852775	2.8297429504	1.1635996323
H	1.0	-1.3326267367	1.7940185716	0.2854329335
H	1.0	-4.3644034554	-2.9549826019	0.8367574685
H	1.0	-6.3023882689	-1.3813028343	0.4781242865
H	1.0	-5.8935197823	1.1204048992	0.2837820064

H	1.0	-3.5550754283	2.0239775799	0.3946528774
H	1.0	-2.0913001454	-3.2085765421	0.9989615936
H	1.0	1.3994208173	-1.9938470026	-1.0863054736
H	1.0	2.0899521467	-3.0443017511	0.0010052980

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1	CO	0.0000000	5.4748426	5.2812162
2	C	5.4748426	0.0000000	1.3986824 *
3	C	5.2812162	1.3986824 *	0.0000000
4	C	4.1034239	2.4368230 *	1.4304345 *
5	C	2.8668116 *	2.8391684 *	2.4749485 *
6	C	3.1701036	2.5425614 *	2.9337450 *
7	C	4.6155124	1.4437942 *	2.4766736 *
8	C	5.5158252	2.4705197 *	3.7658877
9	C	5.3538624	3.7629172	4.9442340
10	C	4.1872830	4.2790897	5.1788426
11	C	2.9017256 *	3.8464497	4.4012953
12	N	1.9274265 *	5.0941457	5.3805145
13	C	2.8422320 *	6.2698391	6.6511247
14	C	3.2578326	7.6089554	7.8517165
15	C	3.0244339	8.1340043	8.1427271
16	C	4.3068560	9.5296580	9.4920326
17	C	5.4620680	10.4067521	10.5082235
18	C	5.6209643	10.0482827	10.3319349
19	C	4.6977621	8.7271693	9.0962317
20	O	1.9630053 *	7.3984051	7.2057205
21	N	1.9747036 *	4.3438027	3.8124960
22	H	6.5423119	1.1052639 *	2.1753779 *
23	H	6.2425555	2.1822259 *	1.1039503 *
24	H	4.4332836	3.4320901	2.1886917 *
25	H	6.5779921	2.6634507 *	4.0607253
26	H	6.3253684	4.6518702	5.9168331
27	H	4.5456340	5.3777871	6.2655196
28	H	3.8677907	6.4298305	7.0075970
29	H	4.6511968	10.0537940	9.8768000
30	H	6.4488878	11.4887073	11.5521298
31	H	6.6847552	10.9022740	11.2628143
32	H	5.2766552	8.6583367	9.1875800
33	H	2.6641134 *	8.1082634	7.7830103
34	H	2.4957059 *	4.7387734	4.2470004
35	H	2.5966469 *	4.7496659	3.9344914

	C	C	C	C
1 CO	2.8668116 *	3.1701036	4.6155124	5.5158252
2 C	2.8391684 *	2.5425614 *	1.4437942 *	2.4705197 *
3 C	2.4749485 *	2.9337450 *	2.4766736 *	3.7658877
4 C	1.4089010 *	2.5137572 *	2.8391436 *	4.2805415
5 C	0.0000000	1.4602212 *	2.4732372 *	3.8184886
6 C	1.4602212 *	0.0000000	1.4740430 *	2.5398339 *
7 C	2.4732372 *	1.4740430 *	0.0000000	1.4430767 *
8 C	3.8184886	2.5398339 *	1.4430767 *	0.0000000
9 C	4.3727403	2.9211561 *	2.4711300 *	1.3985002 *
10 C	3.8956867	2.5025680 *	2.8367098 *	2.4398771 *
11 C	2.6463342 *	1.4735189 *	2.5030232 *	2.8719273 *
12 N	3.1504437	2.5584804 *	3.8643056	4.3336131
13 C	4.4432079	3.7737305	4.9554022	5.1581143
14 C	5.4969335	5.0733281	6.3480904	6.6187499
15 C	5.6865672	5.6138041	7.0143910	7.5186964
16 C	7.0239096	7.0158637	8.4213532	8.9092635
17 C	8.0632933	7.8652063	9.1977910	9.5020269
18 C	7.9733609	7.5301508	8.7436628	8.8478298
19 C	6.8135140	6.2374542	7.3921058	7.4437790
20 O	4.7570247	4.9972346	6.4544522	7.2025200
21 N	1.5139152 *	2.6030694 *	3.8933543	5.1289795
22 H	3.9441034	3.5311622	2.1986689 *	2.6613854 *
23 H	3.4696433	4.0375737	3.4824428	4.6520725
24 H	2.1864956 *	3.5141884	3.9470624	5.3877573
25 H	4.6726683	3.5309647	2.2001794 *	1.1064419 *
26 H	5.4766241	4.0250530	3.4784770	2.1823517 *
27 H	4.8206131	3.5062156	3.9366330	3.4177421
28 H	5.0162181	4.0946451	5.0375451	4.9471267
29 H	7.4170405	7.5993349	9.0431196	9.6540698
30 H	9.0939059	8.9493315	10.2944043	10.6082685
31 H	8.9492305	8.4170406	9.5599103	9.5429997
32 H	7.0564225	6.2736371	7.2650695	7.1083255
33 H	5.3795303	5.8008397	7.2622289	8.0914081
34 H	2.1036514 *	3.0118257	4.2620831	5.4244102
35 H	2.0985147 *	3.4281250	4.5692166	5.9007527

	C	C	C	N
1 CO	5.3538624	4.1872830	2.9017256 *	1.9274265 *
2 C	3.7629172	4.2790897	3.8464497	5.0941457
3 C	4.9442340	5.1788426	4.4012953	5.3805145
4 C	5.1759078	5.0085945	3.9132794	4.5544319
5 C	4.3727403	3.8956867	2.6463342 *	3.1504437
6 C	2.9211561 *	2.5025680 *	1.4735189 *	2.5584804 *

7 C	2.4711300 *	2.8367098 *	2.5030232 *	3.8643056
8 C	1.3985002 *	2.4398771 *	2.8719273 *	4.3336131
9 C	0.0000000	1.4293022 *	2.4922250 *	3.8100442
10 C	1.4293022 *	0.0000000	1.4143337 *	2.4759724 *
11 C	2.4922250 *	1.4143337 *	0.0000000	1.4642406 *
12 N	3.8100442	2.4759724 *	1.4642406 *	0.0000000
13 C	4.3281550	2.9057143 *	2.4597823 *	1.3349977 *
14 C	5.7748637	4.3498749	3.8641318	2.5265168 *
15 C	6.8476399	5.4269955	4.6572900	3.1956991
16 C	8.1881220	6.7602552	6.0550890	4.5972658
17 C	8.6155946	7.1994931	6.7345261	5.3417580
18 C	7.8253454	6.4584653	6.2478261	4.9993305
19 C	6.4118160	5.0491661	4.9026700	3.7481845
20 O	6.7857460	5.4425344	4.3800279	2.9940742 *
21 N	5.4178355	4.6015445	3.1955361	2.9778264 *
22 H	4.0581230	4.8755614	4.7015822	6.0385849
23 H	5.9150225	6.2503094	5.5050761	6.4652894
24 H	6.2660208	6.0149334	4.8263484	5.2447335
25 H	2.1792251 *	3.4508087	3.9783118	5.4399635
26 H	1.1041098 *	2.1976122 *	3.4809838	4.6735053
27 H	2.1673532 *	1.1019334 *	2.1883940 *	2.6938526 *
28 H	3.9112470	2.5785600 *	2.6696452 *	2.0998336 *
29 H	9.0332606	7.6165725	6.7860575	5.3240237
30 H	9.7136193	8.3003465	7.8375164	6.4367740
31 H	8.4336795	7.1271170	7.0791433	5.9227138
32 H	5.9523186	4.6939355	4.8531191	3.9633278
33 H	7.7365436	6.4118931	5.3078710	3.9588337
34 H	5.6532875	4.8142356	3.4651202	3.1807645
35 H	6.3191252	5.5736030	4.1739403	3.9418671

C C C C

1 CO	2.8422320 *	3.2578326	3.0244339	4.3068560
2 C	6.2698391	7.6089554	8.1340043	9.5296580
3 C	6.6511247	7.8517165	8.1427271	9.4920326
4 C	5.8495249	6.8947710	7.0085759	8.3096760
5 C	4.4432079	5.4969335	5.6865672	7.0239096
6 C	3.7737305	5.0733281	5.6138041	7.0158637
7 C	4.9554022	6.3480904	7.0143910	8.4213532
8 C	5.1581143	6.6187499	7.5186964	8.9092635
9 C	4.3281550	5.7748637	6.8476399	8.1881220
10 C	2.9057143 *	4.3498749	5.4269955	6.7602552
11 C	2.4597823 *	3.8641318	4.6572900	6.0550890
12 N	1.3349977 *	2.5265168 *	3.1956991	4.5972658
13 C	0.0000000	1.4696927 *	2.6176400 *	3.8962294
14 C	1.4696927 *	0.0000000	1.4382723 *	2.5057118 *

15 C	2.6176400 *	1.4382723 *	0.0000000	1.4079895 *
16 C	3.8962294	2.5057118 *	1.4079895 *	0.0000000
17 C	4.3476642	2.8843634 *	2.4381990 *	1.4260726 *
18 C	3.7892894	2.4969784 *	2.8206022 *	2.4725414 *
19 C	2.4652988 *	1.4432603 *	2.4438081 *	2.8484694 *
20 O	3.0590501	2.4970360 *	1.4620452 *	2.4575276 *
21 N	4.1280783	4.8331760	4.7012428	5.9311514
22 H	7.1519424	8.5374614	9.1429737	10.5457500
23 H	7.7422648	8.9185868	9.1501873	10.4773740
24 H	6.5182467	7.4104102	7.3271944	8.5417714
25 H	6.2413512	7.7050743	8.6236608	10.0125783
26 H	4.9684509	6.3569171	7.5408304	8.8247248
27 H	2.6050557 *	3.9130926	5.1520617	6.3847182
28 H	1.1066274 *	2.1598037 *	3.5226320	4.6578409
29 H	4.8122024	3.5102557	2.1994639 *	1.1090166 *
30 H	5.4530823	3.9905678	3.4395578	2.1919938 *
31 H	4.6478657	3.4901737	3.9231933	3.4729911
32 H	2.6356786 *	2.2007193 *	3.4510356	3.9551485
33 H	4.0382457	3.3299003	2.0408227 *	2.4964085 *
34 H	4.1372098	4.7841535	4.6913029	5.8615075
35 H	5.0727937	5.6405803	5.2984621	6.4167976

C C C O

1 CO	5.4620680	5.6209643	4.6977621	1.9630053 *
2 C	10.4067521	10.0482827	8.7271693	7.3984051
3 C	10.5082235	10.3319349	9.0962317	7.2057205
4 C	9.4038522	9.3649364	8.2194568	5.9697626
5 C	8.0632933	7.9733609	6.8135140	4.7570247
6 C	7.8652063	7.5301508	6.2374542	4.9972346
7 C	9.1977910	8.7436628	7.3921058	6.4544522
8 C	9.5020269	8.8478298	7.4437790	7.2025200
9 C	8.6155946	7.8253454	6.4118160	6.7857460
10 C	7.1994931	6.4584653	5.0491661	5.4425344
11 C	6.7345261	6.2478261	4.9026700	4.3800279
12 N	5.3417580	4.9993305	3.7481845	2.9940742 *
13 C	4.3476642	3.7892894	2.4652988 *	3.0590501
14 C	2.8843634 *	2.4969784 *	1.4432603 *	2.4970360 *
15 C	2.4381990 *	2.8206022 *	2.4438081 *	1.4620452 *
16 C	1.4260726 *	2.4725414 *	2.8484694 *	2.4575276 *
17 C	0.0000000	1.4254596 *	2.4582814 *	3.7644678
18 C	1.4254596 *	0.0000000	1.4151178 *	4.2824497
19 C	2.4582814 *	1.4151178 *	0.0000000	3.7883871
20 O	3.7644678	4.2824497	3.7883871	0.0000000
21 N	7.0833364	7.2109165	6.2263699	3.6090498
22 H	11.3726685	10.9391281	9.5862152	8.4596199

23 H	11.5326740	11.3988901	10.1796830	8.1475155
24 H	9.7242793	9.8326859	8.7835047	6.1558895
25 H	10.5854882	9.8934414	8.4831398	8.2978094
26 H	9.1074919	8.1860858	6.7880041	7.6305270
27 H	6.6330062	5.7479906	4.3468309	5.4476332
28 H	4.8233065	3.9590768	2.5484915 *	4.1421528
29 H	2.2004567 *	3.4758741	3.9572419	2.6892096 *
30 H	1.1063933 *	2.2027284 *	3.4632629	4.6473120
31 H	2.1990348 *	1.1025944 *	2.1837649 *	5.3850318
32 H	3.4598103	2.1850155 *	1.1071913 *	4.6879638
33 H	3.9166564	4.7213532	4.4837647	0.9914089 *
34 H	6.9404971	7.0458859	6.0984714	3.7587588
35 H	7.6670468	7.9459254	7.0586189	4.0366884

N H H H

1 CO	1.9747036 *	6.5423119	6.2425555	4.4332836
2 C	4.3438027	1.1052639 *	2.1822259 *	3.4320901
3 C	3.8124960	2.1753779 *	1.1039503 *	2.1886917 *
4 C	2.4708352 *	3.4458508	2.2021802 *	1.1085943 *
5 C	1.5139152 *	3.9441034	3.4696433	2.1864956 *
6 C	2.6030694 *	3.5311622	4.0375737	3.5141884
7 C	3.8933543	2.1986689 *	3.4824428	3.9470624
8 C	5.1289795	2.6613854 *	4.6520725	5.3877573
9 C	5.4178355	4.0581230	5.9150225	6.2660208
10 C	4.6015445	4.8755614	6.2503094	6.0149334
11 C	3.1955361	4.7015822	5.5050761	4.8263484
12 N	2.9778264 *	6.0385849	6.4652894	5.2447335
13 C	4.1280783	7.1519424	7.7422648	6.5182467
14 C	4.8331760	8.5374614	8.9185868	7.4104102
15 C	4.7012428	9.1429737	9.1501873	7.3271944
16 C	5.9311514	10.5457500	10.4773740	8.5417714
17 C	7.0833364	11.3726685	11.5326740	9.7242793
18 C	7.2109165	10.9391281	11.3988901	9.8326859
19 C	6.2263699	9.5862152	10.1796830	8.7835047
20 O	3.6090498	8.4596199	8.1475155	6.1558895
21 N	0.0000000	5.4473631	4.6704181	2.6462803 *
22 H	5.4473631	0.0000000	2.5216967 *	4.3507073
23 H	4.6704181	2.5216967 *	0.0000000	2.5142236 *
24 H	2.6462803 *	4.3507073	2.5142236 *	0.0000000
25 H	6.0690282	2.3742472 *	4.7526148	5.9594825
26 H	6.5021791	4.7537736	6.8320662	7.3454719
27 H	5.3105946	5.9451998	7.3428985	6.9844742
28 H	4.9349349	7.1981341	8.1070529	7.1578541
29 H	6.1908859	11.1041151	10.8068030	8.7141240
30 H	8.0480647	12.4641155	12.5622221	10.6793480

31 H	8.2460090	11.7491954	12.3405075	10.8532971
32 H	6.6843066	9.4279154	10.2855012	9.1290244
33 H	4.0963499	9.1885231	8.6597693	6.5086868
34 H	1.0439694 *	5.8110676	5.0747561	3.0943604
35 H	1.0412504 *	5.8330675	4.6061329	2.2426658 *

H H H H

1 CO	6.5779921	6.3253684	4.5456340	3.8677907
2 C	2.6634507 *	4.6518702	5.3777871	6.4298305
3 C	4.0607253	5.9168331	6.2655196	7.0075970
4 C	4.8771610	6.2484735	6.0182751	6.3850951
5 C	4.6726683	5.4766241	4.8206131	5.0162181
6 C	3.5309647	4.0250530	3.5062156	4.0946451
7 C	2.2001794 *	3.4784770	3.9366330	5.0375451
8 C	1.1064419 *	2.1823517 *	3.4177421	4.9471267
9 C	2.1792251 *	1.1041098 *	2.1673532 *	3.9112470
10 C	3.4508087	2.1976122 *	1.1019334 *	2.5785600 *
11 C	3.9783118	3.4809838	2.1883940 *	2.6696452 *
12 N	5.4399635	4.6735053	2.6938526 *	2.0998336 *
13 C	6.2413512	4.9684509	2.6050557 *	1.1066274 *
14 C	7.7050743	6.3569171	3.9130926	2.1598037 *
15 C	8.6236608	7.5408304	5.1520617	3.5226320
16 C	10.0125783	8.8247248	6.3847182	4.6578409
17 C	10.5854882	9.1074919	6.6330062	4.8233065
18 C	9.8934414	8.1860858	5.7479906	3.9590768
19 C	8.4831398	6.7880041	4.3468309	2.5484915 *
20 O	8.2978094	7.6305270	5.4476332	4.1421528
21 N	6.0690282	6.5021791	5.3105946	4.9349349
22 H	2.3742472 *	4.7537736	5.9451998	7.1981341
23 H	4.7526148	6.8320662	7.3428985	8.1070529
24 H	5.9594825	7.3454719	6.9844742	7.1578541
25 H	0.0000000	2.5271615 *	4.3351669	5.9669968
26 H	2.5271615 *	0.0000000	2.4820547 *	4.3589877
27 H	4.3351669	2.4820547 *	0.0000000	1.9892663 *
28 H	5.9669968	4.3589877	1.9892663 *	0.0000000
29 H	10.7597059	9.7310241	7.3273109	5.6611519
30 H	11.6911971	10.1850544	7.7112772	5.9007055
31 H	10.5520612	8.6750614	6.3143796	4.6103691
32 H	8.0873804	6.1718430	3.8411840	2.2369820 *
33 H	9.1766041	8.5994324	6.4329664	5.1098597
34 H	6.3604038	6.7075447	5.4738684	4.8676150
35 H	6.7693528	7.4154585	6.3033692	5.9333202

H H H H

1 CO	4.6511968	6.4488878	6.6847552	5.2766552
2 C	10.0537940	11.4887073	10.9022740	8.6583367
3 C	9.8768000	11.5521298	11.2628143	9.1875800
4 C	8.6145873	10.4128782	10.3481763	8.4564433
5 C	7.4170405	9.0939059	8.9492305	7.0564225
6 C	7.5993349	8.9493315	8.4170406	6.2736371
7 C	9.0431196	10.2944043	9.5599103	7.2650695
8 C	9.6540698	10.6082685	9.5429997	7.1083255
9 C	9.0332606	9.7136193	8.4336795	5.9523186
10 C	7.6165725	8.3003465	7.1271170	4.6939355
11 C	6.7860575	7.8375164	7.0791433	4.8531191
12 N	5.3240237	6.4367740	5.9227138	3.9633278
13 C	4.8122024	5.4530823	4.6478657	2.6356786 *
14 C	3.5102557	3.9905678	3.4901737	2.2007193 *
15 C	2.1994639 *	3.4395578	3.9231933	3.4510356
16 C	1.1090166 *	2.1919938 *	3.4729911	3.9551485
17 C	2.2004567 *	1.1063933 *	2.1990348 *	3.4598103
18 C	3.4758741	2.2027284 *	1.1025944 *	2.1850155 *
19 C	3.9572419	3.4632629	2.1837649 *	1.1071913 *
20 O	2.6892096 *	4.6473120	5.3850318	4.6879638
21 N	6.1908859	8.0480647	8.2460090	6.6843066
22 H	11.1041151	12.4641155	11.7491954	9.4279154
23 H	10.8068030	12.5622221	12.3405075	10.2855012
24 H	8.7141240	10.6793480	10.8532971	9.1290244
25 H	10.7597059	11.6911971	10.5520612	8.0873804
26 H	9.7310241	10.1850544	8.6750614	6.1718430
27 H	7.3273109	7.7112772	6.3143796	3.8411840
28 H	5.6611519	5.9007055	4.6103691	2.2369820 *
29 H	0.0000000	2.5220767 *	4.3877969	5.0636462
30 H	2.5220767 *	0.0000000	2.5423383 *	4.3761433
31 H	4.3877969	2.5423383 *	0.0000000	2.5093939 *
32 H	5.0636462	4.3761433	2.5093939 *	0.0000000
33 H	2.2929498 *	4.6198987	5.8058967	5.4669415
34 H	6.1517171	7.8829255	8.0475268	6.5485254
35 H	6.5088529	8.5688147	9.0089160	7.5966275

H H H

1 CO	2.6641134 *	2.4957059 *	2.5966469 *
2 C	8.1082634	4.7387734	4.7496659
3 C	7.7830103	4.2470004	3.9344914
4 C	6.4759529	2.9760207 *	2.5057094 *
5 C	5.3795303	2.1036514 *	2.0985147 *
6 C	5.8008397	3.0118257	3.4281250
7 C	7.2622289	4.2620831	4.5692166
8 C	8.0914081	5.4244102	5.9007527

9 C	7.7365436	5.6532875	6.3191252
10 C	6.4118931	4.8142356	5.5736030
11 C	5.3078710	3.4651202	4.1739403
12 N	3.9588337	3.1807645	3.9418671
13 C	4.0382457	4.1372098	5.0727937
14 C	3.3299003	4.7841535	5.6405803
15 C	2.0408227 *	4.6913029	5.2984621
16 C	2.4964085 *	5.8615075	6.4167976
17 C	3.9166564	6.9404971	7.6670468
18 C	4.7213532	7.0458859	7.9459254
19 C	4.4837647	6.0984714	7.0586189
20 O	0.9914089 *	3.7587588	4.0366884
21 N	4.0963499	1.0439694 *	1.0412504 *
22 H	9.1885231	5.8110676	5.8330675
23 H	8.6597693	5.0747561	4.6061329
24 H	6.5086868	3.0943604	2.2426658 *
25 H	9.1766041	6.3604038	6.7693528
26 H	8.5994324	6.7075447	7.4154585
27 H	6.4329664	5.4738684	6.3033692
28 H	5.1098597	4.8676150	5.9333202
29 H	2.2929498 *	6.1517171	6.5088529
30 H	4.6198987	7.8829255	8.5688147
31 H	5.8058967	8.0475268	9.0089160
32 H	5.4669415	6.5485254	7.5966275
33 H	0.0000000	4.2437059	4.3018338
34 H	4.2437059	0.0000000	1.6620871 *
35 H	4.3018338	1.6620871 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 3280.9 SECONDS (54.7 MIN)
WALL CLOCK TIME: STEP = 0.79 , TOTAL = 3033.0 SECONDS (50.5 MIN)
CPU UTILIZATION: STEP = 98.40% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.20 , TOTAL = 3282.1 SECONDS (54.7 MIN)
WALL CLOCK TIME: STEP = 1.20 , TOTAL = 3034.2 SECONDS (50.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
 INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.632601601	-284.632601601	0.019017529	0.001346340	196078462
11487222						
2	1	-284.632812343	-0.000210742	0.004853318	0.000143971	159985899
14529326						
3	2	-284.632811353	0.000000989	0.003700428	0.000254700	146936169
15584735						
4	3	-284.632816166	-0.000004812	0.001027428	0.000076840	139436653
16160269						
5	4	-284.632816070	0.000000096	0.000674882	0.000103581	134400772
16576871						
6	5	-284.632816470	-0.000000399	0.000419131	0.000039521	126624907
17189805						
7	6	-284.632816544	-0.000000074	0.000286055	0.000038355	124997213
17303114						
8	7	-284.632816668	-0.000000125	0.000767769	0.000038546	116567963
18015303						
9	8	-284.632816808	-0.000000140	0.000643745	0.000034892	148039978
15606271						
10	9	-284.632816897	-0.000000088	0.000470755	0.000051607	144211069
15981455						
11	10	-284.632816991	-0.000000094	0.000604936	0.000027566	144622738
15871595						
12	11	-284.632817078	-0.000000087	0.000560310	0.000016992	165562527
14214500						
13	12	-284.632817128	-0.000000049	0.000333790	0.000035817	164487325
14293586						
14	13	-284.632817152	-0.000000025	0.000119593	0.000010695	161527540
14504318						
15	14	-284.632817158	-0.000000006	0.000050257	0.000012055	156935201
14839008						
16	15	-284.632817165	-0.000000007	0.000079448	0.000009812	151683065
15257302						

-----DISABLING FDIFF OPTION-----

17	16	-284.632817156	0.000000008	0.000200726	0.000009004	196083146
11486607						
18	17	-284.632817164	-0.000000008	0.000193363	0.000009025	196083052
11486611						
19	18	-284.632817171	-0.000000007	0.000188834	0.000005920	196083185
11486600						
20	19	-284.632817176	-0.000000005	0.000068671	0.000006676	196083071
11486602						

21 20	-284.632817179	-0.000000003	0.000041708	0.000004994	196083032
11486604					
22 21	-284.632817181	-0.000000002	0.000061969	0.000002914	196083023
11486603					
23 22	-284.632817182	-0.000000001	0.000029697	0.000001993	196083133
11486596					
24 23	-284.632817182	0.000000000	0.000023006	0.000001483	196082923
11486599					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 81.3 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 25.8 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.5 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6328171822 AFTER 24 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5955536730
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000333190

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 84.71 , TOTAL = 3366.9 SECONDS (56.1 MIN)
WALL CLOCK TIME: STEP = 77.71 , TOTAL = 3111.9 SECONDS (51.9 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 4.01 , TOTAL = 3370.9 SECONDS (56.2 MIN)
WALL CLOCK TIME: STEP = 3.98 , TOTAL = 3115.9 SECONDS (51.9 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.

USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.83 , TOTAL = 3373.7 SECONDS (56.2 MIN)

WALL CLOCK TIME: STEP = 2.65 , TOTAL = 3118.5 SECONDS (52.0 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 30 ENERGY= -284.6328172

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0002786	0.0009785	0.0001554
2 C	6.0	0.0003318	0.0002438	-0.0001804
3 C	6.0	-0.0011640	0.0005673	0.0000146
4 C	6.0	0.0009587	0.0005403	0.0005816
5 C	6.0	0.0000569	-0.0006259	0.0009905
6 C	6.0	0.0002069	-0.0004114	0.0007605
7 C	6.0	0.0002792	0.0003777	0.0003169
8 C	6.0	-0.0008104	0.0002135	0.0000714
9 C	6.0	0.0017387	-0.0002621	-0.0002210
10 C	6.0	-0.0002521	-0.0009953	-0.0004185
11 C	6.0	0.0000956	-0.0001893	0.0001464
12 N	7.0	-0.0009041	0.0004512	-0.0001818
13 C	6.0	0.0003368	0.0007702	-0.0002844
14 C	6.0	-0.0020086	0.0005550	-0.0001085
15 C	6.0	-0.0004594	-0.0004477	-0.0001394
16 C	6.0	-0.0011906	0.0006353	-0.0004748
17 C	6.0	0.0015698	-0.0018049	-0.0001947
18 C	6.0	-0.0007612	0.0012989	-0.0003108
19 C	6.0	0.0010450	-0.0005116	0.0008384
20 O	8.0	0.0001077	0.0002278	-0.0012558
21 N	7.0	-0.0002325	0.0001936	0.0006573
22 H	1.0	0.0005790	-0.0002443	-0.0003081
23 H	1.0	0.0000613	0.0006446	-0.0004213
24 H	1.0	0.0008988	-0.0002254	-0.0005641
25 H	1.0	0.0006348	0.0010494	-0.0002986
26 H	1.0	0.0003141	0.0000481	-0.0002718
27 H	1.0	0.0007400	-0.0002279	-0.0005227
28 H	1.0	-0.0007484	-0.0000644	-0.0002250
29 H	1.0	-0.0006445	-0.0013066	0.0008697

30 H	1.0	-0.0007230	-0.0003240	-0.0005244
31 H	1.0	0.0010579	-0.0005091	-0.0003814
32 H	1.0	-0.0000382	0.0010822	0.0021278
33 H	1.0	-0.0001758	0.0000104	-0.0004816
34 H	1.0	0.0004950	-0.0004485	0.0004924
35 H	1.0	-0.0011163	-0.0012895	-0.0002536

MAXIMUM GRADIENT = 0.0021278 RMS GRADIENT = 0.0007144
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000618005
 PREDICTED ENERGY CHANGE WAS -0.0000338344 RATIO= 1.827
 GDIIS STEP HAS LENGTH = 0.073438
 RADIUS OF STEP TAKEN= 0.07344 CURRENT TRUST RADIUS= 0.09724

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 3373.7 SECONDS (56.2 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 3118.5 SECONDS (52.0
 MIN)
 CPU UTILIZATION: STEP = 93.66% , TOTAL = 100.00%

INSERCH= 31

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1142776588	-1.7195436630	1.0318004784
C	6.0	4.9977845304	0.6844897402	0.4397991682
C	6.0	5.2245081484	-0.6754591574	0.2060170165
C	6.0	4.1002012222	-1.5518436913	0.0810139602
C	6.0	2.7800410139	-1.0728989020	0.2026766625
C	6.0	2.4819657507	0.3234454615	0.5033124432
C	6.0	3.6597976970	1.2050672494	0.5928505840
C	6.0	3.5118120094	2.6226660259	0.8200865487
C	6.0	2.2467589754	3.1932455231	0.9916559548
C	6.0	1.0908848178	2.3539671348	0.9574664513
C	6.0	1.1708151918	0.9659389223	0.7022759640
N	7.0	-0.0600084584	0.1747671339	0.7211723081
C	6.0	-1.2682125493	0.7134182021	0.5378194914
C	6.0	-2.5792288912	0.0569215861	0.5904277723
C	6.0	-2.8727746106	-1.3426582604	0.7409218042
C	6.0	-4.1775165579	-1.8683915470	0.7176965519
C	6.0	-5.2721801382	-0.9710572124	0.5268038286
C	6.0	-5.0416125679	0.4280096011	0.4052426569
C	6.0	-3.7212877351	0.9320325664	0.4494530254
O	8.0	-1.7645465526	-2.2780923319	0.9314952197

N	7.0	1.6941059681	-2.0818533419	-0.0958148767
H	1.0	5.8477689019	1.3862489133	0.5039480198
H	1.0	6.2491760098	-1.0679175814	0.0853924417
H	1.0	4.2859629023	-2.6176114895	-0.1595141601
H	1.0	4.4197628806	3.2523437507	0.8589253127
H	1.0	2.1326524588	4.2756071443	1.1762701638
H	1.0	0.1182690267	2.8277659323	1.1691854208
H	1.0	-1.3269644478	1.7898955176	0.2855401843
H	1.0	-4.3670574583	-2.9517123873	0.8498610703
H	1.0	-6.2997892718	-1.3767536288	0.4840820543
H	1.0	-5.8883112529	1.1235598919	0.2731903360
H	1.0	-3.5488685874	2.0240657195	0.3858508806
H	1.0	-2.0904899662	-3.2116842191	0.9996992905
H	1.0	1.3959554112	-1.9850129271	-1.0913272212
H	1.0	2.0923454702	-3.0398606759	-0.0123898073

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4752609	5.2807657	4.1011834
2 C	5.4752609	0.0000000	1.3983986 *	2.4363025 *
3 C	5.2807657	1.3983986 *	0.0000000	1.4309932 *
4 C	4.1011834	2.4363025 *	1.4309932 *	0.0000000
5 C	2.8656395 *	2.8395472 *	2.4765680 *	1.4096145 *
6 C	3.1716007	2.5423869 *	2.9338940 *	2.5127140 *
7 C	4.6170053	1.4438263 *	2.4767597 *	2.8383957 *
8 C	5.5175037	2.4716918 *	3.7667014	4.2800656
9 C	5.3557993	3.7638468	4.9448048	5.1749772
10 C	4.1896035	4.2800700	5.1796662	5.0079449
11 C	2.9045954 *	3.8462712	4.4014642	3.9123520
12 N	1.9275059 *	5.0911942	5.3772098	4.5495420
13 C	2.8415840 *	6.2668305	6.6478940	5.8446513
14 C	3.2566265	7.6044502	7.8474496	6.8892971
15 C	3.0247536	8.1330010	8.1423133	7.0072554
16 C	4.3058466	9.5278843	9.4912050	8.3081995
17 C	5.4616098	10.4029121	10.5057483	9.4009347
18 C	5.6202993	10.0427322	10.3271762	9.3593644
19 C	4.6991007	8.7225909	9.0923349	8.2146867
20 O	1.9626559 *	7.3991742	7.2070547	5.9704290
21 N	1.9744980 *	4.3420995	3.8121892	2.4701160 *
22 H	6.5419796	1.1041080 *	2.1743636 *	3.4445978
23 H	6.2415769	2.1823190 *	1.1038651 *	2.2027928 *
24 H	4.4304305	3.4307053	2.1877925 *	1.1082519 *
25 H	6.5792669	2.6652673 *	4.0622087	4.8772413

26 H	6.3274435	4.6526869	5.9172646	6.2474009
27 H	4.5493862	5.3791550	6.2668938	6.0183787
28 H	3.8665549	6.4224736	7.0004350	6.3767687
29 H	4.6512048	10.0543713	9.8789673	8.6165671
30 H	6.4465305	11.4841569	11.5489638	10.4092710
31 H	6.6850431	10.8962206	11.2576968	10.3423932
32 H	5.2773575	8.6511649	9.1810628	8.4491611
33 H	2.6624264 *	8.1078539	7.7827737	6.4748522
34 H	2.4941618 *	4.7374851	4.2492175	2.9790879 *
35 H	2.5973684 *	4.7451909	3.9304630	2.5008806 *

C C C C

1 CO	2.8656395 *	3.1716007	4.6170053	5.5175037
2 C	2.8395472 *	2.5423869 *	1.4438263 *	2.4716918 *
3 C	2.4765680 *	2.9338940 *	2.4767597 *	3.7667014
4 C	1.4096145 *	2.5127140 *	2.8383957 *	4.2800656
5 C	0.0000000	1.4591122 *	2.4729208 *	3.8175757
6 C	1.4591122 *	0.0000000	1.4739614 *	2.5391621 *
7 C	2.4729208 *	1.4739614 *	0.0000000	1.4433025 *
8 C	3.8175757	2.5391621 *	1.4433025 *	0.0000000
9 C	4.3711402	2.9205400 *	2.4715536 *	1.3983405 *
10 C	3.8944020	2.5028744 *	2.8376450 *	2.4396641 *
11 C	2.6450079 *	1.4736011 *	2.5028364 *	2.8703467 *
12 N	3.1450579	2.5556215 *	3.8619869	4.3312694
13 C	4.4375226	3.7705579	4.9527802	5.1549526
14 C	5.4907758	5.0689560	6.3437920	6.6133628
15 C	5.6847869	5.6129853	7.0133680	7.5161832
16 C	7.0217990	7.0141867	8.4193367	8.9053835
17 C	8.0593856	7.8614927	9.1934818	9.4952293
18 C	7.9669332	7.5249440	8.7380522	8.8402310
19 C	6.8079310	6.2332682	7.3875255	7.4372940
20 O	4.7578297	4.9984204	6.4552762	7.2020694
21 N	1.5120652 *	2.6009881 *	3.8912788	5.1259568
22 H	3.9432381	3.5296151	2.1972593 *	2.6618350 *
23 H	3.4711206	4.0376257	3.4826504	4.6533154
24 H	2.1874917 *	3.5133404	3.9460117	5.3869691
25 H	4.6719454	3.5298673	2.1999282 *	1.1056117 *
26 H	5.4748071	4.0242358	3.4786156	2.1820087 *
27 H	4.8202028	3.5074307	3.9379866	3.4176117
28 H	5.0069903	4.0872790	5.0303340	4.9389274
29 H	7.4182076	7.5997285	9.0429683	9.6514851
30 H	9.0892703	8.9448459	10.2893635	10.6007441
31 H	8.9425799	8.4115799	9.5538061	9.5346071
32 H	7.0483927	6.2671261	7.2579940	7.0993023
33 H	5.3788214	5.8009390	7.2621641	8.0905927

34 H	2.1028768 *	3.0085336	4.2588788	5.4185844
35 H	2.0947834 *	3.4248476	4.5653735	5.8967882

	C	C	C	N
--	---	---	---	---

1 CO	5.3557993	4.1896035	2.9045954 *	1.9275059 *
2 C	3.7638468	4.2800700	3.8462712	5.0911942
3 C	4.9448048	5.1796662	4.4014642	5.3772098
4 C	5.1749772	5.0079449	3.9123520	4.5495420
5 C	4.3711402	3.8944020	2.6450079 *	3.1450579
6 C	2.9205400 *	2.5028744 *	1.4736011 *	2.5556215 *
7 C	2.4715536 *	2.8376450 *	2.5028364 *	3.8619869
8 C	1.3983405 *	2.4396641 *	2.8703467 *	4.3312694
9 C	0.0000000	1.4288465 *	2.4904398 *	3.8086151
10 C	1.4288465 *	0.0000000	1.4135535 *	2.4757429 *
11 C	2.4904398 *	1.4135535 *	0.0000000	1.4632965 *
12 N	3.8086151	2.4757429 *	1.4632965 *	0.0000000
13 C	4.3255677	2.9039361 *	2.4575738 *	1.3354851 *
14 C	5.7695468	4.3452123	3.8602659	2.5253620 *
15 C	6.8444806	5.4242536	4.6563648	3.1960324
16 C	8.1833086	6.7558756	6.0529596	4.5965620
17 C	8.6076681	7.1923468	6.7301511	5.3401710
18 C	7.8173378	6.4514950	6.2427442	4.9980319
19 C	6.4050488	5.0435087	4.8987488	3.7486329
20 O	6.7845213	5.4415198	4.3809393	2.9943623 *
21 N	5.4143039	4.5988891	3.1937157	2.9726624 *
22 H	4.0583701	4.8754593	4.6999883	6.0346257
23 H	5.9159248	6.2512220	5.5051672	6.4617560
24 H	6.2649505	6.0143797	4.8258327	5.2402723
25 H	2.1778558 *	3.4493797	3.9759083	5.4368010
26 H	1.1039064 *	2.1967829 *	3.4790380	4.6724474
27 H	2.1669244 *	1.1024027 *	2.1891226 *	2.6964609 *
28 H	3.9037789	2.5720919 *	2.6629826 *	2.0984739 *
29 H	9.0290188	7.6125520	6.7851166	5.3237305
30 H	9.7049477	8.2924323	7.8323526	6.4341505
31 H	8.4249130	7.1197833	7.0739116	5.9219937
32 H	5.9433391	4.6864583	4.8471819	3.9628892
33 H	7.7353034	6.4108817	5.3082113	3.9583437
34 H	5.6459761	4.8080528	3.4606094	3.1732689
35 H	6.3153436	5.5710792	4.1720973	3.9375846

	C	C	C	C
--	---	---	---	---

1 CO	2.8415840 *	3.2566265	3.0247536	4.3058466
2 C	6.2668305	7.6044502	8.1330010	9.5278843
3 C	6.6478940	7.8474496	8.1423133	9.4912050

4 C	5.8446513	6.8892971	7.0072554	8.3081995
5 C	4.4375226	5.4907758	5.6847869	7.0217990
6 C	3.7705579	5.0689560	5.6129853	7.0141867
7 C	4.9527802	6.3437920	7.0133680	8.4193367
8 C	5.1549526	6.6133628	7.5161832	8.9053835
9 C	4.3255677	5.7695468	6.8444806	8.1833086
10 C	2.9039361 *	4.3452123	5.4242536	6.7558756
11 C	2.4575738 *	3.8602659	4.6563648	6.0529596
12 N	1.3354851 *	2.5253620 *	3.1960324	4.5965620
13 C	0.0000000	1.4671466 *	2.6159741 *	3.8938602
14 C	1.4671466 *	0.0000000	1.4379295 *	2.5055042 *
15 C	2.6159741 *	1.4379295 *	0.0000000	1.4068712 *
16 C	3.8938602	2.5055042 *	1.4068712 *	0.0000000
17 C	4.3438848	2.8831883 *	2.4374332 *	1.4282637 *
18 C	3.7865000	2.4970649 *	2.8198942 *	2.4734081 *
19 C	2.4643820 *	1.4456803 *	2.4452294 *	2.8499955 *
20 O	3.0578527	2.4964624 *	1.4627114 *	2.4568250 *
21 N	4.1219372	4.8276990	4.7013760	5.9315527
22 H	7.1477997	8.5316400	9.1406220	10.5425197
23 H	7.7387969	8.9140932	9.1496002	10.4764729
24 H	6.5139004	7.4058354	7.3269239	8.5417395
25 H	6.2371721	7.6986167	8.6202710	10.0077515
26 H	4.9661547	6.3515624	7.5371569	8.8191407
27 H	2.6060354 *	3.9101194	5.1499699	6.3805573
28 H	1.1072037 *	2.1597040 *	3.5227538	4.6578397
29 H	4.8097185	3.5093468	2.1985914 *	1.1076901 *
30 H	5.4487127	3.9886468	3.4367948	2.1909644 *
31 H	4.6458107	3.4911865	3.9235782	3.4750795
32 H	2.6348213 *	2.2026595 *	3.4522469	3.9568350
33 H	4.0368183	3.3301881	2.0425947 *	2.4979273 *
34 H	4.1271589	4.7749227	4.6895428	5.8608666
35 H	5.0678578	5.6371142	5.3009803	6.4200106

C C C O

1 CO	5.4616098	5.6202993	4.6991007	1.9626559 *
2 C	10.4029121	10.0427322	8.7225909	7.3991742
3 C	10.5057483	10.3271762	9.0923349	7.2070547
4 C	9.4009347	9.3593644	8.2146867	5.9704290
5 C	8.0593856	7.9669332	6.8079310	4.7578297
6 C	7.8614927	7.5249440	6.2332682	4.9984204
7 C	9.1934818	8.7380522	7.3875255	6.4552762
8 C	9.4952293	8.8402310	7.4372940	7.2020694
9 C	8.6076681	7.8173378	6.4050488	6.7845213
10 C	7.1923468	6.4514950	5.0435087	5.4415198
11 C	6.7301511	6.2427442	4.8987488	4.3809393

12 N	5.3401710	4.9980319	3.7486329	2.9943623 *
13 C	4.3438848	3.7865000	2.4643820 *	3.0578527
14 C	2.8831883 *	2.4970649 *	1.4456803 *	2.4964624 *
15 C	2.4374332 *	2.8198942 *	2.4452294 *	1.4627114 *
16 C	1.4282637 *	2.4734081 *	2.8499955 *	2.4568250 *
17 C	0.0000000	1.4231397 *	2.4562168 *	3.7650510
18 C	1.4231397 *	0.0000000	1.4139489 *	4.2824165
19 C	2.4562168 *	1.4139489 *	0.0000000	3.7902642
20 O	3.7650510	4.2824165	3.7902642	0.0000000
21 N	7.0817134	7.2055794	6.2215203	3.6133299
22 H	11.3670876	10.9319072	9.5799858	8.4591690
23 H	11.5302157	11.3939462	10.1755829	8.1486295
24 H	9.7231822	9.8284496	8.7799133	6.1574540
25 H	10.5773900	9.8843471	8.4751529	8.2967869
26 H	9.0983976	8.1773204	6.7805877	7.6288303
27 H	6.6257568	5.7416737	4.3421211	5.4471350
28 H	4.8213893	3.9582411	2.5486428 *	4.1421324
29 H	2.2015013 *	3.4749433	3.9573754	2.6895150 *
30 H	1.1056199 *	2.2014528 *	3.4612661	4.6455373
31 H	2.1980351 *	1.1036878 *	2.1825999 *	5.3860968
32 H	3.4583857	2.1854189 *	1.1073888 *	4.6893600
33 H	3.9201010	4.7233330	4.4869434	0.9912037 *
34 H	6.9361723	7.0359563	6.0884592	3.7638383
35 H	7.6685667	7.9431668	7.0560305	4.0431208

N H H H

1 CO	1.9744980 *	6.5419796	6.2415769	4.4304305
2 C	4.3420995	1.1041080 *	2.1823190 *	3.4307053
3 C	3.8121892	2.1743636 *	1.1038651 *	2.1877925 *
4 C	2.4701160 *	3.4445978	2.2027928 *	1.1082519 *
5 C	1.5120652 *	3.9432381	3.4711206	2.1874917 *
6 C	2.6009881 *	3.5296151	4.0376257	3.5133404
7 C	3.8912788	2.1972593 *	3.4826504	3.9460117
8 C	5.1259568	2.6618350 *	4.6533154	5.3869691
9 C	5.4143039	4.0583701	5.9159248	6.2649505
10 C	4.5988891	4.8754593	6.2512220	6.0143797
11 C	3.1937157	4.6999883	5.5051672	4.8258327
12 N	2.9726624 *	6.0346257	6.4617560	5.2402723
13 C	4.1219372	7.1477997	7.7387969	6.5139004
14 C	4.8276990	8.5316400	8.9140932	7.4058354
15 C	4.7013760	9.1406220	9.1496002	7.3269239
16 C	5.9315527	10.5425197	10.4764729	8.5417395
17 C	7.0817134	11.3670876	11.5302157	9.7231822
18 C	7.2055794	10.9319072	11.3939462	9.8284496
19 C	6.2215203	9.5799858	10.1755829	8.7799133

20	O	3.6133299	8.4591690	8.1486295	6.1574540
21	N	0.0000000	5.4442965	4.6700712	2.6474170 *
22	H	5.4442965	0.0000000	2.5217553 *	4.3485996
23	H	4.6700712	2.5217553 *	0.0000000	2.5131128 *
24	H	2.6474170 *	4.3485996	2.5131128 *	0.0000000
25	H	6.0658382	2.3764511 *	4.7549725	5.9591523
26	H	6.4982942	4.7542085	6.8329376	7.3442174
27	H	5.3092230	5.9453916	7.3443160	6.9847870
28	H	4.9257220	7.1893971	8.0996950	7.1504647
29	H	6.1958583	11.1031636	10.8091400	8.7180974
30	H	8.0458565	12.4578388	12.5590948	10.6776446
31	H	8.2403817	11.7412875	12.3351708	10.8489378
32	H	6.6767773	9.4189996	10.2787311	9.1228929
33	H	4.0987602	9.1870949	8.6591986	6.5081372
34	H	1.0437033 *	5.8076633	5.0773500	3.1017092
35	H	1.0408326 *	5.8275429	4.6018867	2.2387267 *

H H H H

1	CO	6.5792669	6.3274435	4.5493862	3.8665549
2	C	2.6652673 *	4.6526869	5.3791550	6.4224736
3	C	4.0622087	5.9172646	6.2668938	7.0004350
4	C	4.8772413	6.2474009	6.0183787	6.3767687
5	C	4.6719454	5.4748071	4.8202028	5.0069903
6	C	3.5298673	4.0242358	3.5074307	4.0872790
7	C	2.1999282 *	3.4786156	3.9379866	5.0303340
8	C	1.1056117 *	2.1820087 *	3.4176117	4.9389274
9	C	2.1778558 *	1.1039064 *	2.1669244 *	3.9037789
10	C	3.4493797	2.1967829 *	1.1024027 *	2.5720919 *
11	C	3.9759083	3.4790380	2.1891226 *	2.6629826 *
12	N	5.4368010	4.6724474	2.6964609 *	2.0984739 *
13	C	6.2371721	4.9661547	2.6060354 *	1.1072037 *
14	C	7.6986167	6.3515624	3.9101194	2.1597040 *
15	C	8.6202710	7.5371569	5.1499699	3.5227538
16	C	10.0077515	8.8191407	6.3805573	4.6578397
17	C	10.5773900	9.0983976	6.6257568	4.8213893
18	C	9.8843471	8.1773204	5.7416737	3.9582411
19	C	8.4751529	6.7805877	4.3421211	2.5486428 *
20	O	8.2967869	7.6288303	5.4471350	4.1421324
21	N	6.0658382	6.4982942	5.3092230	4.9257220
22	H	2.3764511 *	4.7542085	5.9453916	7.1893971
23	H	4.7549725	6.8329376	7.3443160	8.0996950
24	H	5.9591523	7.3442174	6.9847870	7.1504647
25	H	0.0000000	2.5255989 *	4.3335179	5.9575499
26	H	2.5255989 *	0.0000000	2.4807328 *	4.3521387
27	H	4.3335179	2.4807328 *	0.0000000	1.9866312 *

28 H	5.9575499	4.3521387	1.9866312 *	0.0000000
29 H	10.7563287	9.7255807	7.3227380	5.6606951
30 H	11.6823734	10.1751845	7.7031697	5.8988196
31 H	10.5418783	8.6652648	6.3076249	4.6097766
32 H	8.0766053	6.1622953	3.8350287	2.2364606 *
33 H	9.1753402	8.5980022	6.4329076	5.1096765
34 H	6.3542743	6.6992600	5.4685684	4.8538634
35 H	6.7651976	7.4115185	6.3025503	5.9251150

H H H H

1 CO	4.6512048	6.4465305	6.6850431	5.2773575
2 C	10.0543713	11.4841569	10.8962206	8.6511649
3 C	9.8789673	11.5489638	11.2576968	9.1810628
4 C	8.6165671	10.4092710	10.3423932	8.4491611
5 C	7.4182076	9.0892703	8.9425799	7.0483927
6 C	7.5997285	8.9448459	8.4115799	6.2671261
7 C	9.0429683	10.2893635	9.5538061	7.2579940
8 C	9.6514851	10.6007441	9.5346071	7.0993023
9 C	9.0290188	9.7049477	8.4249130	5.9433391
10 C	7.6125520	8.2924323	7.1197833	4.6864583
11 C	6.7851166	7.8323526	7.0739116	4.8471819
12 N	5.3237305	6.4341505	5.9219937	3.9628892
13 C	4.8097185	5.4487127	4.6458107	2.6348213 *
14 C	3.5093468	3.9886468	3.4911865	2.2026595 *
15 C	2.1985914 *	3.4367948	3.9235782	3.4522469
16 C	1.1076901 *	2.1909644 *	3.4750795	3.9568350
17 C	2.2015013 *	1.1056199 *	2.1980351 *	3.4583857
18 C	3.4749433	2.2014528 *	1.1036878 *	2.1854189 *
19 C	3.9573754	3.4612661	2.1825999 *	1.1073888 *
20 O	2.6895150 *	4.6455373	5.3860968	4.6893600
21 N	6.1958583	8.0458565	8.2403817	6.6767773
22 H	11.1031636	12.4578388	11.7412875	9.4189996
23 H	10.8091400	12.5590948	12.3351708	10.2787311
24 H	8.7180974	10.6776446	10.8489378	9.1228929
25 H	10.7563287	11.6823734	10.5418783	8.0766053
26 H	9.7255807	10.1751845	8.6652648	6.1622953
27 H	7.3227380	7.7031697	6.3076249	3.8350287
28 H	5.6606951	5.8988196	4.6097766	2.2364606 *
29 H	0.0000000	2.5198694 *	4.3880071	5.0639023
30 H	2.5198694 *	0.0000000	2.5427067 *	4.3752470
31 H	4.3880071	2.5427067 *	0.0000000	2.5093017 *
32 H	5.0639023	4.3752470	2.5093017 *	0.0000000
33 H	2.2962570 *	4.6207177	5.8090966	5.4696211
34 H	6.1575188	7.8788565	8.0365213	6.5349867
35 H	6.5172949	8.5697337	9.0059152	7.5911292

	H	H	H
1 CO	2.6624264 *	2.4941618 *	2.5973684 *
2 C	8.1078539	4.7374851	4.7451909
3 C	7.7827737	4.2492175	3.9304630
4 C	6.4748522	2.9790879 *	2.5008806 *
5 C	5.3788214	2.1028768 *	2.0947834 *
6 C	5.8009390	3.0085336	3.4248476
7 C	7.2621641	4.2588788	4.5653735
8 C	8.0905927	5.4185844	5.8967882
9 C	7.7353034	5.6459761	6.3153436
10 C	6.4108817	4.8080528	5.5710792
11 C	5.3082113	3.4606094	4.1720973
12 N	3.9583437	3.1732689	3.9375846
13 C	4.0368183	4.1271589	5.0678578
14 C	3.3301881	4.7749227	5.6371142
15 C	2.0425947 *	4.6895428	5.3009803
16 C	2.4979273 *	5.8608666	6.4200106
17 C	3.9201010	6.9361723	7.6685667
18 C	4.7233330	7.0359563	7.9431668
19 C	4.4869434	6.0884592	7.0560305
20 O	0.9912037 *	3.7638383	4.0431208
21 N	4.0987602	1.0437033 *	1.0408326 *
22 H	9.1870949	5.8076633	5.8275429
23 H	8.6591986	5.0773500	4.6018867
24 H	6.5081372	3.1017092	2.2387267 *
25 H	9.1753402	6.3542743	6.7651976
26 H	8.5980022	6.6992600	7.4115185
27 H	6.4329076	5.4685684	6.3025503
28 H	5.1096765	4.8538634	5.9251150
29 H	2.2962570 *	6.1575188	6.5172949
30 H	4.6207177	7.8788565	8.5697337
31 H	5.8090966	8.0365213	9.0059152
32 H	5.4696211	6.5349867	7.5911292
33 H	0.0000000	4.2464592	4.3069664
34 H	4.2464592	0.0000000	1.6618570 *
35 H	4.3069664	1.6618570 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.62 , TOTAL = 3374.3 SECONDS (56.2 MIN)

WALL CLOCK TIME: STEP = 0.62 , TOTAL = 3119.1 SECONDS (52.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.97 , TOTAL = 3375.3 SECONDS (56.3 MIN)

WALL CLOCK TIME: STEP = 0.96 , TOTAL = 3120.1 SECONDS (52.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.632808662 -284.632808662 0.023230088 0.001185990 196164158
11478432

2 1 -284.632936235 -0.000127573 0.002585954 0.000133342 159111407
14614615

3 2 -284.632935344 0.000000891 0.001550691 0.000254837 145103200
15709028

4 3 -284.632939302 -0.000003958 0.000361593 0.000057946 137795099
16256863

5 4 -284.632939359 -0.000000058 0.000298244 0.000051643 128124459
17098703

6 5 -284.632939549 -0.000000190 0.000556385 0.000048550 121282392
17636708

7 6 -284.632939700 -0.000000150 0.000859877 0.000045029 146825951
15727188

8 7 -284.632939875 -0.000000175 0.000690346 0.000039859 167294585
14106414

9 8 -284.632940040 -0.000000165 0.001046111 0.000041662 166407833
14163358

-----DISABLING FDIFF OPTION-----

10 9 -284.632940163 -0.000000122 0.000575921 0.000050987 196180170
11476887

11 10 -284.632940230 -0.000000067 0.000424521 0.000054839 196179783
11476885

12 11 -284.632940296 -0.000000066 0.000161099 0.000018843 196179375
11476887

13 12 -284.632940323 -0.000000028 0.000118351 0.000013983 196179428
11476890

14 13 -284.632940333 -0.000000010 0.000108006 0.000012407 196179407
11476895

15	14	-284.632940340	-0.000000007	0.000150380	0.000011261	196179480
11476884						
16	15	-284.632940350	-0.000000010	0.000255720	0.000010640	196179489
11476886						
17	16	-284.632940363	-0.000000013	0.000219714	0.000009486	196179572
11476885						
18	17	-284.632940371	-0.000000008	0.000139785	0.000006928	196179527
11476890						
19	18	-284.632940377	-0.000000006	0.000091822	0.000005915	196179607
11476886						
20	19	-284.632940380	-0.000000004	0.000037185	0.000003980	196179571
11476889						
21	20	-284.632940383	-0.000000002	0.000038597	0.000002713	196179622
11476887						
22	21	-284.632940383	-0.000000001	0.000030382	0.000002420	196179642
11476885						
23	22	-284.632940384	-0.000000001	0.000017666	0.000001930	196179640
11476885						

 DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 76.6 SECONDS (3.3 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 24.8 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
 TIME TO SOLVE SCF EQUATIONS= 4.0 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6329403839 AFTER 23 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.5985354052
 INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000310837

 SPIN SZ = 1.500
 S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
 PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 81.64 , TOTAL = 3456.9 SECONDS (57.6 MIN)
 WALL CLOCK TIME: STEP = 74.66 , TOTAL = 3194.8 SECONDS (53.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.75 , TOTAL = 3460.7 SECONDS (57.7 MIN)
WALL CLOCK TIME: STEP = 3.73 , TOTAL = 3198.5 SECONDS (53.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.82 , TOTAL = 3463.5 SECONDS (57.7 MIN)
WALL CLOCK TIME: STEP = 2.64 , TOTAL = 3201.1 SECONDS (53.4 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 31 ENERGY= -284.6329404

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0003603	0.0008619	-0.0000520
2 C	6.0	0.0008796	0.0001084	-0.0000707
3 C	6.0	-0.0004468	0.0009305	0.0001401
4 C	6.0	0.0008650	0.0000824	0.0004610
5 C	6.0	-0.0011878	-0.0004894	0.0008504
6 C	6.0	0.0002558	-0.0013525	0.0005952
7 C	6.0	0.0004540	0.0003501	0.0004041
8 C	6.0	-0.0007112	0.0006114	0.0000831
9 C	6.0	0.0015385	-0.0004199	-0.0002710
10 C	6.0	0.0001938	-0.0014653	-0.0004413
11 C	6.0	-0.0003027	0.0008410	0.0004011
12 N	7.0	-0.0000772	0.0003129	-0.0001764
13 C	6.0	-0.0011474	-0.0001678	-0.0001283
14 C	6.0	0.0004252	-0.0004558	0.0001112
15 C	6.0	-0.0013620	0.0000937	-0.0005288
16 C	6.0	0.0003676	-0.0014027	-0.0001486
17 C	6.0	0.0004376	0.0011234	-0.0006535
18 C	6.0	0.0005812	-0.0007627	-0.0000800
19 C	6.0	-0.0012900	0.0003768	0.0006368

20 O	8.0	-0.0001151	-0.0000371	-0.0008508
21 N	7.0	0.0000644	0.0006342	0.0005666
22 H	1.0	-0.0000784	-0.0007058	-0.0004563
23 H	1.0	0.0000209	0.0006857	-0.0005167
24 H	1.0	0.0010311	0.0000300	-0.0003717
25 H	1.0	0.0001104	0.0007910	-0.0003463
26 H	1.0	0.0002712	-0.0000914	-0.0003202
27 H	1.0	0.0004860	0.0000310	-0.0005022
28 H	1.0	-0.0004312	0.0003897	-0.0003029
29 H	1.0	-0.0005166	-0.0005077	0.0008692
30 H	1.0	-0.0001325	-0.0003560	-0.0003560
31 H	1.0	0.0005798	0.0000286	-0.0005107
32 H	1.0	0.0000314	0.0012535	0.0021436
33 H	1.0	0.0000790	0.0000558	-0.0006560
34 H	1.0	0.0004508	-0.0004939	0.0006939
35 H	1.0	-0.0009640	-0.0008835	-0.0002156

MAXIMUM GRADIENT = 0.0021436 RMS GRADIENT = 0.0006494
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001232017
 PREDICTED ENERGY CHANGE WAS -0.0000838709 RATIO= 1.469
 GDIIS STEP HAS LENGTH = 0.179804
 RADIUS OF STEP TAKEN= 0.07344 CURRENT TRUST RADIUS= 0.07344

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 3463.5 SECONDS (57.7 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 3201.2 SECONDS (53.4 MIN)
 CPU UTILIZATION: STEP = 93.24% , TOTAL = 100.00%

INSERCH= 32

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1153052321	-1.7255843856	1.0288327429
C	6.0	4.9953639202	0.6833553646	0.4413178192
C	6.0	5.2239080665	-0.6768052214	0.2078720810
C	6.0	4.0973121993	-1.5513351983	0.0808330912
C	6.0	2.7781012880	-1.0712478013	0.1983160691
C	6.0	2.4799234480	0.3247781934	0.5024292713
C	6.0	3.6579333477	1.2040478944	0.5934650983
C	6.0	3.5083616436	2.6217199457	0.8203993475
C	6.0	2.2417900003	3.1921391784	0.9930187960
C	6.0	1.0873707019	2.3539629025	0.9617464433

C	6.0	1.1698049672	0.9647731737	0.7043032195
N	7.0	-0.0577293744	0.1703508726	0.7231346853
C	6.0	-1.2648514302	0.7093942334	0.5386803318
C	6.0	-2.5765576242	0.0553725814	0.5889095792
C	6.0	-2.8705133450	-1.3437240702	0.7431594677
C	6.0	-4.1766721438	-1.8663742827	0.7219030778
C	6.0	-5.2694101530	-0.9680254566	0.5289832174
C	6.0	-5.0381438019	0.4304398447	0.4005956574
C	6.0	-3.7163427863	0.9317637194	0.4425618430
O	8.0	-1.7645872161	-2.2799324664	0.9410186833
N	7.0	1.6934225934	-2.0791261539	-0.1031730283
H	1.0	5.8442460421	1.3865091338	0.5040591559
H	1.0	6.2482487964	-1.0698793681	0.0872608809
H	1.0	4.2836029567	-2.6171519388	-0.1560287478
H	1.0	4.4142592216	3.2519623001	0.8584833175
H	1.0	2.1279526073	4.2744199289	1.1768993608
H	1.0	0.1146375598	2.8270164767	1.1751247397
H	1.0	-1.3201690250	1.7857780735	0.2871371183
H	1.0	-4.3673959336	-2.9477589182	0.8582613828
H	1.0	-6.2962666862	-1.3726376299	0.4914635219
H	1.0	-5.8838972239	1.1260422074	0.2662627651
H	1.0	-3.5431761668	2.0232928885	0.3732119871
H	1.0	-2.0889148722	-3.2146927872	1.0022953860
H	1.0	1.3918994688	-1.9785348153	-1.0966872070
H	1.0	2.0971807217	-3.0332034194	-0.0231641550

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4738595	5.2793690	4.0970045
2 C	5.4738595	0.0000000	1.3988446 *	2.4352183 *
3 C	5.2793690	1.3988446 *	0.0000000	1.4318379 *
4 C	4.0970045	2.4352183 *	1.4318379 *	0.0000000
5 C	2.8650300 *	2.8379457 *	2.4774275 *	1.4087596 *
6 C	3.1737213	2.5416044 *	2.9358789 *	2.5126661 *
7 C	4.6176297	1.4432567 *	2.4776132 *	2.8368964 *
8 C	5.5186349	2.4722734 *	3.7680973	4.2788094
9 C	5.3579124	3.7657057	4.9475463	5.1745139
10 C	4.1942959	4.2818438	5.1831287	5.0087034
11 C	2.9078021 *	3.8449003	4.4019286	3.9102193
12 N	1.9282020 *	5.0868798	5.3739058	4.5432505
13 C	2.8415142 *	6.2610266	6.6434165	5.8372357
14 C	3.2575245	7.5993514	7.8440129	6.8833270
15 C	3.0236632	8.1284798	8.1394700	7.0023119

16 C	4.3052407	9.5239747	9.4894789	8.3047599
17 C	5.4606689	10.3971309	10.5022687	9.3955615
18 C	5.6214908	10.0367775	10.3234124	9.3534078
19 C	4.6996531	8.7152477	9.0868399	8.2066944
20 O	1.9618891 *	7.3978183	7.2073981	5.9693080
21 N	1.9740525 *	4.3394229	3.8115064	2.4680168 *
22 H	6.5407397	1.1040664 *	2.1748131 *	3.4441004
23 H	6.2393512	2.1837832 *	1.1037791 *	2.2041709 *
24 H	4.4241943	3.4288154	2.1866739 *	1.1075979 *
25 H	6.5792093	2.6663554 *	4.0637471	4.8761524
26 H	6.3303021	4.6539094	5.9193399	6.2465319
27 H	4.5549508	5.3810078	6.2703261	6.0190643
28 H	3.8652768	6.4128827	6.9925349	6.3661597
29 H	4.6494532	10.0508758	9.8779223	8.6142717
30 H	6.4437250	11.4773927	11.5446539	10.4032222
31 H	6.6860839	10.8896712	11.2533109	10.3357281
32 H	5.2790535	8.6433060	9.1749459	8.4404096
33 H	2.6602132 *	8.1053366	7.7813470	6.4718820
34 H	2.4922905 *	4.7366734	4.2521365	2.9813272 *
35 H	2.5969974 *	4.7358229	3.9220421	2.4914403 *

C C C C

1 CO	2.8650300 *	3.1737213	4.6176297	5.5186349
2 C	2.8379457 *	2.5416044 *	1.4432567 *	2.4722734 *
3 C	2.4774275 *	2.9358789 *	2.4776132 *	3.7680973
4 C	1.4087596 *	2.5126661 *	2.8368964 *	4.2788094
5 C	0.0000000	1.4595491 *	2.4712786 *	3.8155312
6 C	1.4595491 *	0.0000000	1.4727899 *	2.5366773 *
7 C	2.4712786 *	1.4727899 *	0.0000000	1.4434905 *
8 C	3.8155312	2.5366773 *	1.4434905 *	0.0000000
9 C	4.3698571	2.9187574 *	2.4733807 *	1.3997783 *
10 C	3.8953131	2.5035507 *	2.8400225 *	2.4398504 *
11 C	2.6434866 *	1.4719909 *	2.5020632 *	2.8684139 *
12 N	3.1398945	2.5519092 *	3.8589498	4.3284727
13 C	4.4308013	3.7646491	4.9478777	5.1497493
14 C	5.4858189	5.0643913	6.3394285	6.6080231
15 C	5.6813682	5.6097259	7.0095768	7.5113753
16 C	7.0196327	7.0113895	8.4157609	8.9001368
17 C	8.0549634	7.8564762	9.1880097	9.4879119
18 C	7.9617630	7.5194993	8.7325498	8.8329326
19 C	6.8006996	6.2262132	7.3808441	7.4293383
20 O	4.7590487	4.9992749	6.4546605	7.2003288
21 N	1.5110401 *	2.6007872 *	3.8889380	5.1229819
22 H	3.9414834	3.5278806	2.1957342 *	2.6612352 *
23 H	3.4719244	4.0395186	3.4837798	4.6553603

24 H	2.1867590 *	3.5130869	3.9439538	5.3851824
25 H	4.6693660	3.5265899	2.1991400 *	1.1042220 *
26 H	5.4732515	4.0222460	3.4797157	2.1826678 *
27 H	4.8212715	3.5083177	3.9404695	3.4183826
28 H	4.9966294	4.0769565	5.0213295	4.9292876
29 H	7.4172065	7.5974929	9.0395535	9.6461436
30 H	9.0841029	8.9388396	10.2827920	10.5921588
31 H	8.9366055	8.4054325	9.5477577	9.5267332
32 H	7.0402642	6.2593433	7.2509070	7.0909997
33 H	5.3785300	5.8010348	7.2607628	8.0886528
34 H	2.1027978 *	3.0076936	4.2568013	5.4145154
35 H	2.0885345 *	3.4203481	4.5574641	5.8890737

C C C N

1 CO	5.3579124	4.1942959	2.9078021 *	1.9282020 *
2 C	3.7657057	4.2818438	3.8449003	5.0868798
3 C	4.9475463	5.1831287	4.4019286	5.3739058
4 C	5.1745139	5.0087034	3.9102193	4.5432505
5 C	4.3698571	3.8953131	2.6434866 *	3.1398945
6 C	2.9187574 *	2.5035507 *	1.4719909 *	2.5519092 *
7 C	2.4733807 *	2.8400225 *	2.5020632 *	3.8589498
8 C	1.3997783 *	2.4398504 *	2.8684139 *	4.3284727
9 C	0.0000000	1.4269553 *	2.4887081 *	3.8068138
10 C	1.4269553 *	0.0000000	1.4152457 *	2.4771660 *
11 C	2.4887081 *	1.4152457 *	0.0000000	1.4622934 *
12 N	3.8068138	2.4771660 *	1.4622934 *	0.0000000
13 C	4.3205301	2.9011274 *	2.4536098 *	1.3348164 *
14 C	5.7635998	4.3413011	3.8568845	2.5250212 *
15 C	6.8390153	5.4208408	4.6534763	3.1944605
16 C	8.1767181	6.7512160	6.0498366	4.5949908
17 C	8.5988619	7.1855100	6.7253207	5.3380907
18 C	7.8086737	6.4449018	6.2382993	4.9976200
19 C	6.3962213	5.0366523	4.8932646	3.7475222
20 O	6.7821332	5.4412388	4.3811878	2.9941152 *
21 N	5.4118926	4.5993077	3.1924155	2.9680742 *
22 H	4.0591958	4.8757879	4.6976971	6.0299543
23 H	5.9191986	6.2547649	5.5055557	6.4581628
24 H	6.2639583	6.0147572	4.8234942	5.2335711
25 H	2.1774529 *	3.4474996	3.9725922	5.4326173
26 H	1.1036769 *	2.1948250 *	3.4778090	4.6718830
27 H	2.1659304 *	1.1025061 *	2.1915751 *	2.7003477 *
28 H	3.8940561	2.5640162 *	2.6548158 *	2.0960565 *
29 H	9.0220755	7.6074597	6.7817553	5.3210989
30 H	9.6946974	8.2841305	7.8263028	6.4306946
31 H	8.4156832	7.1126692	7.0691302	5.9216813

32 H	5.9343235	4.6794957	4.8417225	3.9628499
33 H	7.7332132	6.4109563	5.3081061	3.9575454
34 H	5.6413699	4.8062900	3.4577383	3.1671573
35 H	6.3093922	5.5687814	4.1680993	3.9323478

C C C C

1 CO	2.8415142 *	3.2575245	3.0236632	4.3052407
2 C	6.2610266	7.5993514	8.1284798	9.5239747
3 C	6.6434165	7.8440129	8.1394700	9.4894789
4 C	5.8372357	6.8833270	7.0023119	8.3047599
5 C	4.4308013	5.4858189	5.6813682	7.0196327
6 C	3.7646491	5.0643913	5.6097259	7.0113895
7 C	4.9478777	6.3394285	7.0095768	8.4157609
8 C	5.1497493	6.6080231	7.5113753	8.9001368
9 C	4.3205301	5.7635998	6.8390153	8.1767181
10 C	2.9011274 *	4.3413011	5.4208408	6.7512160
11 C	2.4536098 *	3.8568845	4.6534763	6.0498366
12 N	1.3348164 *	2.5250212 *	3.1944605	4.5949908
13 C	0.0000000	1.4665744 *	2.6144324 *	3.8918959
14 C	1.4665744 *	0.0000000	1.4379410 *	2.5042294 *
15 C	2.6144324 *	1.4379410 *	0.0000000	1.4070060 *
16 C	3.8918959	2.5042294 *	1.4070060 *	0.0000000
17 C	4.3416957	2.8813867 *	2.4375658 *	1.4276992 *
18 C	3.7861086	2.4971071 *	2.8219903 *	2.4740103 *
19 C	2.4634319 *	1.4451952 *	2.4461462 *	2.8494756 *
20 O	3.0573986	2.4973839 *	1.4624319 *	2.4570706 *
21 N	4.1157268	4.8236702	4.6996389	5.9316124
22 H	7.1413549	8.5257879	9.1355555	10.5379081
23 H	7.7340978	8.9103901	9.1464210	10.4745478
24 H	6.5064488	7.3999408	7.3219900	8.5387754
25 H	6.2305075	7.6917083	8.6140318	10.0010062
26 H	4.9626456	6.3465352	7.5323525	8.8127560
27 H	2.6062186 *	3.9074531	5.1471154	6.3756306
28 H	1.1067684 *	2.1596023 *	3.5221169	4.6569140
29 H	4.8065251	3.5069147	2.1970056 *	1.1065089 *
30 H	5.4453857	3.9855921	3.4351088	2.1885062 *
31 H	4.6457928	3.4912648	3.9252590	3.4751665
32 H	2.6352368 *	2.2030858 *	3.4534243	3.9563131
33 H	4.0363942	3.3319680	2.0441555 *	2.5010624 *
34 H	4.1179746	4.7672495	4.6857426	5.8590819
35 H	5.0622097	5.6354029	5.3027895	6.4247837

C C C O

1 CO	5.4606689	5.6214908	4.6996531	1.9618891 *
------	-----------	-----------	-----------	-------------

2 C	10.3971309	10.0367775	8.7152477	7.3978183
3 C	10.5022687	10.3234124	9.0868399	7.2073981
4 C	9.3955615	9.3534078	8.2066944	5.9693080
5 C	8.0549634	7.9617630	6.8006996	4.7590487
6 C	7.8564762	7.5194993	6.2262132	4.9992749
7 C	9.1880097	8.7325498	7.3808441	6.4546605
8 C	9.4879119	8.8329326	7.4293383	7.2003288
9 C	8.5988619	7.8086737	6.3962213	6.7821332
10 C	7.1855100	6.4449018	5.0366523	5.4412388
11 C	6.7253207	6.2382993	4.8932646	4.3811878
12 N	5.3380907	4.9976200	3.7475222	2.9941152 *
13 C	4.3416957	3.7861086	2.4634319 *	3.0573986
14 C	2.8813867 *	2.4971071 *	1.4451952 *	2.4973839 *
15 C	2.4375658 *	2.8219903 *	2.4461462 *	1.4624319 *
16 C	1.4276992 *	2.4740103 *	2.8494756 *	2.4570706 *
17 C	0.0000000	1.4232613 *	2.4553382 *	3.7649246
18 C	1.4232613 *	0.0000000	1.4143001 *	4.2841975
19 C	2.4553382 *	1.4143001 *	0.0000000	3.7911478
20 O	3.7649246	4.2841975	3.7911478	0.0000000
21 N	7.0792094	7.2017838	6.2152108	3.6178020
22 H	11.3603613	10.9247967	9.5715952	8.4574270
23 H	11.5265763	11.3899866	10.1698525	8.1485380
24 H	9.7184834	9.8230652	8.7722429	6.1561217
25 H	10.5683641	9.8751493	8.4654002	8.2937817
26 H	9.0897747	8.1689515	6.7726207	7.6267320
27 H	6.6187470	5.7353841	4.3364780	5.4467622
28 H	4.8206254	3.9589331	2.5485576 *	4.1418680
29 H	2.2003178 *	3.4744190	3.9556759	2.6883925 *
30 H	1.1043338 *	2.2005042 *	3.4595757	4.6434257
31 H	2.1981210 *	1.1032710 *	2.1833730 *	5.3874552
32 H	3.4571858	2.1846874 *	1.1073536 *	4.6907922
33 H	3.9226380	4.7272599	4.4894237	0.9913224 *
34 H	6.9308715	7.0278355	6.0772744	3.7691503
35 H	7.6704946	7.9428744	7.0522990	4.0509650

N H H H

1 CO	1.9740525 *	6.5407397	6.2393512	4.4241943
2 C	4.3394229	1.1040664 *	2.1837832 *	3.4288154
3 C	3.8115064	2.1748131 *	1.1037791 *	2.1866739 *
4 C	2.4680168 *	3.4441004	2.2041709 *	1.1075979 *
5 C	1.5110401 *	3.9414834	3.4719244	2.1867590 *
6 C	2.6007872 *	3.5278806	4.0395186	3.5130869
7 C	3.8889380	2.1957342 *	3.4837798	3.9439538
8 C	5.1229819	2.6612352 *	4.6553603	5.3851824
9 C	5.4118926	4.0591958	5.9191986	6.2639583

10 C	4.5993077	4.8757879	6.2547649	6.0147572
11 C	3.1924155	4.6976971	5.5055557	4.8234942
12 N	2.9680742 *	6.0299543	6.4581628	5.2335711
13 C	4.1157268	7.1413549	7.7340978	6.5064488
14 C	4.8236702	8.5257879	8.9103901	7.3999408
15 C	4.6996389	9.1355555	9.1464210	7.3219900
16 C	5.9316124	10.5379081	10.4745478	8.5387754
17 C	7.0792094	11.3603613	11.5265763	9.7184834
18 C	7.2017838	10.9247967	11.3899866	9.8230652
19 C	6.2152108	9.5715952	10.1698525	8.7722429
20 O	3.6178020	8.4574270	8.1485380	6.1561217
21 N	0.0000000	5.4413872	4.6691847	2.6459969 *
22 H	5.4413872	0.0000000	2.5240411 *	4.3474849
23 H	4.6691847	2.5240411 *	0.0000000	2.5125834 *
24 H	2.6459969 *	4.3474849	2.5125834 *	0.0000000
25 H	6.0620326	2.3770558 *	4.7577954	5.9575841
26 H	6.4957640	4.7543222	6.8356190	7.3428393
27 H	5.3100700	5.9459065	7.3478182	6.9850706
28 H	4.9164582	7.1788101	8.0917043	7.1403396
29 H	6.1977738	11.0990527	10.8079964	8.7165284
30 H	8.0428759	12.4501044	12.5546769	10.6724741
31 H	8.2356155	11.7334451	12.3305750	10.8428729
32 H	6.6692392	9.4099049	10.2723651	9.1144004
33 H	4.1009327	9.1844619	8.6571249	6.5044410
34 H	1.0431228 *	5.8059710	5.0805036	3.1071883
35 H	1.0390791 *	5.8182748	4.5932778	2.2296175 *

H H H H

1 CO	6.5792093	6.3303021	4.5549508	3.8652768
2 C	2.6663554 *	4.6539094	5.3810078	6.4128827
3 C	4.0637471	5.9193399	6.2703261	6.9925349
4 C	4.8761524	6.2465319	6.0190643	6.3661597
5 C	4.6693660	5.4732515	4.8212715	4.9966294
6 C	3.5265899	4.0222460	3.5083177	4.0769565
7 C	2.1991400 *	3.4797157	3.9404695	5.0213295
8 C	1.1042220 *	2.1826678 *	3.4183826	4.9292876
9 C	2.1774529 *	1.1036769 *	2.1659304 *	3.8940561
10 C	3.4474996	2.1948250 *	1.1025061 *	2.5640162 *
11 C	3.9725922	3.4778090	2.1915751 *	2.6548158 *
12 N	5.4326173	4.6718830	2.7003477 *	2.0960565 *
13 C	6.2305075	4.9626456	2.6062186 *	1.1067684 *
14 C	7.6917083	6.3465352	3.9074531	2.1596023 *
15 C	8.6140318	7.5323525	5.1471154	3.5221169
16 C	10.0010062	8.8127560	6.3756306	4.6569140
17 C	10.5683641	9.0897747	6.6187470	4.8206254

18 C	9.8751493	8.1689515	5.7353841	3.9589331
19 C	8.4654002	6.7726207	4.3364780	2.5485576 *
20 O	8.2937817	7.6267320	5.4467622	4.1418680
21 N	6.0620326	6.4957640	5.3100700	4.9164582
22 H	2.3770558 *	4.7543222	5.9459065	7.1788101
23 H	4.7577954	6.8356190	7.3478182	8.0917043
24 H	5.9575841	7.3428393	6.9850706	7.1403396
25 H	0.0000000	2.5246794 *	4.3321573	5.9464107
26 H	2.5246794 *	0.0000000	2.4796002 *	4.3444859
27 H	4.3321573	2.4796002 *	0.0000000	1.9827681 *
28 H	5.9464107	4.3444859	1.9827681 *	0.0000000
29 H	10.7496051	9.7185879	7.3169022	5.6584580
30 H	11.6720604	10.1649669	7.6944253	5.8973627
31 H	10.5319650	8.6562855	6.3009335	4.6112148
32 H	8.0663433	6.1542821	3.8299657	2.2373160 *
33 H	9.1722180	8.5964683	6.4333323	5.1095137
34 H	6.3494449	6.6940580	5.4667953	4.8415222
35 H	6.7564386	7.4055694	6.3014721	5.9158388

H H H H

1 CO	4.6494532	6.4437250	6.6860839	5.2790535
2 C	10.0508758	11.4773927	10.8896712	8.6433060
3 C	9.8779223	11.5446539	11.2533109	9.1749459
4 C	8.6142717	10.4032222	10.3357281	8.4404096
5 C	7.4172065	9.0841029	8.9366055	7.0402642
6 C	7.5974929	8.9388396	8.4054325	6.2593433
7 C	9.0395535	10.2827920	9.5477577	7.2509070
8 C	9.6461436	10.5921588	9.5267332	7.0909997
9 C	9.0220755	9.6946974	8.4156832	5.9343235
10 C	7.6074597	8.2841305	7.1126692	4.6794957
11 C	6.7817553	7.8263028	7.0691302	4.8417225
12 N	5.3210989	6.4306946	5.9216813	3.9628499
13 C	4.8065251	5.4453857	4.6457928	2.6352368 *
14 C	3.5069147	3.9855921	3.4912648	2.2030858 *
15 C	2.1970056 *	3.4351088	3.9252590	3.4534243
16 C	1.1065089 *	2.1885062 *	3.4751665	3.9563131
17 C	2.2003178 *	1.1043338 *	2.1981210 *	3.4571858
18 C	3.4744190	2.2005042 *	1.1032710 *	2.1846874 *
19 C	3.9556759	3.4595757	2.1833730 *	1.1073536 *
20 O	2.6883925 *	4.6434257	5.3874552	4.6907922
21 N	6.1977738	8.0428759	8.2356155	6.6692392
22 H	11.0990527	12.4501044	11.7334451	9.4099049
23 H	10.8079964	12.5546769	12.3305750	10.2723651
24 H	8.7165284	10.6724741	10.8428729	9.1144004
25 H	10.7496051	11.6720604	10.5319650	8.0663433

26 H	9.7185879	10.1649669	8.6562855	6.1542821
27 H	7.3169022	7.6944253	6.3009335	3.8299657
28 H	5.6584580	5.8973627	4.6112148	2.2373160 *
29 H	0.0000000	2.5171591 *	4.3870371	5.0622097
30 H	2.5171591 *	0.0000000	2.5424722 *	4.3733094
31 H	4.3870371	2.5424722 *	0.0000000	2.5090779 *
32 H	5.0622097	4.3733094	2.5090779 *	0.0000000
33 H	2.2985812 *	4.6212472	5.8125395	5.4723958
34 H	6.1587907	7.8738322	8.0270324	6.5215182
35 H	6.5249493	8.5715973	9.0044821	7.5854397

H H H

1 CO	2.6602132 *	2.4922905 *	2.5969974 *
2 C	8.1053366	4.7366734	4.7358229
3 C	7.7813470	4.2521365	3.9220421
4 C	6.4718820	2.9813272 *	2.4914403 *
5 C	5.3785300	2.1027978 *	2.0885345 *
6 C	5.8010348	3.0076936	3.4203481
7 C	7.2607628	4.2568013	4.5574641
8 C	8.0886528	5.4145154	5.8890737
9 C	7.7332132	5.6413699	6.3093922
10 C	6.4109563	4.8062900	5.5687814
11 C	5.3081061	3.4577383	4.1680993
12 N	3.9575454	3.1671573	3.9323478
13 C	4.0363942	4.1179746	5.0622097
14 C	3.3319680	4.7672495	5.6354029
15 C	2.0441555 *	4.6857426	5.3027895
16 C	2.5010624 *	5.8590819	6.4247837
17 C	3.9226380	6.9308715	7.6704946
18 C	4.7272599	7.0278355	7.9428744
19 C	4.4894237	6.0772744	7.0522990
20 O	0.9913224 *	3.7691503	4.0509650
21 N	4.1009327	1.0431228 *	1.0390791 *
22 H	9.1844619	5.8059710	5.8182748
23 H	8.6571249	5.0805036	4.5932778
24 H	6.5044410	3.1071883	2.2296175 *
25 H	9.1722180	6.3494449	6.7564386
26 H	8.5964683	6.6940580	7.4055694
27 H	6.4333323	5.4667953	6.3014721
28 H	5.1095137	4.8415222	5.9158388
29 H	2.2985812 *	6.1587907	6.5249493
30 H	4.6212472	7.8738322	8.5715973
31 H	5.8125395	8.0270324	9.0044821
32 H	5.4723958	6.5215182	7.5854397
33 H	0.0000000	4.2485154	4.3136877

34 H	4.2485154	0.0000000	1.6619865 *
35 H	4.3136877	1.6619865 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.76, TOTAL = 3464.3 SECONDS (57.7 MIN)
 WALL CLOCK TIME: STEP = 0.76, TOTAL = 3201.9 SECONDS (53.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.94, TOTAL = 3465.2 SECONDS (57.8 MIN)
 WALL CLOCK TIME: STEP = 0.94, TOTAL = 3202.9 SECONDS (53.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
INTEGRALS	SKIPPED				

-----START SECOND ORDER SCF-----

1	0	-284.632966373	-284.632966373	0.017115839	0.000982061	196282323
11466854						
2	1	-284.633102541	-0.000136168	0.007253479	0.000125779	160017068
14546275						
3	2	-284.633101911	0.000000630	0.001812055	0.000204026	146233693
15651854						
4	3	-284.633105272	-0.000003361	0.002198200	0.000114750	138091987
16293656						
5	4	-284.633104844	0.000000428	0.000627920	0.000203069	134682955
16592042						
6	5	-284.633105646	-0.000000802	0.000378959	0.000041753	128070507
17093536						
7	6	-284.633105709	-0.000000062	0.000403359	0.000043665	121291075
17642525						
8	7	-284.633105854	-0.000000145	0.000994152	0.000038166	140704727
16265882						
9	8	-284.633106012	-0.000000158	0.000532172	0.000043284	168070170
14062281						
10	9	-284.633106116	-0.000000104	0.000428613	0.000044578	165642061
14184142						

11 10	-284.633106201	-0.000000085	0.000729850	0.000030077	163510553
14360510					
-----DISABLING FDIFF OPTION-----					
12 11	-284.633106313	-0.000000112	0.000505890	0.000014110	196296819
11465458					
13 12	-284.633106343	-0.000000030	0.000209416	0.000011290	196296545
11465467					
14 13	-284.633106348	-0.000000005	0.000077324	0.000012651	196296728
11465467					
15 14	-284.633106355	-0.000000008	0.000087139	0.000009659	196296715
11465466					
16 15	-284.633106360	-0.000000004	0.000126697	0.000007638	196296567
11465469					
17 16	-284.633106367	-0.000000007	0.000265177	0.000007658	196296612
11465467					
18 17	-284.633106375	-0.000000008	0.000197466	0.000006157	196296564
11465464					
19 18	-284.633106380	-0.000000005	0.000072126	0.000005710	196296706
11465463					
20 19	-284.633106384	-0.000000004	0.000113886	0.000004064	196296733
11465461					
21 20	-284.633106387	-0.000000003	0.000038960	0.000003154	196296793
11465460					
22 21	-284.633106389	-0.000000001	0.000017055	0.000002297	196296760
11465463					
23 22	-284.633106389	0.000000000	0.000013393	0.000001509	196296785
11465459					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 76.9 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 24.8 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 3.5 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6331063890 AFTER 23 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6024645654
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000281876

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 81.63 , TOTAL = 3546.9 SECONDS (59.1 MIN)
WALL CLOCK TIME: STEP = 74.90 , TOTAL = 3277.8 SECONDS (54.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.69 , TOTAL = 3550.6 SECONDS (59.2 MIN)
WALL CLOCK TIME: STEP = 3.66 , TOTAL = 3281.4 SECONDS (54.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.90 , TOTAL = 3553.5 SECONDS (59.2 MIN)
WALL CLOCK TIME: STEP = 2.72 , TOTAL = 3284.1 SECONDS (54.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 32 ENERGY= -284.6331064

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0004836	0.0005960	-0.0002666
2 C	6.0	-0.0000866	0.0003635	0.0002535
3 C	6.0	0.0007036	0.0003822	0.0001151
4 C	6.0	-0.0003474	-0.0002072	0.0003073
5 C	6.0	-0.0007012	-0.0011467	0.0003898
6 C	6.0	-0.0001782	-0.0004356	0.0006738
7 C	6.0	0.0009433	-0.0007206	0.0003168
8 C	6.0	0.0006179	0.0008736	0.0000048
9 C	6.0	-0.0003445	-0.0006008	-0.0002214
10 C	6.0	0.0008120	0.0004375	-0.0000315

11 C	6.0	-0.0001326	-0.0001596	0.0002343
12 N	7.0	-0.0000551	0.0004053	-0.0001977
13 C	6.0	-0.0006722	-0.0004435	0.0000198
14 C	6.0	-0.0000708	-0.0001381	0.0000305
15 C	6.0	-0.0005452	-0.0000171	-0.0007483
16 C	6.0	-0.0004120	-0.0017868	-0.0001728
17 C	6.0	0.0002325	0.0005919	-0.0006304
18 C	6.0	-0.0001567	-0.0002066	-0.0002064
19 C	6.0	-0.0005079	0.0002278	0.0006624
20 O	8.0	-0.0004036	0.0000229	-0.0003167
21 N	7.0	0.0003258	-0.0001043	0.0000977
22 H	1.0	-0.0001985	-0.0006518	-0.0005710
23 H	1.0	-0.0000011	0.0006707	-0.0006190
24 H	1.0	0.0011004	0.0004801	-0.0000411
25 H	1.0	-0.0006856	0.0002516	-0.0003961
26 H	1.0	0.0001953	-0.0002673	-0.0003763
27 H	1.0	0.0004070	0.0001655	-0.0005489
28 H	1.0	-0.0001605	0.0001937	-0.0001728
29 H	1.0	-0.0002707	0.0002481	0.0007636
30 H	1.0	0.0007252	-0.0000881	-0.0001981
31 H	1.0	0.0007472	-0.0001650	-0.0004538
32 H	1.0	-0.0001738	0.0012643	0.0020491
33 H	1.0	0.0003301	-0.0001785	-0.0008485
34 H	1.0	0.0003859	-0.0004379	0.0010984
35 H	1.0	-0.0009385	0.0005811	0.0000005

MAXIMUM GRADIENT = 0.0020491 RMS GRADIENT = 0.0005508
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001660051
 PREDICTED ENERGY CHANGE WAS -0.0004505786 RATIO= 0.368
 GDIIS STEP HAS LENGTH = 0.152982
 RADIUS OF STEP TAKEN= 0.07344 CURRENT TRUST RADIUS= 0.07344

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 3553.5 SECONDS (59.2 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 3284.2 SECONDS (54.7
 MIN)
 CPU UTILIZATION: STEP = 91.62%, TOTAL = 100.00%

INSERCH= 33

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1169958944	-1.7319548897	1.0264081847

C	6.0	4.9937072843	0.6817829002	0.4423889146
C	6.0	5.2225495267	-0.6789308424	0.2093626274
C	6.0	4.0949201564	-1.5507182342	0.0799804215
C	6.0	2.7765235754	-1.0683941032	0.1930009627
C	6.0	2.4780292753	0.3264361823	0.5001578012
C	6.0	3.6551643508	1.2041310926	0.5934024300
C	6.0	3.5041707394	2.6201187220	0.8207820837
C	6.0	2.2378514423	3.1918275350	0.9945129555
C	6.0	1.0830085472	2.3536102389	0.9656399703
C	6.0	1.1684507078	0.9647628720	0.7057237755
N	7.0	-0.0551305001	0.1657561881	0.7250358018
C	6.0	-1.2613639990	0.7064339659	0.5394254575
C	6.0	-2.5735163105	0.0540866812	0.5873829622
C	6.0	-2.8680693451	-1.3445059874	0.7458489543
C	6.0	-4.1747989776	-1.8636135701	0.7253704362
C	6.0	-5.2669223092	-0.9648059024	0.5317420444
C	6.0	-5.0343470809	0.4322896108	0.3972460703
C	6.0	-3.7123713301	0.9314959133	0.4351174915
O	8.0	-1.7641833361	-2.2816694140	0.9512088161
N	7.0	1.6927316631	-2.0762881520	-0.1103833741
H	1.0	5.8406708002	1.3871589983	0.5051069225
H	1.0	6.2474732793	-1.0731965321	0.0899189093
H	1.0	4.2794238091	-2.6173445020	-0.1524661820
H	1.0	4.4100328655	3.2507929503	0.8589780175
H	1.0	2.1235316810	4.2739369927	1.1782055737
H	1.0	0.1104897071	2.8266911187	1.1812928823
H	1.0	-1.3131794065	1.7819735561	0.2892376168
H	1.0	-4.3665480601	-2.9439715975	0.8633703158
H	1.0	-6.2937474358	-1.3692685107	0.4989343956
H	1.0	-5.8812906032	1.1286107387	0.2617433117
H	1.0	-3.5379194270	2.0213629124	0.3579411454
H	1.0	-2.0875730084	-3.2173357227	1.0061611496
H	1.0	1.3876144686	-1.9732004361	-1.1025951137
H	1.0	2.1036183556	-3.0269557727	-0.0322967318

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4726157	5.2766562	4.0929761
2 C	5.4726157	0.0000000	1.3993613 *	2.4337665 *
3 C	5.2766562	1.3993613 *	0.0000000	1.4311887 *
4 C	4.0929761	2.4337665 *	1.4311887 *	0.0000000
5 C	2.8649551 *	2.8357041 *	2.4768917 *	1.4083962 *
6 C	3.1762229	2.5413076 *	2.9372974 *	2.5128856 *

7 C	4.6180874	1.4447664 *	2.4799405 *	2.8365793 *
8 C	5.5186756	2.4736706 *	3.7696668	4.2771080
9 C	5.3612199	3.7682763	4.9505206	5.1746318
10 C	4.1986564	4.2851328	5.1869124	5.0099686
11 C	2.9121611 *	3.8447381	4.4027061	3.9094019
12 N	1.9291864 *	5.0830046	5.3696668	4.5371027
13 C	2.8430210 *	6.2558725	6.6384721	5.8305751
14 C	3.2590710	7.5945967	7.8395699	6.8775651
15 C	3.0231514	8.1243748	8.1356574	6.9977945
16 C	4.3043537	9.5194868	9.4857734	8.3007642
17 C	5.4607497	10.3922932	10.4983176	9.3910317
18 C	5.6228226	10.0312591	10.3186258	9.3475397
19 C	4.7018771	8.7096621	9.0816986	8.2000799
20 O	1.9612945 *	7.3966231	7.2064931	5.9684523
21 N	1.9732723 *	4.3369290	3.8097847	2.4663681 *
22 H	6.5391957	1.1040091 *	2.1767558 *	3.4437625
23 H	6.2364836	2.1854329 *	1.1046180 *	2.2049061 *
24 H	4.4158199	3.4275786	2.1858302 *	1.1071425 *
25 H	6.5792078	2.6672148 *	4.0650846	4.8744890
26 H	6.3340323	4.6564907	5.9222857	6.2465254
27 H	4.5612811	5.3844614	6.2743278	6.0208212
28 H	3.8647788	6.4039593	6.9841380	6.3559550
29 H	4.6473360	10.0467757	9.8746609	8.6111149
30 H	6.4426237	11.4724297	11.5406028	10.3986951
31 H	6.6893190	10.8856726	11.2501207	10.3313418
32 H	5.2813491	8.6365653	9.1683956	8.4319195
33 H	2.6583623 *	8.1034249	7.7792210	6.4698258
34 H	2.4910492 *	4.7370685	4.2547731	2.9843727 *
35 H	2.5970276 *	4.7257468	3.9114386	2.4813638 *

C C C C

1 CO	2.8649551 *	3.1762229	4.6180874	5.5186756
2 C	2.8357041 *	2.5413076 *	1.4447664 *	2.4736706 *
3 C	2.4768917 *	2.9372974 *	2.4799405 *	3.7696668
4 C	1.4083962 *	2.5128856 *	2.8365793 *	4.2771080
5 C	0.0000000	1.4591078 *	2.4691500 *	3.8116540
6 C	1.4591078 *	0.0000000	1.4712885 *	2.5331297 *
7 C	2.4691500 *	1.4712885 *	0.0000000	1.4420546 *
8 C	3.8116540	2.5331297 *	1.4420546 *	0.0000000
9 C	4.3683037	2.9176257 *	2.4739852 *	1.4002135 *
10 C	3.8955202	2.5044343 *	2.8418038 *	2.4400895 *
11 C	2.6424440 *	1.4712968 *	2.5007315 *	2.8651404 *
12 N	3.1343983	2.5481928 *	3.8551054	4.3245448
13 C	4.4243147	3.7588565	4.9419497	5.1431189
14 C	5.4807323	5.0596339	6.3339641	6.6013086

15	C	5.6783191	5.6065303	7.0050959	7.5052853
16	C	7.0168851	7.0076503	8.4105171	8.8926675
17	C	8.0512420	7.8519156	9.1821414	9.4798366
18	C	7.9563477	7.5138269	8.7259283	8.8245264
19	C	6.7944049	6.2202401	7.3742773	7.4215001
20	O	4.7607705	5.0002030	6.4535386	7.1972281
21	N	1.5107936 *	2.6004879 *	3.8868505	5.1190447
22	H	3.9390544	3.5259772	2.1949337 *	2.6606527 *
23	H	3.4724834	4.0417788	3.4870879	4.6583739
24	H	2.1857045 *	3.5123760	3.9433102	5.3832379
25	H	4.6655391	3.5232446	2.1975399 *	1.1044433 *
26	H	5.4715197	4.0209675	3.4801726	2.1838110 *
27	H	4.8224627	3.5100518	3.9424655	3.4190220
28	H	4.9859330	4.0664898	5.0110735	4.9185251
29	H	7.4155686	7.5944538	9.0347943	9.6389382
30	H	9.0804150	8.9341750	10.2767775	10.5838555
31	H	8.9324858	8.4011044	9.5425193	9.5196641
32	H	7.0317846	6.2517710	7.2431874	7.0826382
33	H	5.3794623	5.8016448	7.2593919	8.0856563
34	H	2.1038803 *	3.0076818	4.2560105	5.4108938
35	H	2.0831525 *	3.4159814	4.5498231	5.8803691

C C C N

1	CO	5.3612199	4.1986564	2.9121611 *	1.9291864 *
2	C	3.7682763	4.2851328	3.8447381	5.0830046
3	C	4.9505206	5.1869124	4.4027061	5.3696668
4	C	5.1746318	5.0099686	3.9094019	4.5371027
5	C	4.3683037	3.8955202	2.6424440 *	3.1343983
6	C	2.9176257 *	2.5044343 *	1.4712968 *	2.5481928 *
7	C	2.4739852 *	2.8418038 *	2.5007315 *	3.8551054
8	C	1.4002135 *	2.4400895 *	2.8651404 *	4.3245448
9	C	0.0000000	1.4272715 *	2.4873347 *	3.8062438
10	C	1.4272715 *	0.0000000	1.4155401 *	2.4778935 *
11	C	2.4873347 *	1.4155401 *	0.0000000	1.4614840 *
12	N	3.8062438	2.4778935 *	1.4614840 *	0.0000000
13	C	4.3161087	2.8967104 *	2.4491608 *	1.3348344 *
14	C	5.7585095	4.3360190	3.8530057	2.5246159 *
15	C	6.8345141	5.4162153	4.6505727	3.1927966
16	C	8.1701902	6.7444233	6.0456940	4.5923861
17	C	8.5914718	7.1778670	6.7206794	5.3365070
18	C	7.8010671	6.4371255	6.2332485	4.9971076
19	C	6.3896145	5.0298640	4.8884311	3.7477754
20	O	6.7806583	5.4399014	4.3817722	2.9936446 *
21	N	5.4102675	4.5993030	3.1920045	2.9630576 *
22	H	4.0591445	4.8766247	4.6955624	6.0250034

23 H	5.9233258	6.2595198	5.5071739	6.4545481
24 H	6.2633903	6.0147837	4.8214248	5.2253249
25 H	2.1772043 *	3.4475215	3.9695435	5.4289111
26 H	1.1035275 *	2.1944310 *	3.4765000	4.6721602
27 H	2.1665362 *	1.1027713 *	2.1936782 *	2.7048429 *
28 H	3.8852184	2.5546047 *	2.6457101 *	2.0939832 *
29 H	9.0157264	7.6008223	6.7778514	5.3176936
30 H	9.6869693	8.2761204	7.8214363	6.4286674
31 H	8.4091785	7.1061633	7.0656081	5.9233327
32 H	5.9274565	4.6725434	4.8360393	3.9633135
33 H	7.7321928	6.4101223	5.3086629	3.9566608
34 H	5.6389963	4.8053795	3.4568307	3.1617848
35 H	6.3044129	5.5666878	4.1656969	3.9277422

C C C C

1 CO	2.8430210 *	3.2590710	3.0231514	4.3043537
2 C	6.2558725	7.5945967	8.1243748	9.5194868
3 C	6.6384721	7.8395699	8.1356574	9.4857734
4 C	5.8305751	6.8775651	6.9977945	8.3007642
5 C	4.4243147	5.4807323	5.6783191	7.0168851
6 C	3.7588565	5.0596339	5.6065303	7.0076503
7 C	4.9419497	6.3339641	7.0050959	8.4105171
8 C	5.1431189	6.6013086	7.5052853	8.8926675
9 C	4.3161087	5.7585095	6.8345141	8.1701902
10 C	2.8967104 *	4.3360190	5.4162153	6.7444233
11 C	2.4491608 *	3.8530057	4.6505727	6.0456940
12 N	1.3348344 *	2.5246159 *	3.1927966	4.5923861
13 C	0.0000000	1.4661516 *	2.6135163 *	3.8894502
14 C	1.4661516 *	0.0000000	1.4380314 *	2.5021433 *
15 C	2.6135163 *	1.4380314 *	0.0000000	1.4062128 *
16 C	3.8894502	2.5021433 *	1.4062128 *	0.0000000
17 C	4.3402303	2.8802212 *	2.4381365 *	1.4276136 *
18 C	3.7856005	2.4969737 *	2.8233466 *	2.4733904 *
19 C	2.4635280 *	1.4456910 *	2.4473628 *	2.8479331 *
20 O	3.0579658	2.4986288 *	1.4625362 *	2.4569985 *
21 N	4.1100456	4.8193616	4.6978234	5.9305675
22 H	7.1346663	8.5195303	9.1302851	10.5321258
23 H	7.7299274	8.9066321	9.1431379	10.4715002
24 H	6.4981957	7.3923413	7.3153090	8.5330294
25 H	6.2241962	7.6852231	8.6081556	9.9937152
26 H	4.9590964	6.3418032	7.5279423	8.8058819
27 H	2.6056605 *	3.9043505	5.1439587	6.3694994
28 H	1.1054701 *	2.1593825 *	3.5215126	4.6550385
29 H	4.8033914	3.5042097	2.1948895 *	1.1058866 *
30 H	5.4438096	3.9842042	3.4346543	2.1875998 *

31 H	4.6474791	3.4931381	3.9281251	3.4756971
32 H	2.6352759 *	2.2029282 *	3.4537292	3.9539426
33 H	4.0368840	3.3337247	2.0455875 *	2.5035813 *
34 H	4.1102018	4.7598819	4.6821840	5.8561003
35 H	5.0584752	5.6349281	5.3060180	6.4300816

C C C O

1 CO	5.4607497	5.6228226	4.7018771	1.9612945 *
2 C	10.3922932	10.0312591	8.7096621	7.3966231
3 C	10.4983176	10.3186258	9.0816986	7.2064931
4 C	9.3910317	9.3475397	8.2000799	5.9684523
5 C	8.0512420	7.9563477	6.7944049	4.7607705
6 C	7.8519156	7.5138269	6.2202401	5.0002030
7 C	9.1821414	8.7259283	7.3742773	6.4535386
8 C	9.4798366	8.8245264	7.4215001	7.1972281
9 C	8.5914718	7.8010671	6.3896145	6.7806583
10 C	7.1778670	6.4371255	5.0298640	5.4399014
11 C	6.7206794	6.2332485	4.8884311	4.3817722
12 N	5.3365070	4.9971076	3.7477754	2.9936446 *
13 C	4.3402303	3.7856005	2.4635280 *	3.0579658
14 C	2.8802212 *	2.4969737 *	1.4456910 *	2.4986288 *
15 C	2.4381365 *	2.8233466 *	2.4473628 *	1.4625362 *
16 C	1.4276136 *	2.4733904 *	2.8479331 *	2.4569985 *
17 C	0.0000000	1.4226933 *	2.4539612 *	3.7655361
18 C	1.4226933 *	0.0000000	1.4135986 *	4.2856061
19 C	2.4539612 *	1.4135986 *	0.0000000	3.7929168
20 O	3.7655361	4.2856061	3.7929168	0.0000000
21 N	7.0770404	7.1975161	6.2096276	3.6220741
22 H	11.3539012	10.9173909	9.5641592	8.4553601
23 H	11.5233789	11.3859742	10.1654542	8.1479365
24 H	9.7124533	9.8157414	8.7640352	6.1527200
25 H	10.5603891	9.8667862	8.4576738	8.2908137
26 H	9.0819135	8.1610894	6.7662291	7.6250791
27 H	6.6116508	5.7286328	4.3316058	5.4463460
28 H	4.8203411	3.9598487	2.5496500 *	4.1418359
29 H	2.1994881 *	3.4730919	3.9535549	2.6867568 *
30 H	1.1040997 *	2.2004639 *	3.4584812	4.6426262
31 H	2.1983496 *	1.1047794 *	2.1847480 *	5.3903567
32 H	3.4549764	2.1831158 *	1.1064356 *	4.6919285
33 H	3.9252040	4.7301184	4.4920891	0.9914999 *
34 H	6.9260939	7.0197932	6.0672627	3.7745322
35 H	7.6743385	7.9436412	7.0507838	4.0598799

N H H H

1 CO	1.9732723 *	6.5391957	6.2364836	4.4158199
2 C	4.3369290	1.1040091 *	2.1854329 *	3.4275786
3 C	3.8097847	2.1767558 *	1.1046180 *	2.1858302 *
4 C	2.4663681 *	3.4437625	2.2049061 *	1.1071425 *
5 C	1.5107936 *	3.9390544	3.4724834	2.1857045 *
6 C	2.6004879 *	3.5259772	4.0417788	3.5123760
7 C	3.8868505	2.1949337 *	3.4870879	3.9433102
8 C	5.1190447	2.6606527 *	4.6583739	5.3832379
9 C	5.4102675	4.0591445	5.9233258	6.2633903
10 C	4.5993030	4.8766247	6.2595198	6.0147837
11 C	3.1920045	4.6955624	5.5071739	4.8214248
12 N	2.9630576 *	6.0250034	6.4545481	5.2253249
13 C	4.1100456	7.1346663	7.7299274	6.4981957
14 C	4.8193616	8.5195303	8.9066321	7.3923413
15 C	4.6978234	9.1302851	9.1431379	7.3153090
16 C	5.9305675	10.5321258	10.4715002	8.5330294
17 C	7.0770404	11.3539012	11.5233789	9.7124533
18 C	7.1975161	10.9173909	11.3859742	9.8157414
19 C	6.2096276	9.5641592	10.1654542	8.7640352
20 O	3.6220741	8.4553601	8.1479365	6.1527200
21 N	0.0000000	5.4387217	4.6681886	2.6430076 *
22 H	5.4387217	0.0000000	2.5280860 *	4.3480965
23 H	4.6681886	2.5280860 *	0.0000000	2.5132374 *
24 H	2.6430076 *	4.3480965	2.5132374 *	0.0000000
25 H	6.0581499	2.3759380 *	4.7607273	5.9560990
26 H	6.4939518	4.7543319	6.8398172	7.3422285
27 H	5.3114144	5.9468021	7.3527402	6.9854455
28 H	4.9072784	7.1679879	8.0842559	7.1292575
29 H	6.1980595	11.0938885	10.8053448	8.7115692
30 H	8.0408329	12.4435540	12.5513812	10.6664880
31 H	8.2325979	11.7273378	12.3281950	10.8371522
32 H	6.6610647	9.4011609	10.2665498	9.1043384
33 H	4.1035795	9.1820192	8.6550465	6.4993119
34 H	1.0431719 *	5.8057241	5.0843214	3.1113065
35 H	1.0386021 *	5.8085087	4.5829734	2.2172847 *

H H H H

1 CO	6.5792078	6.3340323	4.5612811	3.8647788
2 C	2.6672148 *	4.6564907	5.3844614	6.4039593
3 C	4.0650846	5.9222857	6.2743278	6.9841380
4 C	4.8744890	6.2465254	6.0208212	6.3559550
5 C	4.6655391	5.4715197	4.8224627	4.9859330
6 C	3.5232446	4.0209675	3.5100518	4.0664898
7 C	2.1975399 *	3.4801726	3.9424655	5.0110735
8 C	1.1044433 *	2.1838110 *	3.4190220	4.9185251

9 C	2.1772043 *	1.1035275 *	2.1665362 *	3.8852184
10 C	3.4475215	2.1944310 *	1.1027713 *	2.5546047 *
11 C	3.9695435	3.4765000	2.1936782 *	2.6457101 *
12 N	5.4289111	4.6721602	2.7048429 *	2.0939832 *
13 C	6.2241962	4.9590964	2.6056605 *	1.1054701 *
14 C	7.6852231	6.3418032	3.9043505	2.1593825 *
15 C	8.6081556	7.5279423	5.1439587	3.5215126
16 C	9.9937152	8.8058819	6.3694994	4.6550385
17 C	10.5603891	9.0819135	6.6116508	4.8203411
18 C	9.8667862	8.1610894	5.7286328	3.9598487
19 C	8.4576738	6.7662291	4.3316058	2.5496500 *
20 O	8.2908137	7.6250791	5.4463460	4.1418359
21 N	6.0581499	6.4939518	5.3114144	4.9072784
22 H	2.3759380 *	4.7543319	5.9468021	7.1679879
23 H	4.7607273	6.8398172	7.3527402	8.0842559
24 H	5.9560990	7.3422285	6.9854455	7.1292575
25 H	0.0000000	2.5252362 *	4.3324151	5.9360924
26 H	2.5252362 *	0.0000000	2.4792878 *	4.3371798
27 H	4.3324151	2.4792878 *	0.0000000	1.9783910 *
28 H	5.9360924	4.3371798	1.9783910 *	0.0000000
29 H	10.7426021	9.7117692	7.3106423	5.6557268
30 H	11.6638549	10.1566611	7.6867382	5.8974874
31 H	10.5248128	8.6492867	6.2952744	4.6146808
32 H	8.0580694	6.1480853	3.8258791	2.2386370 *
33 H	9.1693639	8.5954737	6.4336934	5.1094773
34 H	6.3460924	6.6910651	5.4668227	4.8304055
35 H	6.7471511	7.4005910	6.3016302	5.9079347

H H H H

1 CO	4.6473360	6.4426237	6.6893190	5.2813491
2 C	10.0467757	11.4724297	10.8856726	8.6365653
3 C	9.8746609	11.5406028	11.2501207	9.1683956
4 C	8.6111149	10.3986951	10.3313418	8.4319195
5 C	7.4155686	9.0804150	8.9324858	7.0317846
6 C	7.5944538	8.9341750	8.4011044	6.2517710
7 C	9.0347943	10.2767775	9.5425193	7.2431874
8 C	9.6389382	10.5838555	9.5196641	7.0826382
9 C	9.0157264	9.6869693	8.4091785	5.9274565
10 C	7.6008223	8.2761204	7.1061633	4.6725434
11 C	6.7778514	7.8214363	7.0656081	4.8360393
12 N	5.3176936	6.4286674	5.9233327	3.9633135
13 C	4.8033914	5.4438096	4.6474791	2.6352759 *
14 C	3.5042097	3.9842042	3.4931381	2.2029282 *
15 C	2.1948895 *	3.4346543	3.9281251	3.4537292
16 C	1.1058866 *	2.1875998 *	3.4756971	3.9539426

17 C	2.1994881 *	1.1040997 *	2.1983496 *	3.4549764
18 C	3.4730919	2.2004639 *	1.1047794 *	2.1831158 *
19 C	3.9535549	3.4584812	2.1847480 *	1.1064356 *
20 O	2.6867568 *	4.6426262	5.3903567	4.6919285
21 N	6.1980595	8.0408329	8.2325979	6.6610647
22 H	11.0938885	12.4435540	11.7273378	9.4011609
23 H	10.8053448	12.5513812	12.3281950	10.2665498
24 H	8.7115692	10.6664880	10.8371522	9.1043384
25 H	10.7426021	11.6638549	10.5248128	8.0580694
26 H	9.7117692	10.1566611	8.6492867	6.1480853
27 H	7.3106423	7.6867382	6.2952744	3.8258791
28 H	5.6557268	5.8974874	4.6146808	2.2386370 *
29 H	0.0000000	2.5152735 *	4.3866077	5.0593113
30 H	2.5152735 *	0.0000000	2.5427900 *	4.3715957
31 H	4.3866077	2.5427900 *	0.0000000	2.5095117 *
32 H	5.0593113	4.3715957	2.5095117 *	0.0000000
33 H	2.2997488 *	4.6221786	5.8166745	5.4742723
34 H	6.1577433	7.8697491	8.0199522	6.5077328
35 H	6.5323931	8.5758898	9.0063291	7.5805511

H H H

1 CO	2.6583623 *	2.4910492 *	2.5970276 *
2 C	8.1034249	4.7370685	4.7257468
3 C	7.7792210	4.2547731	3.9114386
4 C	6.4698258	2.9843727 *	2.4813638 *
5 C	5.3794623	2.1038803 *	2.0831525 *
6 C	5.8016448	3.0076818	3.4159814
7 C	7.2593919	4.2560105	4.5498231
8 C	8.0856563	5.4108938	5.8803691
9 C	7.7321928	5.6389963	6.3044129
10 C	6.4101223	4.8053795	5.5666878
11 C	5.3086629	3.4568307	4.1656969
12 N	3.9566608	3.1617848	3.9277422
13 C	4.0368840	4.1102018	5.0584752
14 C	3.3337247	4.7598819	5.6349281
15 C	2.0455875 *	4.6821840	5.3060180
16 C	2.5035813 *	5.8561003	6.4300816
17 C	3.9252040	6.9260939	7.6743385
18 C	4.7301184	7.0197932	7.9436412
19 C	4.4920891	6.0672627	7.0507838
20 O	0.9914999 *	3.7745322	4.0598799
21 N	4.1035795	1.0431719 *	1.0386021 *
22 H	9.1820192	5.8057241	5.8085087
23 H	8.6550465	5.0843214	4.5829734
24 H	6.4993119	3.1113065	2.2172847 *

25 H	9.1693639	6.3460924	6.7471511
26 H	8.5954737	6.6910651	7.4005910
27 H	6.4336934	5.4668227	6.3016302
28 H	5.1094773	4.8304055	5.9079347
29 H	2.2997488 *	6.1577433	6.5323931
30 H	4.6221786	7.8697491	8.5758898
31 H	5.8166745	8.0199522	9.0063291
32 H	5.4742723	6.5077328	7.5805511
33 H	0.0000000	4.2510768	4.3221204
34 H	4.2510768	0.0000000	1.6639112 *
35 H	4.3221204	1.6639112 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.76 , TOTAL = 3554.2 SECONDS (59.2 MIN)
WALL CLOCK TIME: STEP = 0.75 , TOTAL = 3284.9 SECONDS (54.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.91 , TOTAL = 3555.1 SECONDS (59.3 MIN)
WALL CLOCK TIME: STEP = 0.91 , TOTAL = 3285.8 SECONDS (54.8 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.633111301	-284.633111301	0.020435029	0.000958307	196438924
11454108						
2	1	-284.633248926	-0.000137625	0.003756878	0.000127632	160884317
14473583						
3	2	-284.633248017	0.000000909	0.001637062	0.000243038	145207949
15743036						
4	3	-284.633251895	-0.000003877	0.000987578	0.000074164	138018059
16271562						
5	4	-284.633251893	0.000000002	0.000452081	0.000046683	131874976
16778181						

6 5	-284.633252178	-0.000000285	0.000395053	0.000040819	124097797
17352543					
7 6	-284.633252284	-0.000000105	0.000700284	0.000038180	121327081
17662851					
8 7	-284.633252442	-0.000000159	0.000551701	0.000035130	145608657
15885595					
9 8	-284.633252567	-0.000000125	0.000743419	0.000033144	145485679
15861804					
10 9	-284.633252694	-0.000000126	0.000598981	0.000040295	167210580
14117601					
11 10	-284.633252785	-0.000000091	0.000856149	0.000036586	164217359
14367858					
-----DISABLING FDIFF OPTION-----					
12 11	-284.633252875	-0.000000090	0.000453817	0.000024664	196455713
11452579					
13 12	-284.633252909	-0.000000033	0.000147847	0.000011753	196455700
11452584					
14 13	-284.633252919	-0.000000011	0.000071490	0.000010363	196455606
11452587					
15 14	-284.633252927	-0.000000007	0.000085100	0.000009538	196455621
11452586					
16 15	-284.633252931	-0.000000004	0.000143805	0.000007780	196455670
11452582					
17 16	-284.633252939	-0.000000008	0.000305160	0.000007987	196455582
11452587					
18 17	-284.633252949	-0.000000010	0.000145689	0.000009277	196455765
11452579					
19 18	-284.633252954	-0.000000004	0.000086460	0.000009652	196455724
11452580					
20 19	-284.633252958	-0.000000005	0.000093001	0.000005293	196455731
11452581					
21 20	-284.633252962	-0.000000004	0.000050164	0.000002926	196455732
11452580					
22 21	-284.633252963	-0.000000001	0.000025913	0.000001932	196455684
11452584					
23 22	-284.633252964	-0.000000001	0.000016484	0.000001277	196455726
11452581					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 75.9 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 24.8 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.3
TIME TO SOLVE SCF EQUATIONS= 3.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6332529636 AFTER 23 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6046688843
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000259042

SPIN SZ = 1.500
S-SQUARED = 3.758

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 80.08 , TOTAL = 3635.2 SECONDS (60.6 MIN)
WALL CLOCK TIME: STEP = 74.36 , TOTAL = 3360.2 SECONDS (56.0
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.70 , TOTAL = 3638.9 SECONDS (60.6 MIN)
WALL CLOCK TIME: STEP = 3.70 , TOTAL = 3363.9 SECONDS (56.1
MIN)
CPU UTILIZATION: STEP = 99.92% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.77 , TOTAL = 3641.7 SECONDS (60.7 MIN)
WALL CLOCK TIME: STEP = 2.68 , TOTAL = 3366.6 SECONDS (56.1
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 33 ENERGY= -284.6332530

GRADIENT (HARTREE/BOHR)

ATOM ZNUC DE/DX DE/DY DE/DZ

1	CO	27.0	-0.0004992	0.0001823	-0.0004426
2	C	6.0	0.0005610	-0.0001192	0.0003442
3	C	6.0	0.0001227	-0.0005620	0.0000762
4	C	6.0	-0.0002486	-0.0000345	0.0001974
5	C	6.0	-0.0001220	-0.0010457	0.0000622
6	C	6.0	-0.0001480	-0.0002924	0.0005185
7	C	6.0	-0.0001772	0.0002465	0.0006118
8	C	6.0	0.0002380	-0.0006111	-0.0002171
9	C	6.0	-0.0001997	-0.0000527	-0.0002008
10	C	6.0	0.0002551	0.0005004	0.0001494
11	C	6.0	-0.0002521	0.0002225	0.0002634
12	N	7.0	0.0005789	-0.0000951	-0.0000750
13	C	6.0	-0.0004234	0.0005668	-0.0001076
14	C	6.0	-0.0000774	-0.0002931	0.0000319
15	C	6.0	-0.0006049	-0.0005032	-0.0008776
16	C	6.0	-0.0001056	-0.0013832	-0.0002210
17	C	6.0	0.0001466	0.0009816	-0.0006388
18	C	6.0	0.0011766	-0.0008745	-0.0000316
19	C	6.0	-0.0011626	0.0007692	0.0005057
20	O	8.0	-0.0004947	0.0000393	0.0002345
21	N	7.0	0.0000574	-0.0002181	-0.0001184
22	H	1.0	-0.0004465	-0.0004472	-0.0006280
23	H	1.0	0.0005376	0.0004302	-0.0007556
24	H	1.0	0.0010084	0.0007427	0.0002670
25	H	1.0	-0.0005715	0.0002687	-0.0003993
26	H	1.0	0.0000184	-0.0003683	-0.0004145
27	H	1.0	0.0002302	0.0003812	-0.0005695
28	H	1.0	0.0001031	-0.0005174	0.0001123
29	H	1.0	-0.0000902	0.0006534	0.0006124
30	H	1.0	0.0008882	-0.0001022	-0.0000986
31	H	1.0	-0.0001320	0.0003975	-0.0005035
32	H	1.0	-0.0003625	0.0006798	0.0019179
33	H	1.0	0.0005191	-0.0004188	-0.0010468
34	H	1.0	0.0001598	-0.0002942	0.0010469
35	H	1.0	-0.0004830	0.0011708	0.0003948

MAXIMUM GRADIENT = 0.0019179 RMS GRADIENT = 0.0005417
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001465745
 PREDICTED ENERGY CHANGE WAS -0.0001857909 RATIO= 0.789
 GDIIS STEP HAS LENGTH = 0.120074
 RADIUS OF STEP TAKEN= 0.10386 CURRENT TRUST RADIUS= 0.10386

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 0.02 , TOTAL = 3641.7 SECONDS (60.7 MIN)

WALL CLOCK TIME: STEP = 0.03 , TOTAL = 3366.6 SECONDS (56.1 MIN)

CPU UTILIZATION: STEP = 79.36%, TOTAL = 100.00%

INSERCH= 34

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1200167270	-1.7409283253	1.0237764565
C	6.0	4.9909683953	0.6802089061	0.4435118564
C	6.0	5.2213268012	-0.6809255553	0.2113155676
C	6.0	4.0914939505	-1.5501736411	0.0785310169
C	6.0	2.7739260823	-1.0638673624	0.1855125770
C	6.0	2.4756192728	0.3286124506	0.4963597106
C	6.0	3.6524415873	1.2034641666	0.5924684175
C	6.0	3.4988601576	2.6199221066	0.8217033599
C	6.0	2.2319475580	3.1913806308	0.9968503346
C	6.0	1.0774922229	2.3530414105	0.9708208057
C	6.0	1.1664878859	0.9648043732	0.7074249709
N	7.0	-0.0520109363	0.1597399927	0.7276316543
C	6.0	-1.2566610388	0.7010364626	0.5406696776
C	6.0	-2.5684445183	0.0526534066	0.5852819050
C	6.0	-2.8641671664	-1.3448513495	0.7504092300
C	6.0	-4.1721982090	-1.8594890516	0.7305061704
C	6.0	-5.2640134571	-0.9608063408	0.5361395458
C	6.0	-5.0311939605	0.4356031763	0.3926925502
C	6.0	-3.7060757159	0.9302386178	0.4242891876
O	8.0	-1.7632606269	-2.2840820925	0.9650499947
N	7.0	1.6922763729	-2.0721772940	-0.1203476899
H	1.0	5.8360352768	1.3882269076	0.5072615150
H	1.0	6.2456947565	-1.0782304873	0.0944874314
H	1.0	4.2725412468	-2.6184302235	-0.1479158083
H	1.0	4.4045454645	3.2485857434	0.8601454447
H	1.0	2.1175244150	4.2737150316	1.1805047957
H	1.0	0.1043916979	2.8257816755	1.1904243065
H	1.0	-1.3037516161	1.7779086733	0.2918479912
H	1.0	-4.3651648040	-2.9391356169	0.8694997272
H	1.0	-6.2911634318	-1.3645239274	0.5093399983
H	1.0	-5.8773958980	1.1315319265	0.2562858544
H	1.0	-3.5302167687	2.0181873518	0.3347288662
H	1.0	-2.0863955420	-3.2204788186	1.0127117751
H	1.0	1.3816782922	-1.9657688733	-1.1116052577
H	1.0	2.1128425262	-3.0196690508	-0.0454269395

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C	
1	CO	0.0000000	5.4703549	5.2732403	4.0868702
2	C	5.4703549	0.0000000	1.3998811 *	2.4324620 *
3	C	5.2732403	1.3998811 *	0.0000000	1.4316935 *
4	C	4.0868702	2.4324620 *	1.4316935 *	0.0000000
5	C	2.8643206 *	2.8326034 *	2.4773132 *	1.4085183 *
6	C	3.1796275	2.5403532 *	2.9392732 *	2.5130597 *
7	C	4.6188201	1.4448661 *	2.4814518 *	2.8353871 *
8	C	5.5203653	2.4762680 *	3.7729378	4.2770572
9	C	5.3655054	3.7715200	4.9546149	5.1752836
10	C	4.2047773	4.2885568	5.1916441	5.0115342
11	C	2.9182477 *	3.8441249	4.4041197	3.9084885
12	N	1.9312782 *	5.0777212	5.3648291	4.5292128
13	C	2.8446135 *	6.2484196	6.6319394	5.8210206
14	C	3.2614470	7.5867416	7.8331683	6.8688159
15	C	3.0227405	8.1177712	8.1305985	6.9910514
16	C	4.3038556	9.5129414	9.4813967	8.2951405
17	C	5.4620656	10.3858636	10.4941033	9.3852159
18	C	5.6276574	10.0252757	10.3147330	9.3415974
19	C	4.7046255	8.7006586	9.0741238	8.1898771
20	O	1.9609177 *	7.3945002	7.2057399	5.9667989
21	N	1.9724975 *	4.3330055	3.8078575	2.4633890 *
22	H	6.5369158	1.1043059 *	2.1787250 *	3.4440430
23	H	6.2311057	2.1882105 *	1.1049116 *	2.2053494 *
24	H	4.4029913	3.4273816	2.1870449 *	1.1069004 *
25	H	6.5786938	2.6672148 *	4.0656083	4.8720647
26	H	6.3396006	4.6597345	5.9263294	6.2472859
27	H	4.5697763	5.3888767	6.2800218	6.0234771
28	H	3.8658827	6.3915136	6.9734496	6.3427368
29	H	4.6450356	10.0408341	9.8708429	8.6063886
30	H	6.4427910	11.4661137	11.5366181	10.3932496
31	H	6.6939546	10.8793423	11.2458290	10.3248199
32	H	5.2848786	8.6262748	9.1591460	8.4195791
33	H	2.6565856 *	8.1011378	7.7778128	6.4675290
34	H	2.4904213 *	4.7377804	4.2595590	2.9886861 *
35	H	2.5980239 *	4.7129361	3.8985013	2.4677609 *
	C	C	C	C	
1	CO	2.8643206 *	3.1796275	4.6188201	5.5203653
2	C	2.8326034 *	2.5403532 *	1.4448661 *	2.4762680 *
3	C	2.4773132 *	2.9392732 *	2.4814518 *	3.7729378

4 C	1.4085183 *	2.5130597 *	2.8353871 *	4.2770572
5 C	0.0000000	1.4576052 *	2.4653995 *	3.8079618
6 C	1.4576052 *	0.0000000	1.4695282 *	2.5304091 *
7 C	2.4653995 *	1.4695282 *	0.0000000	1.4430832 *
8 C	3.8079618	2.5304091 *	1.4430832 *	0.0000000
9 C	4.3656781	2.9163862 *	2.4765177 *	1.4008243 *
10 C	3.8948508	2.5056307 *	2.8451788 *	2.4405909 *
11 C	2.6404089 *	1.4707528 *	2.5000279 *	2.8622429 *
12 N	3.1268240	2.5438001 *	3.8510515	4.3208831
13 C	4.4143691	3.7510771	4.9350183	5.1357652
14 C	5.4724179	5.0523895	6.3264398	6.5923402
15 C	5.6732844	5.6016374	6.9989318	7.4975081
16 C	7.0127509	7.0025774	8.4039113	8.8836129
17 C	8.0462434	7.8464067	9.1755332	9.4705394
18 C	7.9505493	7.5082913	8.7198078	8.8157315
19 C	6.7840914	6.2113204	7.3655084	7.4110775
20 O	4.7626322	5.0013944	6.4522575	7.1944229
21 N	1.5100349 *	2.5995664 *	3.8833209	5.1153692
22 H	3.9360896	3.5235348	2.1930524 *	2.6605139 *
23 H	3.4729914	4.0440299	3.4898535	4.6637191
24 H	2.1848770 *	3.5112790	3.9420260	5.3832220
25 H	4.6595387	3.5184287	2.1954119 *	1.1031598 *
26 H	5.4690638	4.0199653	3.4825562	2.1844583 *
27 H	4.8234460	3.5128763	3.9469131	3.4206358
28 H	4.9713634	4.0528914	4.9984208	4.9045706
29 H	7.4129001	7.5903714	9.0288367	9.6305917
30 H	9.0758529	8.9287938	10.2701876	10.5744004
31 H	8.9258142	8.3949495	9.5360367	9.5104774
32 H	7.0187993	6.2410620	7.2333108	7.0715735
33 H	5.3812599	5.8029861	7.2582455	8.0834305
34 H	2.1057766 *	3.0077307	4.2549114	5.4082070
35 H	2.0773841 *	3.4111770	4.5400584	5.8717926

C C C N

1 CO	5.3655054	4.2047773	2.9182477 *	1.9312782 *
2 C	3.7715200	4.2885568	3.8441249	5.0777212
3 C	4.9546149	5.1916441	4.4041197	5.3648291
4 C	5.1752836	5.0115342	3.9084885	4.5292128
5 C	4.3656781	3.8948508	2.6404089 *	3.1268240
6 C	2.9163862 *	2.5056307 *	1.4707528 *	2.5438001 *
7 C	2.4765177 *	2.8451788 *	2.5000279 *	3.8510515
8 C	1.4008243 *	2.4405909 *	2.8622429 *	4.3208831
9 C	0.0000000	1.4269749 *	2.4852793 *	3.8052319
10 C	1.4269749 *	0.0000000	1.4158035 *	2.4790098 *
11 C	2.4852793 *	1.4158035 *	0.0000000	1.4605740 *

12 N	3.8052319	2.4790098 *	1.4605740 *	0.0000000
13 C	4.3104878	2.8917852 *	2.4431602 *	1.3338435 *
14 C	5.7501966	4.3281959	3.8466425	2.5227305 *
15 C	6.8270432	5.4092209	4.6457010	3.1894414
16 C	8.1605948	6.7351625	6.0397629	4.5883807
17 C	8.5815117	7.1683491	6.7148092	5.3345350
18 C	7.7918252	6.4285962	6.2281916	4.9980545
19 C	6.3797108	5.0205166	4.8809053	3.7467151
20 O	6.7781555	5.4380901	4.3823578	2.9928263 *
21 N	5.4078109	4.5990400	3.1913820	2.9568669 *
22 H	4.0596193	4.8774467	4.6929761	6.0188729
23 H	5.9290813	6.2651340	5.5089043	6.4493829
24 H	6.2632591	6.0146022	4.8185834	5.2140737
25 H	2.1776460 *	3.4472499	3.9653496	5.4239675
26 H	1.1037524 *	2.1942246 *	3.4752215	4.6729828
27 H	2.1674011 *	1.1039174 *	2.1964911 *	2.7104275 *
28 H	3.8724798	2.5420669 *	2.6336146 *	2.0917055 *
29 H	9.0067385	7.5920958	6.7724587	5.3128573
30 H	9.6766396	8.2662170	7.8154700	6.4263563
31 H	8.3995752	7.0974019	7.0602849	5.9246651
32 H	5.9175438	4.6634453	4.8277896	3.9630941
33 H	7.7304774	6.4090614	5.3095241	3.9554861
34 H	5.6360211	4.8042845	3.4559279	3.1553201
35 H	6.2990210	5.5651350	4.1639406	3.9233725

C C C C

1 CO	2.8446135 *	3.2614470	3.0227405	4.3038556
2 C	6.2484196	7.5867416	8.1177712	9.5129414
3 C	6.6319394	7.8331683	8.1305985	9.4813967
4 C	5.8210206	6.8688159	6.9910514	8.2951405
5 C	4.4143691	5.4724179	5.6732844	7.0127509
6 C	3.7510771	5.0523895	5.6016374	7.0025774
7 C	4.9350183	6.3264398	6.9989318	8.4039113
8 C	5.1357652	6.5923402	7.4975081	8.8836129
9 C	4.3104878	5.7501966	6.8270432	8.1605948
10 C	2.8917852 *	4.3281959	5.4092209	6.7351625
11 C	2.4431602 *	3.8466425	4.6457010	6.0397629
12 N	1.3338435 *	2.5227305 *	3.1894414	4.5883807
13 C	0.0000000	1.4639559 *	2.6103110 *	3.8849306
14 C	1.4639559 *	0.0000000	1.4379633 *	2.4998810 *
15 C	2.6103110 *	1.4379633 *	0.0000000	1.4057714 *
16 C	3.8849306	2.4998810 *	1.4057714 *	0.0000000
17 C	4.3382733	2.8802096 *	2.4398082 *	1.4273996 *
18 C	3.7867467	2.4997752 *	2.8273636 *	2.4737502 *
19 C	2.4628663 *	1.4457798 *	2.4476925 *	2.8449287 *

20	O	3.0573967	2.5005755 *	1.4629492 *	2.4572892 *
21	N	4.1016936	4.8131654	4.6955722	5.9296923
22	H	7.1259868	8.5102952	9.1226290	10.5243639
23	H	7.7233550	8.8999342	9.1373357	10.4664884
24	H	6.4857603	7.3804710	7.3049023	8.5241563
25	H	6.2162152	7.6754233	8.5991796	9.9834747
26	H	4.9556582	6.3348209	7.5213377	8.7965506
27	H	2.6056070 *	3.8987807	5.1381062	6.3602286
28	H	1.1062475 *	2.1591798 *	3.5209097	4.6530709
29	H	4.7981015	3.5013976	2.1929247 *	1.1055279 *
30	H	5.4418504	3.9840676	3.4355210	2.1872171 *
31	H	4.6494506	3.4959085	3.9314348	3.4754554
32	H	2.6355936 *	2.2025227 *	3.4534680	3.9503360
33	H	4.0360333	3.3359350	2.0473665 *	2.5064928 *
34	H	4.0991094	4.7494131	4.6775891	5.8523682
35	H	5.0537821	5.6348387	5.3112141	6.4381540

C C C O

1	CO	5.4620656	5.6276574	4.7046255	1.9609177 *
2	C	10.3858636	10.0252757	8.7006586	7.3945002
3	C	10.4941033	10.3147330	9.0741238	7.2057399
4	C	9.3852159	9.3415974	8.1898771	5.9667989
5	C	8.0462434	7.9505493	6.7840914	4.7626322
6	C	7.8464067	7.5082913	6.2113204	5.0013944
7	C	9.1755332	8.7198078	7.3655084	6.4522575
8	C	9.4705394	8.8157315	7.4110775	7.1944229
9	C	8.5815117	7.7918252	6.3797108	6.7781555
10	C	7.1683491	6.4285962	5.0205166	5.4380901
11	C	6.7148092	6.2281916	4.8809053	4.3823578
12	N	5.3345350	4.9980545	3.7467151	2.9928263 *
13	C	4.3382733	3.7867467	2.4628663 *	3.0573967
14	C	2.8802096 *	2.4997752 *	1.4457798 *	2.5005755 *
15	C	2.4398082 *	2.8273636 *	2.4476925 *	1.4629492 *
16	C	1.4273996 *	2.4737502 *	2.8449287 *	2.4572892 *
17	C	0.0000000	1.4229341 *	2.4526988 *	3.7670006
18	C	1.4229341 *	0.0000000	1.4147795 *	4.2899498
19	C	2.4526988 *	1.4147795 *	0.0000000	3.7945764
20	O	3.7670006	4.2899498	3.7945764	0.0000000
21	N	7.0750328	7.1942495	6.2010754	3.6281852
22	H	11.3459188	10.9095045	9.5534559	8.4524980
23	H	11.5187772	11.3819523	10.1577779	8.1458777
24	H	9.7036861	9.8070825	8.7509312	6.1466565
25	H	10.5501182	9.8572086	8.4467082	8.2863291
26	H	9.0720737	8.1520504	6.7575894	7.6230976
27	H	6.6019778	5.7204518	4.3243159	5.4451471

28 H	4.8211941	3.9630519	2.5509305 *	4.1429601
29 H	2.1983732 *	3.4727225	3.9502744	2.6847961 *
30 H	1.1039670 *	2.2003607 *	3.4577228	4.6427538
31 H	2.1982801 *	1.1040749 *	2.1870929 *	5.3939665
32 H	3.4526831	2.1819406 *	1.1057033 *	4.6935020
33 H	3.9281671	4.7353138	4.4942252	0.9917291 *
34 H	6.9202768	7.0110220	6.0523609	3.7821239
35 H	7.6808293	7.9478369	7.0485611	4.0726315

N H H H

1 CO	1.9724975 *	6.5369158	6.2311057	4.4029913
2 C	4.3330055	1.1043059 *	2.1882105 *	3.4273816
3 C	3.8078575	2.1787250 *	1.1049116 *	2.1870449 *
4 C	2.4633890 *	3.4440430	2.2053494 *	1.1069004 *
5 C	1.5100349 *	3.9360896	3.4729914	2.1848770 *
6 C	2.5995664 *	3.5235348	4.0440299	3.5112790
7 C	3.8833209	2.1930524 *	3.4898535	3.9420260
8 C	5.1153692	2.6605139 *	4.6637191	5.3832220
9 C	5.4078109	4.0596193	5.9290813	6.2632591
10 C	4.5990400	4.8774467	6.2651340	6.0146022
11 C	3.1913820	4.6929761	5.5089043	4.8185834
12 N	2.9568669 *	6.0188729	6.4493829	5.2140737
13 C	4.1016936	7.1259868	7.7233550	6.4857603
14 C	4.8131654	8.5102952	8.8999342	7.3804710
15 C	4.6955722	9.1226290	9.1373357	7.3049023
16 C	5.9296923	10.5243639	10.4664884	8.5241563
17 C	7.0750328	11.3459188	11.5187772	9.7036861
18 C	7.1942495	10.9095045	11.3819523	9.8070825
19 C	6.2010754	9.5534559	10.1577779	8.7509312
20 O	3.6281852	8.4524980	8.1458777	6.1466565
21 N	0.0000000	5.4349819	4.6655871	2.6375972 *
22 H	5.4349819	0.0000000	2.5340906 *	4.3505255
23 H	4.6655871	2.5340906 *	0.0000000	2.5148180 *
24 H	2.6375972 *	4.3505255	2.5148180 *	0.0000000
25 H	6.0521310	2.3737365 *	4.7641790	5.9544512
26 H	6.4917950	4.7546421	6.8457684	7.3423746
27 H	5.3131444	5.9485303	7.3592114	6.9859908
28 H	4.8958402	7.1536572	8.0740710	7.1145084
29 H	6.1987102	11.0870089	10.8006459	8.7033299
30 H	8.0394397	12.4356982	12.5469869	10.6581482
31 H	8.2283379	11.7189313	12.3239018	10.8280570
32 H	6.6492565	9.3889986	10.2573859	9.0892355
33 H	4.1086228	9.1793550	8.6519416	6.4919640
34 H	1.0442152 *	5.8061445	5.0893064	3.1163685
35 H	1.0393410 *	5.7963071	4.5682849	2.1990441 *

	H	H	H	H
1 CO	6.5786938	6.3396006	4.5697763	3.8658827
2 C	2.6672148 *	4.6597345	5.3888767	6.3915136
3 C	4.0656083	5.9263294	6.2800218	6.9734496
4 C	4.8720647	6.2472859	6.0234771	6.3427368
5 C	4.6595387	5.4690638	4.8234460	4.9713634
6 C	3.5184287	4.0199653	3.5128763	4.0528914
7 C	2.1954119 *	3.4825562	3.9469131	4.9984208
8 C	1.1031598 *	2.1844583 *	3.4206358	4.9045706
9 C	2.1776460 *	1.1037524 *	2.1674011 *	3.8724798
10 C	3.4472499	2.1942246 *	1.1039174 *	2.5420669 *
11 C	3.9653496	3.4752215	2.1964911 *	2.6336146 *
12 N	5.4239675	4.6729828	2.7104275 *	2.0917055 *
13 C	6.2162152	4.9556582	2.6056070 *	1.1062475 *
14 C	7.6754233	6.3348209	3.8987807	2.1591798 *
15 C	8.5991796	7.5213377	5.1381062	3.5209097
16 C	9.9834747	8.7965506	6.3602286	4.6530709
17 C	10.5501182	9.0720737	6.6019778	4.8211941
18 C	9.8572086	8.1520504	5.7204518	3.9630519
19 C	8.4467082	6.7575894	4.3243159	2.5509305 *
20 O	8.2863291	7.6230976	5.4451471	4.1429601
21 N	6.0521310	6.4917950	5.3131444	4.8958402
22 H	2.3737365 *	4.7546421	5.9485303	7.1536572
23 H	4.7641790	6.8457684	7.3592114	8.0740710
24 H	5.9544512	7.3423746	6.9859908	7.1145084
25 H	0.0000000	2.5266550 *	4.3334940	5.9220358
26 H	2.5266550 *	0.0000000	2.4797808 *	4.3271110
27 H	4.3334940	2.4797808 *	0.0000000	1.9718886 *
28 H	5.9220358	4.3271110	1.9718886 *	0.0000000
29 H	10.7329307	9.7029479	7.3016573	5.6530027
30 H	11.6534130	10.1462423	7.6763053	5.8988526
31 H	10.5149837	8.6398059	6.2868816	4.6192304
32 H	8.0467630	6.1400100	3.8203144	2.2398035 *
33 H	9.1653908	8.5944191	6.4333814	5.1103868
34 H	6.3415314	6.6877797	5.4671526	4.8162575
35 H	6.7352047	7.3957002	6.3032132	5.8994595

	H	H	H	H
1 CO	4.6450356	6.4427910	6.6939546	5.2848786
2 C	10.0408341	11.4661137	10.8793423	8.6262748
3 C	9.8708429	11.5366181	11.2458290	9.1591460
4 C	8.6063886	10.3932496	10.3248199	8.4195791
5 C	7.4129001	9.0758529	8.9258142	7.0187993

6 C	7.5903714	8.9287938	8.3949495	6.2410620
7 C	9.0288367	10.2701876	9.5360367	7.2333108
8 C	9.6305917	10.5744004	9.5104774	7.0715735
9 C	9.0067385	9.6766396	8.3995752	5.9175438
10 C	7.5920958	8.2662170	7.0974019	4.6634453
11 C	6.7724587	7.8154700	7.0602849	4.8277896
12 N	5.3128573	6.4263563	5.9246651	3.9630941
13 C	4.7981015	5.4418504	4.6494506	2.6355936 *
14 C	3.5013976	3.9840676	3.4959085	2.2025227 *
15 C	2.1929247 *	3.4355210	3.9314348	3.4534680
16 C	1.1055279 *	2.1872171 *	3.4754554	3.9503360
17 C	2.1983732 *	1.1039670 *	2.1982801 *	3.4526831
18 C	3.4727225	2.2003607 *	1.1040749 *	2.1819406 *
19 C	3.9502744	3.4577228	2.1870929 *	1.1057033 *
20 O	2.6847961 *	4.6427538	5.3939665	4.6935020
21 N	6.1987102	8.0394397	8.2283379	6.6492565
22 H	11.0870089	12.4356982	11.7189313	9.3889986
23 H	10.8006459	12.5469869	12.3239018	10.2573859
24 H	8.7033299	10.6581482	10.8280570	9.0892355
25 H	10.7329307	11.6534130	10.5149837	8.0467630
26 H	9.7029479	10.1462423	8.6398059	6.1400100
27 H	7.3016573	7.6763053	6.2868816	3.8203144
28 H	5.6530027	5.8988526	4.6192304	2.2398035 *
29 H	0.0000000	2.5136801 *	4.3855682	5.0555088
30 H	2.5136801 *	0.0000000	2.5427416 *	4.3699029
31 H	4.3855682	2.5427416 *	0.0000000	2.5102910 *
32 H	5.0555088	4.3699029	2.5102910 *	0.0000000
33 H	2.3005332 *	4.6236376	5.8209846	5.4761212
34 H	6.1561697	7.8652056	8.0099036	6.4877194
35 H	6.5427942	8.5833902	9.0092958	7.5742085

H H H

1 CO	2.6565856 *	2.4904213 *	2.5980239 *
2 C	8.1011378	4.7377804	4.7129361
3 C	7.7778128	4.2595590	3.8985013
4 C	6.4675290	2.9886861 *	2.4677609 *
5 C	5.3812599	2.1057766 *	2.0773841 *
6 C	5.8029861	3.0077307	3.4111770
7 C	7.2582455	4.2549114	4.5400584
8 C	8.0834305	5.4082070	5.8717926
9 C	7.7304774	5.6360211	6.2990210
10 C	6.4090614	4.8042845	5.5651350
11 C	5.3095241	3.4559279	4.1639406
12 N	3.9554861	3.1553201	3.9233725
13 C	4.0360333	4.0991094	5.0537821

14 C	3.3359350	4.7494131	5.6348387
15 C	2.0473665 *	4.6775891	5.3112141
16 C	2.5064928 *	5.8523682	6.4381540
17 C	3.9281671	6.9202768	7.6808293
18 C	4.7353138	7.0110220	7.9478369
19 C	4.4942252	6.0523609	7.0485611
20 O	0.9917291 *	3.7821239	4.0726315
21 N	4.1086228	1.0442152 *	1.0393410 *
22 H	9.1793550	5.8061445	5.7963071
23 H	8.6519416	5.0893064	4.5682849
24 H	6.4919640	3.1163685	2.1990441 *
25 H	9.1653908	6.3415314	6.7352047
26 H	8.5944191	6.6877797	7.3957002
27 H	6.4333814	5.4671526	6.3032132
28 H	5.1103868	4.8162575	5.8994595
29 H	2.3005332 *	6.1561697	6.5427942
30 H	4.6236376	7.8652056	8.5833902
31 H	5.8209846	8.0099036	9.0092958
32 H	5.4761212	6.4877194	7.5742085
33 H	0.0000000	4.2561198	4.3351566
34 H	4.2561198	0.0000000	1.6679457 *
35 H	4.3351566	1.6679457 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.79 , TOTAL = 3642.5 SECONDS (60.7 MIN)
WALL CLOCK TIME: STEP = 0.78 , TOTAL = 3367.4 SECONDS (56.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.17 , TOTAL = 3643.7 SECONDS (60.7 MIN)
WALL CLOCK TIME: STEP = 1.17 , TOTAL = 3368.5 SECONDS (56.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.633098871	-284.633098871	0.031443012	0.001366886	196577737
11440396					
2 1	-284.633370062	-0.000271191	0.004841487	0.000147977	163423533
14270556					
3 2	-284.633370205	-0.000000143	0.002034950	0.000272645	147967133
15540431					
4 3	-284.633374259	-0.000004053	0.002195252	0.000109513	140811794
16108433					
5 4	-284.633374157	0.000000102	0.000505297	0.000165935	138420960
16308750					
6 5	-284.633374959	-0.000000802	0.000693111	0.000060185	129924479
16947869					
7 6	-284.633375045	-0.000000086	0.000399284	0.000058924	151989646
15234880					
8 7	-284.633375317	-0.000000271	0.000749924	0.000049731	144927790
15831199					
9 8	-284.633375554	-0.000000238	0.000974216	0.000045972	170269407
13808937					

-----DISABLING FDIFF OPTION-----

10 9	-284.633375746	-0.000000191	0.000940613	0.000049104	196595776
11438586					
11 10	-284.633375951	-0.000000206	0.000986451	0.000049380	196595993
11438565					
12 11	-284.633376127	-0.000000176	0.000802203	0.000035943	196596142
11438550					
13 12	-284.633376229	-0.000000102	0.000287125	0.000031970	196596125
11438554					
14 13	-284.633376269	-0.000000040	0.000177066	0.000012265	196596049
11438561					
15 14	-284.633376281	-0.000000012	0.000100445	0.000012262	196596167
11438553					
16 15	-284.633376290	-0.000000009	0.000118633	0.000011346	196596139
11438551					
17 16	-284.633376301	-0.000000011	0.000293439	0.000009931	196596143
11438554					
18 17	-284.633376316	-0.000000016	0.000245837	0.000007670	196595879
11438564					
19 18	-284.633376327	-0.000000011	0.000162740	0.000009819	196595924
11438556					
20 19	-284.633376335	-0.000000008	0.000174712	0.000007854	196595978
11438557					
21 20	-284.633376342	-0.000000007	0.000057231	0.000004234	196595983
11438559					
22 21	-284.633376346	-0.000000003	0.000051200	0.000003521	196595921
11438559					

23 22 -284.633376347 -0.000000002 0.000031362 0.000003124 196596004
11438556
24 23 -284.633376348 -0.000000001 0.000036246 0.000002350 196596032
11438553
25 24 -284.633376348 0.000000000 0.000015558 0.000001424 196596050
11438554

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 84.3 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 27.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.6 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6333763483 AFTER 25 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6057838871
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000193846

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 88.04 , TOTAL = 3731.7 SECONDS (62.2 MIN)
WALL CLOCK TIME: STEP = 81.14 , TOTAL = 3449.7 SECONDS (57.5
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.56 , TOTAL = 3735.3 SECONDS (62.3 MIN)
WALL CLOCK TIME: STEP = 3.53 , TOTAL = 3453.2 SECONDS (57.6
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.80 , TOTAL = 3738.1 SECONDS (62.3 MIN)

WALL CLOCK TIME: STEP = 2.66 , TOTAL = 3455.9 SECONDS (57.6 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 34 ENERGY= -284.6333763

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0004696	-0.0004724	-0.0005798
2 C	6.0	0.0000443	-0.0006226	0.0004898
3 C	6.0	0.0008435	-0.0006571	0.0001327
4 C	6.0	-0.0005882	-0.0006549	-0.0000730
5 C	6.0	-0.0001198	-0.0001313	-0.0001913
6 C	6.0	-0.0000323	-0.0005253	0.0001775
7 C	6.0	-0.0000483	-0.0009445	0.0004664
8 C	6.0	0.0005728	0.0003285	-0.0000808
9 C	6.0	-0.0010082	-0.0001689	-0.0002029
10 C	6.0	0.0005885	0.0007829	0.0002346
11 C	6.0	-0.0005772	0.0006946	0.0003598
12 N	7.0	0.0004855	-0.0000003	-0.0001155
13 C	6.0	-0.0001857	-0.0010271	0.0003528
14 C	6.0	0.0007923	0.0003889	-0.0000915
15 C	6.0	-0.0001455	-0.0005739	-0.0009430
16 C	6.0	-0.0001103	-0.0006751	-0.0003155
17 C	6.0	0.0003083	0.0004709	-0.0004989
18 C	6.0	-0.0005426	0.0001288	-0.0002408
19 C	6.0	-0.0001070	0.0008849	0.0004337
20 O	8.0	-0.0005626	-0.0000894	0.0009186
21 N	7.0	-0.0000628	0.0005489	0.0001966
22 H	1.0	-0.0005387	-0.0000852	-0.0006556
23 H	1.0	0.0006653	0.0001189	-0.0008623
24 H	1.0	0.0008022	0.0008179	0.0006119
25 H	1.0	-0.0011411	-0.0005131	-0.0004689
26 H	1.0	-0.0000850	-0.0002232	-0.0004470
27 H	1.0	-0.0004895	0.0008385	-0.0004675
28 H	1.0	0.0004197	0.0001105	0.0001562
29 H	1.0	0.0000706	0.0008899	0.0003869
30 H	1.0	0.0009537	0.0000042	-0.0000137
31 H	1.0	0.0000514	-0.0000194	-0.0003090

32 H	1.0	-0.0006427	0.0001772	0.0016754
33 H	1.0	0.0007302	-0.0007072	-0.0013044
34 H	1.0	-0.0003404	-0.0000319	0.0002910
35 H	1.0	0.0004691	0.0009373	0.0009769

MAXIMUM GRADIENT = 0.0016754 RMS GRADIENT = 0.0005610
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001233847
 PREDICTED ENERGY CHANGE WAS -0.0001038481 RATIO= 1.188
 GDIIS STEP HAS LENGTH = 0.059269
 RADIUS OF STEP TAKEN= 0.05927 CURRENT TRUST RADIUS= 0.14688

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 3738.1 SECONDS (62.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 3455.9 SECONDS (57.6 MIN)
 CPU UTILIZATION: STEP = 92.23% , TOTAL = 100.00%

INSERCH= 35

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1224302281	-1.7452135126	1.0231687269
C	6.0	4.9895778220	0.6806056308	0.4435889577
C	6.0	5.2197476087	-0.6813227910	0.2122016099
C	6.0	4.0899482652	-1.5491924010	0.0779965139
C	6.0	2.7726992187	-1.0621500484	0.1819072528
C	6.0	2.4743503751	0.3302528832	0.4943712388
C	6.0	3.6511441785	1.2043982632	0.5915380463
C	6.0	3.4956588541	2.6197506610	0.8222990454
C	6.0	2.2288302192	3.1915734091	0.9985418079
C	6.0	1.0746876712	2.3522576031	0.9735120789
C	6.0	1.1658753960	0.9640101351	0.7080834189
N	7.0	-0.0504853913	0.1565027895	0.7291527737
C	6.0	-1.2540655525	0.6993646669	0.5408057814
C	6.0	-2.5660309438	0.0512387901	0.5841832923
C	6.0	-2.8615268421	-1.3445555159	0.7538220611
C	6.0	-4.1708370586	-1.8569683500	0.7342598729
C	6.0	-5.2633816912	-0.9588042288	0.5391461766
C	6.0	-5.0285258730	0.4368566669	0.3902474827
C	6.0	-3.7026763541	0.9283904229	0.4178211515
O	8.0	-1.7621294175	-2.2852412008	0.9706498292
N	7.0	1.6923215593	-2.0710701174	-0.1263155886
H	1.0	5.8339584457	1.3889022150	0.5091584375

H	1.0	6.2438583955	-1.0808967132	0.0980100003
H	1.0	4.2677470092	-2.6199952664	-0.1463664306
H	1.0	4.4027703199	3.2481088825	0.8611728839
H	1.0	2.1140499246	4.2738006491	1.1822662840
H	1.0	0.1013196054	2.8238018739	1.1960632201
H	1.0	-1.2994158268	1.7757131422	0.2930042291
H	1.0	-4.3644084784	-2.9373540563	0.8731399425
H	1.0	-6.2905212481	-1.3615609534	0.5150637742
H	1.0	-5.8751698790	1.1334956478	0.2529578963
H	1.0	-3.5245523317	2.0160937514	0.3204512576
H	1.0	-2.0866525797	-3.2211424461	1.0181782805
H	1.0	1.3790763865	-1.9613354258	-1.1168549476
H	1.0	2.1163249850	-3.0172100568	-0.0543393579

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4689704	5.2699313	4.0832553
2 C	5.4689704	0.0000000	1.4004882 *	2.4320753 *
3 C	5.2699313	1.4004882 *	0.0000000	1.4309630 *
4 C	4.0832553	2.4320753 *	1.4309630 *	0.0000000
5 C	2.8632538 *	2.8320002 *	2.4766899 *	1.4082446 *
6 C	3.1809929	2.5400187 *	2.9394066 *	2.5131333 *
7 C	4.6193438	1.4448710 *	2.4820066 *	2.8352311 *
8 C	5.5201388	2.4769939 *	3.7738292	4.2763597
9 C	5.3674382	3.7728847	4.9561318	5.1755217
10 C	4.2069620	4.2897090	5.1926607	5.0114925
11 C	2.9202653 *	3.8433027	4.4030557	3.9068400
12 N	1.9320637 *	5.0752801	5.3613940	4.5251068
13 C	2.8466431 *	6.2444284	6.6275588	5.8162432
14 C	3.2630925	7.5830794	7.8290079	6.8643765
15 C	3.0227594	8.1140228	8.1265138	6.9872471
16 C	4.3044281	9.5098355	9.4782787	8.2925257
17 C	5.4644018	10.3836398	10.4918963	9.3832829
18 C	5.6297752	10.0212105	10.3106321	9.3374762
19 C	4.7059584	8.6958234	9.0687985	8.1840635
20 O	1.9611102 *	7.3932125	7.2037771	5.9653509
21 N	1.9728293 *	4.3322522	3.8064059	2.4622578 *
22 H	6.5351697	1.1040661 *	2.1797408 *	3.4438165
23 H	6.2264852	2.1898710 *	1.1052158 *	2.2043208 *
24 H	4.3950776	3.4297308	2.1893668 *	1.1084087 *
25 H	6.5788162	2.6666069 *	4.0655933	4.8708647
26 H	6.3419549	4.6610466	5.9278691	6.2474662
27 H	4.5723342	5.3902297	6.2810977	6.0234799

28 H	3.8667442	6.3854035	6.9672840	6.3361242
29 H	4.6449359	10.0384862	9.8682605	8.6043822
30 H	6.4444788	11.4636900	11.5343287	10.3913609
31 H	6.6971186	10.8758536	11.2424384	10.3213859
32 H	5.2859934	8.6191127	9.1515330	8.4113417
33 H	2.6567721 *	8.1010387	7.7771310	6.4675928
34 H	2.4910981 *	4.7382020	4.2609364	2.9910463 *
35 H	2.5989643 *	4.7092840	3.8934105	2.4632859 *

C C C C

1 CO	2.8632538 *	3.1809929	4.6193438	5.5201388
2 C	2.8320002 *	2.5400187 *	1.4448710 *	2.4769939 *
3 C	2.4766899 *	2.9394066 *	2.4820066 *	3.7738292
4 C	1.4082446 *	2.5131333 *	2.8352311 *	4.2763597
5 C	0.0000000	1.4578860 *	2.4650972 *	3.8064636
6 C	1.4578860 *	0.0000000	1.4691546 *	2.5283211 *
7 C	2.4650972 *	1.4691546 *	0.0000000	1.4424454 *
8 C	3.8064636	2.5283211 *	1.4424454 *	0.0000000
9 C	4.3654151	2.9157543 *	2.4773966 *	1.4010345 *
10 C	3.8946195	2.5054211 *	2.8463333 *	2.4403933 *
11 C	2.6389523 *	1.4694992 *	2.4995860 *	2.8604917 *
12 N	3.1232937	2.5416741 *	3.8495564	4.3187273
13 C	4.4098273	3.7469301	4.9314009	5.1309846
14 C	5.4684093	5.0488968	6.3232189	6.5877185
15 C	5.6702154	5.5985608	6.9955976	7.4922775
16 C	7.0106723	7.0000000	8.4009360	8.8782838
17 C	8.0446812	7.8444994	9.1733833	9.4660986
18 C	7.9466685	7.5043559	8.7158654	8.8098479
19 C	6.7785246	6.2063909	7.3610485	7.4054258
20 O	4.7626398	5.0015409	6.4517316	7.1920297
21 N	1.5100122 *	2.6006102 *	3.8834254	5.1142638
22 H	3.9352330	3.5224882	2.1921465 *	2.6609566 *
23 H	3.4722235	4.0444575	3.4911760	4.6660461
24 H	2.1839902 *	3.5115211	3.9434361	5.3841778
25 H	4.6579894	3.5167073	2.1941736 *	1.1041723 *
26 H	5.4687208	4.0192767	3.4832240	2.1850174 *
27 H	4.8234224	3.5130376	3.9483127	3.4209466
28 H	4.9646683	4.0461359	4.9923509	4.8974783
29 H	7.4116462	7.5887643	9.0267656	9.6262483
30 H	9.0742826	8.9266812	10.2677508	10.5695107
31 H	8.9225304	8.3915414	9.5325927	9.5050268
32 H	7.0107173	6.2337101	7.2265454	7.0639662
33 H	5.3827407	5.8042683	7.2587702	8.0818687
34 H	2.1065380 *	3.0078318	4.2547348	5.4061622
35 H	2.0757888 *	3.4109784	4.5381499	5.8691041

	C	C	C	N
1 CO	5.3674382	4.2069620	2.9202653 *	1.9320637 *
2 C	3.7728847	4.2897090	3.8433027	5.0752801
3 C	4.9561318	5.1926607	4.4030557	5.3613940
4 C	5.1755217	5.0114925	3.9068400	4.5251068
5 C	4.3654151	3.8946195	2.6389523 *	3.1232937
6 C	2.9157543 *	2.5054211 *	1.4694992 *	2.5416741 *
7 C	2.4773966 *	2.8463333 *	2.4995860 *	3.8495564
8 C	1.4010345 *	2.4403933 *	2.8604917 *	4.3187273
9 C	0.0000000	1.4272780 *	2.4852117 *	3.8051943
10 C	1.4272780 *	0.0000000	1.4163328 *	2.4793275 *
11 C	2.4852117 *	1.4163328 *	0.0000000	1.4601526 *
12 N	3.8051943	2.4793275 *	1.4601526 *	0.0000000
13 C	4.3071092	2.8883181 *	2.4401093 *	1.3337087 *
14 C	5.7466589	4.3244764	3.8439079	2.5219171 *
15 C	6.8226159	5.4044866	4.6423632	3.1868070
16 C	8.1555723	6.7298109	6.0364811	4.5859993
17 C	8.5772908	7.1640022	6.7127566	5.3342572
18 C	7.7863794	6.4232526	6.2249110	4.9974336
19 C	6.3751082	5.0159144	4.8773268	3.7458292
20 O	6.7767275	5.4363531	4.3817562	2.9916818 *
21 N	5.4081940	4.5996653	3.1914071	2.9548745 *
22 H	4.0603041	4.8779439	4.6915993	6.0161354
23 H	5.9317291	6.2668476	5.5081526	6.4457942
24 H	6.2643696	6.0144039	4.8163043	5.2079369
25 H	2.1790094 *	3.4483770	3.9645974	5.4228170
26 H	1.1036961 *	2.1945797 *	3.4754277	4.6736139
27 H	2.1680803 *	1.1042320 *	2.1977781 *	2.7121089 *
28 H	3.8666476	2.5361116 *	2.6284622 *	2.0909077 *
29 H	9.0027926	7.5877423	6.7699281	5.3106134
30 H	9.6718216	8.2612908	7.8130268	6.4256050
31 H	8.3944265	7.0926088	7.0577747	5.9252195
32 H	5.9112579	4.6575211	4.8225772	3.9615977
33 H	7.7295991	6.4077184	5.3094820	3.9544911
34 H	5.6346654	4.8030586	3.4544900	3.1522421
35 H	6.2984290	5.5653095	4.1635030	3.9219103

	C	C	C	C
1 CO	2.8466431 *	3.2630925	3.0227594	4.3044281
2 C	6.2444284	7.5830794	8.1140228	9.5098355
3 C	6.6275588	7.8290079	8.1265138	9.4782787
4 C	5.8162432	6.8643765	6.9872471	8.2925257
5 C	4.4098273	5.4684093	5.6702154	7.0106723

6 C	3.7469301	5.0488968	5.5985608	7.0000000
7 C	4.9314009	6.3232189	6.9955976	8.4009360
8 C	5.1309846	6.5877185	7.4922775	8.8782838
9 C	4.3071092	5.7466589	6.8226159	8.1555723
10 C	2.8883181 *	4.3244764	5.4044866	6.7298109
11 C	2.4401093 *	3.8439079	4.6423632	6.0364811
12 N	1.3337087 *	2.5219171 *	3.1868070	4.5859993
13 C	0.0000000	1.4639679 *	2.6090070 *	3.8832743
14 C	1.4639679 *	0.0000000	1.4367800 *	2.4978351 *
15 C	2.6090070 *	1.4367800 *	0.0000000	1.4061447 *
16 C	3.8832743	2.4978351 *	1.4061447 *	0.0000000
17 C	4.3386798	2.8806104 *	2.4420886 *	1.4277331 *
18 C	3.7865722	2.5000387 *	2.8286924 *	2.4729755 *
19 C	2.4623714 *	1.4453491 *	2.4467759 *	2.8420998 *
20 O	3.0579024	2.5009504 *	1.4630716 *	2.4578792 *
21 N	4.0989702	4.8106725	4.6946779	5.9298447
22 H	7.1215552	8.5061621	9.1182847	10.5205646
23 H	7.7190843	8.8956307	9.1327786	10.4629337
24 H	6.4792569	7.3735823	7.2981937	8.5186509
25 H	6.2127711	7.6720853	8.5950046	9.9792116
26 H	4.9530058	6.3317366	7.5170376	8.7912936
27 H	2.6037789 *	3.8956722	5.1331510	6.3540692
28 H	1.1054358 *	2.1593774 *	3.5197472	4.6514666
29 H	4.7969159	3.4999064	2.1931478 *	1.1063412 *
30 H	5.4418713	3.9840443	3.4373387	2.1878155 *
31 H	4.6503689	3.4973405	3.9336557	3.4755254
32 H	2.6339024 *	2.2020383 *	3.4527346	3.9483581
33 H	4.0362683	3.3356610	2.0474113 *	2.5070711 *
34 H	4.0939712	4.7442447	4.6757423	5.8514150
35 H	5.0523913	5.6344961	5.3131824	6.4417743

C C C O

1 CO	5.4644018	5.6297752	4.7059584	1.9611102 *
2 C	10.3836398	10.0212105	8.6958234	7.3932125
3 C	10.4918963	10.3106321	9.0687985	7.2037771
4 C	9.3832829	9.3374762	8.1840635	5.9653509
5 C	8.0446812	7.9466685	6.7785246	4.7626398
6 C	7.8444994	7.5043559	6.2063909	5.0015409
7 C	9.1733833	8.7158654	7.3610485	6.4517316
8 C	9.4660986	8.8098479	7.4054258	7.1920297
9 C	8.5772908	7.7863794	6.3751082	6.7767275
10 C	7.1640022	6.4232526	5.0159144	5.4363531
11 C	6.7127566	6.2249110	4.8773268	4.3817562
12 N	5.3342572	4.9974336	3.7458292	2.9916818 *
13 C	4.3386798	3.7865722	2.4623714 *	3.0579024

14 C	2.8806104 *	2.5000387 *	1.4453491 *	2.5009504 *
15 C	2.4420886 *	2.8286924 *	2.4467759 *	1.4630716 *
16 C	1.4277331 *	2.4729755 *	2.8420998 *	2.4578792 *
17 C	0.0000000	1.4230943 *	2.4519430 *	3.7688722
18 C	1.4230943 *	0.0000000	1.4142994 *	4.2913902
19 C	2.4519430 *	1.4142994 *	0.0000000	3.7945711
20 O	3.7688722	4.2913902	3.7945711	0.0000000
21 N	7.0754351	7.1921015	6.1966806	3.6307622
22 H	11.3429971	10.9047740	9.5481840	8.4506127
23 H	11.5163398	11.3778568	10.1524907	8.1429593
24 H	9.6990668	9.8006626	8.7428255	6.1415955
25 H	10.5468627	9.8526269	8.4425068	8.2846809
26 H	9.0675385	8.1465221	6.7535510	7.6217175
27 H	6.5969439	5.7150819	4.3207211	5.4429380
28 H	4.8219494	3.9633641	2.5513126 *	4.1430252
29 H	2.1987187 *	3.4726841	3.9483142	2.6845140 *
30 H	1.1035437 *	2.2005721 *	3.4569169	4.6440367
31 H	2.1986149 *	1.1049708 *	2.1883729 *	5.3962899
32 H	3.4527341	2.1819252 *	1.1064843 *	4.6936526
33 H	3.9292816	4.7360187	4.4933934	0.9917083 *
34 H	6.9187902	7.0057155	6.0440017	3.7854676
35 H	7.6843562	7.9484041	7.0463803	4.0778413

N H H H

1 CO	1.9728293 *	6.5351697	6.2264852	4.3950776
2 C	4.3322522	1.1040661 *	2.1898710 *	3.4297308
3 C	3.8064059	2.1797408 *	1.1052158 *	2.1893668 *
4 C	2.4622578 *	3.4438165	2.2043208 *	1.1084087 *
5 C	1.5100122 *	3.9352330	3.4722235	2.1839902 *
6 C	2.6006102 *	3.5224882	4.0444575	3.5115211
7 C	3.8834254	2.1921465 *	3.4911760	3.9434361
8 C	5.1142638	2.6609566 *	4.6660461	5.3841778
9 C	5.4081940	4.0603041	5.9317291	6.2643696
10 C	4.5996653	4.8779439	6.2668476	6.0144039
11 C	3.1914071	4.6915993	5.5081526	4.8163043
12 N	2.9548745 *	6.0161354	6.4457942	5.2079369
13 C	4.0989702	7.1215552	7.7190843	6.4792569
14 C	4.8106725	8.5061621	8.8956307	7.3735823
15 C	4.6946779	9.1182847	9.1327786	7.2981937
16 C	5.9298447	10.5205646	10.4629337	8.5186509
17 C	7.0754351	11.3429971	11.5163398	9.6990668
18 C	7.1921015	10.9047740	11.3778568	9.8006626
19 C	6.1966806	9.5481840	10.1524907	8.7428255
20 O	3.6307622	8.4506127	8.1429593	6.1415955
21 N	0.0000000	5.4340033	4.6633950	2.6333509 *

22 H	5.4340033	0.0000000	2.5371180 *	4.3536181
23 H	4.6633950	2.5371180 *	0.0000000	2.5166566 *
24 H	2.6333509 *	4.3536181	2.5166566 *	0.0000000
25 H	6.0510603	2.3725225 *	4.7657436	5.9555028
26 H	6.4921203	4.7553583	6.8486286	7.3435753
27 H	5.3141081	5.9492792	7.3609221	6.9854250
28 H	4.8912231	7.1471235	8.0684093	7.1069403
29 H	6.1994627	11.0840274	10.7973416	8.6979433
30 H	8.0399347	12.4325416	12.5444561	10.6535522
31 H	8.2267865	11.7147154	12.3206489	10.8225190
32 H	6.6423100	9.3814020	10.2500087	9.0791613
33 H	4.1125634	9.1786541	8.6501315	6.4881381
34 H	1.0446686 *	5.8063746	5.0908912	3.1177073
35 H	1.0392980 *	5.7924221	4.5616940	2.1897181 *

H H H H

1 CO	6.5788162	6.3419549	4.5723342	3.8667442
2 C	2.6666069 *	4.6610466	5.3902297	6.3854035
3 C	4.0655933	5.9278691	6.2810977	6.9672840
4 C	4.8708647	6.2474662	6.0234799	6.3361242
5 C	4.6579894	5.4687208	4.8234224	4.9646683
6 C	3.5167073	4.0192767	3.5130376	4.0461359
7 C	2.1941736 *	3.4832240	3.9483127	4.9923509
8 C	1.1041723 *	2.1850174 *	3.4209466	4.8974783
9 C	2.1790094 *	1.1036961 *	2.1680803 *	3.8666476
10 C	3.4483770	2.1945797 *	1.1042320 *	2.5361116 *
11 C	3.9645974	3.4754277	2.1977781 *	2.6284622 *
12 N	5.4228170	4.6736139	2.7121089 *	2.0909077 *
13 C	6.2127711	4.9530058	2.6037789 *	1.1054358 *
14 C	7.6720853	6.3317366	3.8956722	2.1593774 *
15 C	8.5950046	7.5170376	5.1331510	3.5197472
16 C	9.9792116	8.7912936	6.3540692	4.6514666
17 C	10.5468627	9.0675385	6.5969439	4.8219494
18 C	9.8526269	8.1465221	5.7150819	3.9633641
19 C	8.4425068	6.7535510	4.3207211	2.5513126 *
20 O	8.2846809	7.6217175	5.4429380	4.1430252
21 N	6.0510603	6.4921203	5.3141081	4.8912231
22 H	2.3725225 *	4.7553583	5.9492792	7.1471235
23 H	4.7657436	6.8486286	7.3609221	8.0684093
24 H	5.9555028	7.3435753	6.9854250	7.1069403
25 H	0.0000000	2.5285145 *	4.3352816	5.9165608
26 H	2.5285145 *	0.0000000	2.4806794 *	4.3223809
27 H	4.3352816	2.4806794 *	0.0000000	1.9687725 *
28 H	5.9165608	4.3223809	1.9687725 *	0.0000000
29 H	10.7295629	9.6988007	7.2964323	5.6518793

30 H	11.6496924	10.1409702	7.6705053	5.8994010
31 H	10.5108310	8.6343942	6.2821182	4.6207761
32 H	8.0406894	6.1346394	3.8165477	2.2382512 *
33 H	9.1645225	8.5934276	6.4311910	5.1102040
34 H	6.3398446	6.6860352	5.4662411	4.8091117
35 H	6.7320291	7.3951360	6.3040601	5.8957651

H H H H

1 CO	4.6449359	6.4444788	6.6971186	5.2859934
2 C	10.0384862	11.4636900	10.8758536	8.6191127
3 C	9.8682605	11.5343287	11.2424384	9.1515330
4 C	8.6043822	10.3913609	10.3213859	8.4113417
5 C	7.4116462	9.0742826	8.9225304	7.0107173
6 C	7.5887643	8.9266812	8.3915414	6.2337101
7 C	9.0267656	10.2677508	9.5325927	7.2265454
8 C	9.6262483	10.5695107	9.5050268	7.0639662
9 C	9.0027926	9.6718216	8.3944265	5.9112579
10 C	7.5877423	8.2612908	7.0926088	4.6575211
11 C	6.7699281	7.8130268	7.0577747	4.8225772
12 N	5.3106134	6.4256050	5.9252195	3.9615977
13 C	4.7969159	5.4418713	4.6503689	2.6339024 *
14 C	3.4999064	3.9840443	3.4973405	2.2020383 *
15 C	2.1931478 *	3.4373387	3.9336557	3.4527346
16 C	1.1063412 *	2.1878155 *	3.4755254	3.9483581
17 C	2.1987187 *	1.1035437 *	2.1986149 *	3.4527341
18 C	3.4726841	2.2005721 *	1.1049708 *	2.1819252 *
19 C	3.9483142	3.4569169	2.1883729 *	1.1064843 *
20 O	2.6845140 *	4.6440367	5.3962899	4.6936526
21 N	6.1994627	8.0399347	8.2267865	6.6423100
22 H	11.0840274	12.4325416	11.7147154	9.3814020
23 H	10.7973416	12.5444561	12.3206489	10.2500087
24 H	8.6979433	10.6535522	10.8225190	9.0791613
25 H	10.7295629	11.6496924	10.5108310	8.0406894
26 H	9.6988007	10.1409702	8.6343942	6.1346394
27 H	7.2964323	7.6705053	6.2821182	3.8165477
28 H	5.6518793	5.8994010	4.6207761	2.2382512 *
29 H	0.0000000	2.5142102 *	4.3862106	5.0544503
30 H	2.5142102 *	0.0000000	2.5429360 *	4.3700125
31 H	4.3862106	2.5429360 *	0.0000000	2.5117599 *
32 H	5.0544503	4.3700125	2.5117599 *	0.0000000
33 H	2.2999443 *	4.6242491	5.8224822	5.4756755
34 H	6.1563228	7.8641984	8.0049020	6.4754434
35 H	6.5472514	8.5872264	9.0103707	7.5692874

H H H

1	CO	2.6567721 *	2.4910981 *	2.5989643 *
2	C	8.1010387	4.7382020	4.7092840
3	C	7.7771310	4.2609364	3.8934105
4	C	6.4675928	2.9910463 *	2.4632859 *
5	C	5.3827407	2.1065380 *	2.0757888 *
6	C	5.8042683	3.0078318	3.4109784
7	C	7.2587702	4.2547348	4.5381499
8	C	8.0818687	5.4061622	5.8691041
9	C	7.7295991	5.6346654	6.2984290
10	C	6.4077184	4.8030586	5.5653095
11	C	5.3094820	3.4544900	4.1635030
12	N	3.9544911	3.1522421	3.9219103
13	C	4.0362683	4.0939712	5.0523913
14	C	3.3356610	4.7442447	5.6344961
15	C	2.0474113 *	4.6757423	5.3131824
16	C	2.5070711 *	5.8514150	6.4417743
17	C	3.9292816	6.9187902	7.6843562
18	C	4.7360187	7.0057155	7.9484041
19	C	4.4933934	6.0440017	7.0463803
20	O	0.9917083 *	3.7854676	4.0778413
21	N	4.1125634	1.0446686 *	1.0392980 *
22	H	9.1786541	5.8063746	5.7924221
23	H	8.6501315	5.0908912	4.5616940
24	H	6.4881381	3.1177073	2.1897181 *
25	H	9.1645225	6.3398446	6.7320291
26	H	8.5934276	6.6860352	7.3951360
27	H	6.4311910	5.4662411	6.3040601
28	H	5.1102040	4.8091117	5.8957651
29	H	2.2999443 *	6.1563228	6.5472514
30	H	4.6242491	7.8641984	8.5872264
31	H	5.8224822	8.0049020	9.0103707
32	H	5.4756755	6.4754434	7.5692874
33	H	0.0000000	4.2610747	4.3424536
34	H	4.2610747	0.0000000	1.6695347 *
35	H	4.3424536	1.6695347 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.86 , TOTAL = 3739.0 SECONDS (62.3 MIN)
WALL CLOCK TIME: STEP = 0.86 , TOTAL = 3456.7 SECONDS (57.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.09 , TOTAL = 3740.0 SECONDS (62.3 MIN)
WALL CLOCK TIME: STEP = 1.08 , TOTAL = 3457.8 SECONDS (57.6 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.633366828	-284.633366828	0.014571168	0.000878882	196664740
11431991						
2	1	-284.633448795	-0.000081967	0.003636979	0.000121750	157998075
14695423						
3	2	-284.633448157	0.000000638	0.000791167	0.000250940	142407524
15960884						
4	3	-284.633450236	-0.000002079	0.000981223	0.000087603	135308245
16517894						
5	4	-284.633450020	0.000000216	0.000453750	0.000144100	132000700
16803824						
6	5	-284.633450449	-0.000000429	0.000208097	0.000029897	125462137
17289225						
7	6	-284.633450467	-0.000000018	0.000165615	0.000024177	121289266
17576018						
8	7	-284.633450537	-0.000000070	0.000300685	0.000023613	113433028
18205419						
9	8	-284.633450591	-0.000000054	0.000349393	0.000023744	142236750
16095480						
10	9	-284.633450623	-0.000000033	0.000218719	0.000021117	161773450
14557649						
11	10	-284.633450661	-0.000000038	0.000482803	0.000019057	158433895
14772847						
-----DISABLING FDIFF OPTION-----						
12	11	-284.633450708	-0.000000047	0.000298461	0.000023776	196671914
11431199						
13	12	-284.633450730	-0.000000022	0.000183499	0.000015937	196671803
11431205						
14	13	-284.633450737	-0.000000008	0.000076478	0.000010742	196671867
11431205						
15	14	-284.633450742	-0.000000005	0.000039937	0.000003803	196671883
11431198						

16 15	-284.633450743	-0.000000001	0.000035158	0.000003314	196671880
11431201					
17 16	-284.633450744	-0.000000001	0.000046892	0.000003210	196671877
11431203					
18 17	-284.633450745	-0.000000001	0.000076580	0.000002843	196671861
11431204					
19 18	-284.633450747	-0.000000001	0.000062632	0.000002569	196671910
11431202					
20 19	-284.633450748	-0.000000001	0.000038929	0.000002912	196671820
11431203					
21 20	-284.633450748	-0.000000001	0.000046883	0.000002980	196671634
11431205					
22 21	-284.633450749	-0.000000001	0.000057885	0.000002850	196671733
11431204					
23 22	-284.633450750	-0.000000001	0.000030571	0.000002204	196671722
11431204					
24 23	-284.633450750	0.000000000	0.000031324	0.000001741	196671722
11431204					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 80.8 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 25.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.1 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6334507503 AFTER 24 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6056141499
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000176262

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 84.49 , TOTAL = 3824.5 SECONDS (63.7 MIN)
WALL CLOCK TIME: STEP = 77.66 , TOTAL = 3535.5 SECONDS (58.9 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.84, TOTAL = 3828.4 SECONDS (63.8 MIN)
WALL CLOCK TIME: STEP = 3.82, TOTAL = 3539.3 SECONDS (59.0 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.92, TOTAL = 3831.3 SECONDS (63.9 MIN)
WALL CLOCK TIME: STEP = 2.75, TOTAL = 3542.1 SECONDS (59.0 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 35 ENERGY= -284.6334508

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0004390	-0.0006430	-0.0004816
2 C	6.0	0.0000309	-0.0002531	0.0005050
3 C	6.0	0.0003167	-0.0011809	0.0000176
4 C	6.0	-0.0002614	0.0006512	0.0001674
5 C	6.0	0.0001794	-0.0003063	-0.0003650
6 C	6.0	-0.0004319	0.0002069	0.0002235
7 C	6.0	0.0002521	-0.0005784	0.0004728
8 C	6.0	-0.0004287	-0.0006523	-0.0001148
9 C	6.0	-0.0009050	0.0002659	-0.0001222
10 C	6.0	0.0003564	0.0008805	0.0002438
11 C	6.0	-0.0003871	0.0001838	0.0002233
12 N	7.0	0.0006179	-0.0003622	0.0000343
13 C	6.0	0.0002042	-0.0001119	0.0002144
14 C	6.0	0.0001997	-0.0001784	-0.0000716
15 C	6.0	0.0006678	0.0001157	-0.0008272
16 C	6.0	0.0000831	0.0002132	-0.0003826
17 C	6.0	-0.0006056	0.0003228	-0.0005109
18 C	6.0	0.0003419	0.0001618	-0.0001766
19 C	6.0	-0.0002576	-0.0003253	0.0004211

20 O	8.0	-0.0005359	-0.0002633	0.0010365
21 N	7.0	0.0001071	0.0002913	0.0002170
22 H	1.0	-0.0007601	-0.0000871	-0.0006054
23 H	1.0	0.0007923	-0.0001467	-0.0008719
24 H	1.0	0.0006015	-0.0002236	0.0005160
25 H	1.0	-0.0004833	-0.0003199	-0.0004683
26 H	1.0	-0.0001376	-0.0002418	-0.0005048
27 H	1.0	-0.0007054	0.0009503	-0.0004151
28 H	1.0	0.0005169	-0.0003026	0.0003940
29 H	1.0	0.0000053	0.0003830	0.0003084
30 H	1.0	0.0011740	0.0001615	0.0000028
31 H	1.0	-0.0005262	0.0002595	-0.0002867
32 H	1.0	-0.0005079	0.0006728	0.0014683
33 H	1.0	0.0007631	-0.0006962	-0.0013811
34 H	1.0	-0.0005205	0.0001190	-0.0000566
35 H	1.0	0.0006829	0.0010338	0.0011764

MAXIMUM GRADIENT = 0.0014683 RMS GRADIENT = 0.0005260
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000744020
 PREDICTED ENERGY CHANGE WAS -0.0000452809 RATIO= 1.643
 GDIIS STEP HAS LENGTH = 0.136253
 RADIUS OF STEP TAKEN= 0.05927 CURRENT TRUST RADIUS= 0.05927

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 3831.3 SECONDS (63.9 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 3542.1 SECONDS (59.0
 MIN)
 CPU UTILIZATION: STEP = 92.22% , TOTAL = 100.00%

INSERCH= 36

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z

CO	27.0	0.1252089344	-1.7486898980	1.0233406504
C	6.0	4.9883879498	0.6815354738	0.4431029012
C	6.0	5.2182145513	-0.6802700333	0.2130445110
C	6.0	4.0890017023	-1.5493132427	0.0774980020
C	6.0	2.7719411996	-1.0606727207	0.1795539022
C	6.0	2.4740509690	0.3312566715	0.4927565635
C	6.0	3.6496735652	1.2060265386	0.5903455670
C	6.0	3.4935981781	2.6205248750	0.8228727198
C	6.0	2.2263227900	3.1912698705	1.0002703115
C	6.0	1.0726997166	2.3504014776	0.9758787316

C	6.0	1.1656933252	0.9628416453	0.7087769448
N	7.0	-0.0494827425	0.1538758894	0.7307740727
C	6.0	-1.2519169678	0.6975004929	0.5407214099
C	6.0	-2.5638223146	0.0501156914	0.5835098680
C	6.0	-2.8599922010	-1.3448823521	0.7582935952
C	6.0	-4.1703106338	-1.8548844501	0.7393136814
C	6.0	-5.2627274636	-0.9572890081	0.5425723349
C	6.0	-5.0265176347	0.4377974718	0.3876049365
C	6.0	-3.6991599587	0.9271484422	0.4114403958
O	8.0	-1.7609842283	-2.2863501917	0.9740817942
N	7.0	1.6923004659	-2.0703037977	-0.1321366147
H	1.0	5.8332710824	1.3900520001	0.5114351501
H	1.0	6.2415909887	-1.0825875936	0.1022196298
H	1.0	4.2632148820	-2.6207509727	-0.1457350614
H	1.0	4.4016283233	3.2482931253	0.8622783409
H	1.0	2.1107724221	4.2740015014	1.1843177649
H	1.0	0.0991471538	2.8202143911	1.2019541278
H	1.0	-1.2963070179	1.7737832911	0.2930254217
H	1.0	-4.3644230878	-2.9359917088	0.8780365802
H	1.0	-6.2914747091	-1.3584688412	0.5198829429
H	1.0	-5.8724121084	1.1353496924	0.2486092453
H	1.0	-3.5184164812	2.0129594917	0.3060565095
H	1.0	-2.0881310492	-3.2208180323	1.0242668423
H	1.0	1.3773511227	-1.9558645373	-1.1218262727
H	1.0	2.1180062759	-3.0167056527	-0.0652504997

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4674657	5.2665745	4.0799537
2 C	5.4674657	0.0000000	1.4000933 *	2.4329506 *
3 C	5.2665745	1.4000933 *	0.0000000	1.4313387 *
4 C	4.0799537	2.4329506 *	1.4313387 *	0.0000000
5 C	2.8619111 *	2.8314985 *	2.4759001 *	1.4084862 *
6 C	3.1819422	2.5391044 *	2.9380025 *	2.5133740 *
7 C	4.6194897	1.4453122 *	2.4820942 *	2.8368855 *
8 C	5.5205318	2.4775596 *	3.7737831	4.2775739
9 C	5.3682785	3.7733548	4.9558008	5.1763124
10 C	4.2074388	4.2897061	5.1915488	5.0112813
11 C	2.9212945 *	3.8422272	4.4009652	3.9057864
12 N	1.9328396 *	5.0735905	5.3584026	4.5226846
13 C	2.8483758 *	6.2410888	6.6233093	5.8127584
14 C	3.2649719	7.5798605	7.8250115	6.8610705
15 C	3.0240265	8.1118916	8.1238187	6.9852552

16 C	4.3062091	9.5080454	9.4763434	8.2914181
17 C	5.4669290	10.3817632	10.4897795	9.3819841
18 C	5.6325104	10.0180249	10.3070405	9.3347452
19 C	4.7074760	8.6910769	9.0632623	8.1792324
20 O	1.9619454 *	7.3921789	7.2019363	5.9640105
21 N	1.9734080 *	4.3321718	3.8057081	2.4616163 *
22 H	6.5341963	1.1047590 *	2.1802671 *	3.4453803
23 H	6.2211161	2.1906276 *	1.1051882 *	2.2027448 *
24 H	4.3875189	3.4318657	2.1923078 *	1.1082247 *
25 H	6.5790230	2.6661282 *	4.0647172	4.8714107
26 H	6.3435942	4.6621758	5.9282691	6.2489548
27 H	4.5724685	5.3902206	6.2798236	6.0229654
28 H	3.8680596	6.3806676	6.9618795	6.3317433
29 H	4.6462452	10.0374670	9.8669873	8.6037277
30 H	6.4482223	11.4631067	11.5337353	10.3916513
31 H	6.6999516	10.8720170	11.2383157	10.3182585
32 H	5.2858782	8.6114571	9.1428036	8.4032635
33 H	2.6582016 *	8.1020513	7.7778629	6.4689465
34 H	2.4924932 *	4.7375594	4.2616022	2.9927766 *
35 H	2.6007952 *	4.7089809	3.8920009	2.4613900 *

C C C C

1 CO	2.8619111 *	3.1819422	4.6194897	5.5205318
2 C	2.8314985 *	2.5391044 *	1.4453122 *	2.4775596 *
3 C	2.4759001 *	2.9380025 *	2.4820942 *	3.7737831
4 C	1.4084862 *	2.5133740 *	2.8368855 *	4.2775739
5 C	0.0000000	1.4574985 *	2.4651753 *	3.8060299
6 C	1.4574985 *	0.0000000	1.4686165 *	2.5276871 *
7 C	2.4651753 *	1.4686165 *	0.0000000	1.4419549 *
8 C	3.8060299	2.5276871 *	1.4419549 *	0.0000000
9 C	4.3646639	2.9152384 *	2.4769249 *	1.4011448 *
10 C	3.8931969	2.5048230 *	2.8458784 *	2.4407226 *
11 C	2.6371802 *	1.4687968 *	2.4986642 *	2.8600826 *
12 N	3.1208020	2.5409326 *	3.8484411	4.3181317
13 C	4.4060242	3.7442319	4.9281488	5.1281133
14 C	5.4651078	5.0465279	6.3201035	6.5845760
15 C	5.6687202	5.5974966	6.9936465	7.4897754
16 C	7.0099190	6.9991103	8.3990190	8.8753461
17 C	8.0435298	7.8435051	9.1713199	9.4632214
18 C	7.9438441	7.5020622	8.7124952	8.8060281
19 C	6.7735039	6.2024376	7.3562989	7.4008493
20 O	4.7624545	5.0019059	6.4512918	7.1910308
21 N	1.5106720 *	2.6017529 *	3.8842799	5.1147424
22 H	3.9354717	3.5221806	2.1927586 *	2.6617900 *
23 H	3.4705807	4.0429980	3.4919991	4.6673169

24 H	2.1825568 *	3.5104313	3.9449301	5.3853025
25 H	4.6571643	3.5158502	2.1932251 *	1.1046106 *
26 H	5.4685870	4.0193861	3.4833160	2.1855971 *
27 H	4.8218684	3.5125546	3.9478988	3.4213852
28 H	4.9596028	4.0418282	4.9873310	4.8929440
29 H	7.4116391	7.5886811	9.0257867	9.6242619
30 H	9.0746909	8.9269451	10.2668413	10.5674900
31 H	8.9191999	8.3886602	9.5284781	9.5004038
32 H	7.0022723	6.2267686	7.2189664	7.0572363
33 H	5.3851713	5.8063106	7.2600029	8.0819272
34 H	2.1070928 *	3.0067510	4.2535323	5.4040444
35 H	2.0769268 *	3.4127689	4.5395240	5.8702116

C C C N

1 CO	5.3682785	4.2074388	2.9212945 *	1.9328396 *
2 C	3.7733548	4.2897061	3.8422272	5.0735905
3 C	4.9558008	5.1915488	4.4009652	5.3584026
4 C	5.1763124	5.0112813	3.9057864	4.5226846
5 C	4.3646639	3.8931969	2.6371802 *	3.1208020
6 C	2.9152384 *	2.5048230 *	1.4687968 *	2.5409326 *
7 C	2.4769249 *	2.8458784 *	2.4986642 *	3.8484411
8 C	1.4011448 *	2.4407226 *	2.8600826 *	4.3181317
9 C	0.0000000	1.4277608 *	2.4851148 *	3.8049548
10 C	1.4277608 *	0.0000000	1.4160909 *	2.4787284 *
11 C	2.4851148 *	1.4160909 *	0.0000000	1.4599871 *
12 N	3.8049548	2.4787284 *	1.4599871 *	0.0000000
13 C	4.3044422	2.8853572 *	2.4379270 *	1.3332276 *
14 C	5.7433465	4.3208287	3.8416204	2.5207849 *
15 C	6.8195183	5.4007899	4.6404941	3.1852782
16 C	8.1516066	6.7252918	6.0343559	4.5843662
17 C	8.5735583	7.1600425	6.7111191	5.3336693
18 C	7.7820732	6.4190788	6.2227244	4.9969243
19 C	6.3705818	5.0114753	4.8740620	3.7443382
20 O	6.7752214	5.4340808	4.3809903	2.9905082 *
21 N	5.4084825	4.5993737	3.1913041	2.9538786 *
22 H	4.0612094	4.8786288	4.6912402	6.0152335
23 H	5.9325148	6.2662693	5.5060357	6.4421682
24 H	6.2643311	6.0124671	4.8132075	5.2025170
25 H	2.1804237 *	3.4497652	3.9646092	5.4226471
26 H	1.1043247 *	2.1957411 *	3.4760744	4.6741672
27 H	2.1686942 *	1.1043726 *	2.1978576 *	2.7117268 *
28 H	3.8624324	2.5319894 *	2.6252469 *	2.0905250 *
29 H	8.9997893	7.5840511	6.7684369	5.3092069
30 H	9.6687005	8.2580092	7.8123952	6.4260505
31 H	8.3893569	7.0880075	7.0552421	5.9247177

32 H	5.9052839	4.6519756	4.8172415	3.9585450
33 H	7.7285160	6.4055975	5.3094176	3.9535786
34 H	5.6317883	4.7996985	3.4517753	3.1494424
35 H	6.2996847	5.5661885	4.1644706	3.9222763

C C C C

1 CO	2.8483758 *	3.2649719	3.0240265	4.3062091
2 C	6.2410888	7.5798605	8.1118916	9.5080454
3 C	6.6233093	7.8250115	8.1238187	9.4763434
4 C	5.8127584	6.8610705	6.9852552	8.2914181
5 C	4.4060242	5.4651078	5.6687202	7.0099190
6 C	3.7442319	5.0465279	5.5974966	6.9991103
7 C	4.9281488	6.3201035	6.9936465	8.3990190
8 C	5.1281133	6.5845760	7.4897754	8.8753461
9 C	4.3044422	5.7433465	6.8195183	8.1516066
10 C	2.8853572 *	4.3208287	5.4007899	6.7252918
11 C	2.4379270 *	3.8416204	4.6404941	6.0343559
12 N	1.3332276 *	2.5207849 *	3.1852782	4.5843662
13 C	0.0000000	1.4635688 *	2.6085573 *	3.8821552
14 C	1.4635688 *	0.0000000	1.4367622 *	2.4968190 *
15 C	2.6085573 *	1.4367622 *	0.0000000	1.4061994 *
16 C	3.8821552	2.4968190 *	1.4061994 *	0.0000000
17 C	4.3387709	2.8810812 *	2.4433381 *	1.4275011 *
18 C	3.7866213	2.5007087 *	2.8300512 *	2.4724846 *
19 C	2.4613919 *	1.4449173 *	2.4467598 *	2.8406321 *
20 O	3.0578286	2.5012333 *	1.4631284 *	2.4588885 *
21 N	4.0965711	4.8086287	4.6949410	5.9309392
22 H	7.1190150	8.5036346	9.1166678	10.5191819
23 H	7.7145096	8.8910045	9.1289675	10.4599248
24 H	6.4729201	7.3670729	7.2928175	8.5143535
25 H	6.2106776	7.6696514	8.5929742	9.9767569
26 H	4.9510863	6.3288243	7.5141103	8.7871085
27 H	2.6016374 *	3.8919566	5.1284863	6.3481379
28 H	1.1053092 *	2.1591679 *	3.5196109	4.6504085
29 H	4.7962216	3.4993923	2.1930070 *	1.1071209 *
30 H	5.4428473	3.9854173	3.4397815	2.1895012 *
31 H	4.6503781	3.4980934	3.9352259	3.4755489
32 H	2.6310682 *	2.2002241 *	3.4515421	3.9462507
33 H	4.0356276	3.3345999	2.0458852 *	2.5064805 *
34 H	4.0886992	4.7397232	4.6758131	5.8524004
35 H	5.0516247	5.6343413	5.3154197	6.4451595

C C C O

1 CO	5.4669290	5.6325104	4.7074760	1.9619454 *
------	-----------	-----------	-----------	-------------

2 C	10.3817632	10.0180249	8.6910769	7.3921789
3 C	10.4897795	10.3070405	9.0632623	7.2019363
4 C	9.3819841	9.3347452	8.1792324	5.9640105
5 C	8.0435298	7.9438441	6.7735039	4.7624545
6 C	7.8435051	7.5020622	6.2024376	5.0019059
7 C	9.1713199	8.7124952	7.3562989	6.4512918
8 C	9.4632214	8.8060281	7.4008493	7.1910308
9 C	8.5735583	7.7820732	6.3705818	6.7752214
10 C	7.1600425	6.4190788	5.0114753	5.4340808
11 C	6.7111191	6.2227244	4.8740620	4.3809903
12 N	5.3336693	4.9969243	3.7443382	2.9905082 *
13 C	4.3387709	3.7866213	2.4613919 *	3.0578286
14 C	2.8810812 *	2.5007087 *	1.4449173 *	2.5012333 *
15 C	2.4433381 *	2.8300512 *	2.4467598 *	1.4631284 *
16 C	1.4275011 *	2.4724846 *	2.8406321 *	2.4588885 *
17 C	0.0000000	1.4234031 *	2.4521508 *	3.7702533
18 C	1.4234031 *	0.0000000	1.4148890 *	4.2928597
19 C	2.4521508 *	1.4148890 *	0.0000000	3.7946889
20 O	3.7702533	4.2928597	3.7946889	0.0000000
21 N	7.0757648	7.1904951	6.1925795	3.6325708
22 H	11.3416120	10.9021619	9.5441878	8.4500112
23 H	11.5134249	11.3737983	10.1465849	8.1394348
24 H	9.6945578	9.7948099	8.7348410	6.1365127
25 H	10.5446150	9.8495755	8.4388233	8.2838741
26 H	9.0634838	8.1419974	6.7493762	7.6205586
27 H	6.5919660	5.7106492	4.3169141	5.4395787
28 H	4.8221904	3.9633666	2.5503951 *	4.1429997
29 H	2.1988068 *	3.4729448	3.9476751	2.6849865 *
30 H	1.1044369 *	2.2009513 *	3.4577307	4.6467843
31 H	2.1993786 *	1.1051861 *	2.1892662 *	5.3979792
32 H	3.4526710	2.1822362 *	1.1057846 *	4.6924290
33 H	3.9285692	4.7354959	4.4918366	0.9913494 *
34 H	6.9179491	7.0012524	6.0360281	3.7882978
35 H	7.6867338	7.9487667	7.0441921	4.0816906

N H H H

1 CO	1.9734080 *	6.5341963	6.2211161	4.3875189
2 C	4.3321718	1.1047590 *	2.1906276 *	3.4318657
3 C	3.8057081	2.1802671 *	1.1051882 *	2.1923078 *
4 C	2.4616163 *	3.4453803	2.2027448 *	1.1082247 *
5 C	1.5106720 *	3.9354717	3.4705807	2.1825568 *
6 C	2.6017529 *	3.5221806	4.0429980	3.5104313
7 C	3.8842799	2.1927586 *	3.4919991	3.9449301
8 C	5.1147424	2.6617900 *	4.6673169	5.3853025
9 C	5.4084825	4.0612094	5.9325148	6.2643311

10 C	4.5993737	4.8786288	6.2662693	6.0124671
11 C	3.1913041	4.6912402	5.5060357	4.8132075
12 N	2.9538786 *	6.0152335	6.4421682	5.2025170
13 C	4.0965711	7.1190150	7.7145096	6.4729201
14 C	4.8086287	8.5036346	8.8910045	7.3670729
15 C	4.6949410	9.1166678	9.1289675	7.2928175
16 C	5.9309392	10.5191819	10.4599248	8.5143535
17 C	7.0757648	11.3416120	11.5134249	9.6945578
18 C	7.1904951	10.9021619	11.3737983	9.7948099
19 C	6.1925795	9.5441878	10.1465849	8.7348410
20 O	3.6325708	8.4500112	8.1394348	6.1365127
21 N	0.0000000	5.4346927	4.6611748	2.6292162 *
22 H	5.4346927	0.0000000	2.5393166 *	4.3570047
23 H	4.6611748	2.5393166 *	0.0000000	2.5182137 *
24 H	2.6292162 *	4.3570047	2.5182137 *	0.0000000
25 H	6.0511810	2.3718668 *	4.7665165	5.9565869
26 H	6.4929485	4.7567775	6.8503755	7.3443625
27 H	5.3136714	5.9499881	7.3600880	6.9828239
28 H	4.8876930	7.1432371	8.0631984	7.1001920
29 H	6.2011100	11.0834118	10.7946530	8.6938842
30 H	8.0419217	12.4323730	12.5430574	10.6507218
31 H	8.2247224	11.7114034	12.3162391	10.8164104
32 H	6.6345025	9.3746602	10.2411770	9.0680304
33 H	4.1173553	9.1799635	8.6490733	6.4860296
34 H	1.0448804 *	5.8067136	5.0913388	3.1181786
35 H	1.0398921 *	5.7926913	4.5577198	2.1829287 *

H H H H

1 CO	6.5790230	6.3435942	4.5724685	3.8680596
2 C	2.6661282 *	4.6621758	5.3902206	6.3806676
3 C	4.0647172	5.9282691	6.2798236	6.9618795
4 C	4.8714107	6.2489548	6.0229654	6.3317433
5 C	4.6571643	5.4685870	4.8218684	4.9596028
6 C	3.5158502	4.0193861	3.5125546	4.0418282
7 C	2.1932251 *	3.4833160	3.9478988	4.9873310
8 C	1.1046106 *	2.1855971 *	3.4213852	4.8929440
9 C	2.1804237 *	1.1043247 *	2.1686942 *	3.8624324
10 C	3.4497652	2.1957411 *	1.1043726 *	2.5319894 *
11 C	3.9646092	3.4760744	2.1978576 *	2.6252469 *
12 N	5.4226471	4.6741672	2.7117268 *	2.0905250 *
13 C	6.2106776	4.9510863	2.6016374 *	1.1053092 *
14 C	7.6696514	6.3288243	3.8919566	2.1591679 *
15 C	8.5929742	7.5141103	5.1284863	3.5196109
16 C	9.9767569	8.7871085	6.3481379	4.6504085
17 C	10.5446150	9.0634838	6.5919660	4.8221904

18 C	9.8495755	8.1419974	5.7106492	3.9633666
19 C	8.4388233	6.7493762	4.3169141	2.5503951 *
20 O	8.2838741	7.6205586	5.4395787	4.1429997
21 N	6.0511810	6.4929485	5.3136714	4.8876930
22 H	2.3718668 *	4.7567775	5.9499881	7.1432371
23 H	4.7665165	6.8503755	7.3600880	8.0631984
24 H	5.9565869	7.3443625	6.9828239	7.1001920
25 H	0.0000000	2.5305746 *	4.3370468	5.9130952
26 H	2.5305746 *	0.0000000	2.4820242 *	4.3189910
27 H	4.3370468	2.4820242 *	0.0000000	1.9668406 *
28 H	5.9130952	4.3189910	1.9668406 *	0.0000000
29 H	10.7279674	9.6956674	7.2912475	5.6513321
30 H	11.6482592	10.1372557	7.6659417	5.9003532
31 H	10.5069989	8.6289003	6.2775119	4.6206394
32 H	8.0350819	6.1295531	3.8132741	2.2349822 *
33 H	9.1647486	8.5923644	6.4272725	5.1095735
34 H	6.3376794	6.6833703	5.4630294	4.8021377
35 H	6.7324178	7.3970186	6.3048581	5.8936136

H H H H

1 CO	4.6462452	6.4482223	6.6999516	5.2858782
2 C	10.0374670	11.4631067	10.8720170	8.6114571
3 C	9.8669873	11.5337353	11.2383157	9.1428036
4 C	8.6037277	10.3916513	10.3182585	8.4032635
5 C	7.4116391	9.0746909	8.9191999	7.0022723
6 C	7.5886811	8.9269451	8.3886602	6.2267686
7 C	9.0257867	10.2668413	9.5284781	7.2189664
8 C	9.6242619	10.5674900	9.5004038	7.0572363
9 C	8.9997893	9.6687005	8.3893569	5.9052839
10 C	7.5840511	8.2580092	7.0880075	4.6519756
11 C	6.7684369	7.8123952	7.0552421	4.8172415
12 N	5.3092069	6.4260505	5.9247177	3.9585450
13 C	4.7962216	5.4428473	4.6503781	2.6310682 *
14 C	3.4993923	3.9854173	3.4980934	2.2002241 *
15 C	2.1930070 *	3.4397815	3.9352259	3.4515421
16 C	1.1071209 *	2.1895012 *	3.4755489	3.9462507
17 C	2.1988068 *	1.1044369 *	2.1993786 *	3.4526710
18 C	3.4729448	2.2009513 *	1.1051861 *	2.1822362 *
19 C	3.9476751	3.4577307	2.1892662 *	1.1057846 *
20 O	2.6849865 *	4.6467843	5.3979792	4.6924290
21 N	6.2011100	8.0419217	8.2247224	6.6345025
22 H	11.0834118	12.4323730	11.7114034	9.3746602
23 H	10.7946530	12.5430574	12.3162391	10.2411770
24 H	8.6938842	10.6507218	10.8164104	9.0680304
25 H	10.7279674	11.6482592	10.5069989	8.0350819

26 H	9.6956674	10.1372557	8.6289003	6.1295531
27 H	7.2912475	7.6659417	6.2775119	3.8132741
28 H	5.6513321	5.9003532	4.6206394	2.2349822 *
29 H	0.0000000	2.5160247 *	4.3870298	5.0532174
30 H	2.5160247 *	0.0000000	2.5432919 *	4.3705952
31 H	4.3870298	2.5432919 *	0.0000000	2.5129255 *
32 H	5.0532174	4.3705952	2.5129255 *	0.0000000
33 H	2.2986985 *	4.6250238	5.8222526	5.4730220
34 H	6.1585771	7.8653023	7.9995479	6.4621168
35 H	6.5511980	8.5913620	9.0102640	7.5633764

H H H

1 CO	2.6582016 *	2.4924932 *	2.6007952 *
2 C	8.1020513	4.7375594	4.7089809
3 C	7.7778629	4.2616022	3.8920009
4 C	6.4689465	2.9927766 *	2.4613900 *
5 C	5.3851713	2.1070928 *	2.0769268 *
6 C	5.8063106	3.0067510	3.4127689
7 C	7.2600029	4.2535323	4.5395240
8 C	8.0819272	5.4040444	5.8702116
9 C	7.7285160	5.6317883	6.2996847
10 C	6.4055975	4.7996985	5.5661885
11 C	5.3094176	3.4517753	4.1644706
12 N	3.9535786	3.1494424	3.9222763
13 C	4.0356276	4.0886992	5.0516247
14 C	3.3345999	4.7397232	5.6343413
15 C	2.0458852 *	4.6758131	5.3154197
16 C	2.5064805 *	5.8524004	6.4451595
17 C	3.9285692	6.9179491	7.6867338
18 C	4.7354959	7.0012524	7.9487667
19 C	4.4918366	6.0360281	7.0441921
20 O	0.9913494 *	3.7882978	4.0816906
21 N	4.1173553	1.0448804 *	1.0398921 *
22 H	9.1799635	5.8067136	5.7926913
23 H	8.6490733	5.0913388	4.5577198
24 H	6.4860296	3.1181786	2.1829287 *
25 H	9.1647486	6.3376794	6.7324178
26 H	8.5923644	6.6833703	7.3970186
27 H	6.4272725	5.4630294	6.3048581
28 H	5.1095735	4.8021377	5.8936136
29 H	2.2986985 *	6.1585771	6.5511980
30 H	4.6250238	7.8653023	8.5913620
31 H	5.8222526	7.9995479	9.0102640
32 H	5.4730220	6.4621168	7.5633764
33 H	0.0000000	4.2679491	4.3497472

34 H 4.2679491 0.0000000 1.6704210 *
35 H 4.3497472 1.6704210 * 0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80, TOTAL = 3832.1 SECONDS (63.9 MIN)
WALL CLOCK TIME: STEP = 0.79, TOTAL = 3542.9 SECONDS (59.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.05, TOTAL = 3833.2 SECONDS (63.9 MIN)
WALL CLOCK TIME: STEP = 1.05, TOTAL = 3543.9 SECONDS (59.1 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.633466651	-284.633466651	0.012008787	0.000999756	196724244
11425967						
2	1	-284.633543128	-0.000076477	0.005033356	0.000125432	157209939
14787252						
3	2	-284.633541754	0.000001374	0.001450769	0.000310182	143163832
15890735						
4	3	-284.633544712	-0.000002958	0.001303397	0.000100948	137046439
16402452						
5	4	-284.633544323	0.000000389	0.000853222	0.000160935	133842981
16645641						
6	5	-284.633544954	-0.000000631	0.000209341	0.000029585	128771885
17031596						
7	6	-284.633544960	-0.000000006	0.000132391	0.000023416	118834422
17770241						
8	7	-284.633545013	-0.000000053	0.000308598	0.000023851	111550235
18380293						
9	8	-284.633545056	-0.000000044	0.000331743	0.000024123	142121857
16098832						
10	9	-284.633545085	-0.000000029	0.000175918	0.000022540	162142643
14498627						

11 10 -284.633545113 -0.000000028 0.000327584 0.000019226 158319782
14745968

-----DISABLING FDIFF OPTION-----

12 11 -284.633545193 -0.000000080 0.000281856 0.000010757 196727763
11425516

13 12 -284.633545213 -0.000000020 0.000239083 0.000010391 196727721
11425518

14 13 -284.633545218 -0.000000006 0.000058512 0.000009428 196727636
11425519

15 14 -284.633545222 -0.000000004 0.000051590 0.000003966 196727602
11425519

16 15 -284.633545222 -0.000000001 0.000019734 0.000002592 196727586
11425523

17 16 -284.633545223 -0.000000001 0.000036435 0.000002283 196727589
11425522

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 57.0 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 18.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6335452231 AFTER 17 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6050789834
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000172517

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 59.65 , TOTAL = 3892.8 SECONDS (64.9 MIN)
WALL CLOCK TIME: STEP = 54.71 , TOTAL = 3598.6 SECONDS (60.0
MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.94, TOTAL = 3896.8 SECONDS (64.9 MIN)
 WALL CLOCK TIME: STEP = 3.92, TOTAL = 3602.6 SECONDS (60.0 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
 USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84, TOTAL = 3899.6 SECONDS (65.0 MIN)
 WALL CLOCK TIME: STEP = 2.68, TOTAL = 3605.2 SECONDS (60.1 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 36 ENERGY= -284.6335452

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0003060	-0.0007355	-0.0002675
2 C	6.0	-0.0000532	-0.0009501	0.0002206
3 C	6.0	0.0001942	-0.0001148	0.0001002
4 C	6.0	0.0002562	-0.0002179	0.0000242
5 C	6.0	-0.0000639	0.0005383	-0.0001567
6 C	6.0	-0.0001545	0.0003006	0.0001602
7 C	6.0	-0.0002497	-0.0000120	0.0004873
8 C	6.0	-0.0006490	-0.0010353	-0.0000896
9 C	6.0	-0.0007624	0.0000168	-0.0001305
10 C	6.0	0.0000395	0.0004478	0.0001007
11 C	6.0	-0.0002657	0.0000986	0.0001992
12 N	7.0	0.0002512	-0.0003093	0.0001078
13 C	6.0	0.0005910	0.0000208	0.0002090
14 C	6.0	0.0002014	0.0000460	-0.0001036
15 C	6.0	0.0007658	-0.0002509	-0.0004602
16 C	6.0	-0.0000090	0.0014019	-0.0004697
17 C	6.0	-0.0000953	-0.0001499	-0.0003808
18 C	6.0	-0.0000625	0.0001964	-0.0002099
19 C	6.0	0.0003942	-0.0000200	0.0002957
20 O	8.0	-0.0003428	-0.0006039	0.0009190
21 N	7.0	0.0001112	0.0002231	0.0000833
22 H	1.0	-0.0004413	0.0002531	-0.0004571

23 H	1.0	0.0006416	-0.0004200	-0.0008137
24 H	1.0	0.0001438	-0.0002380	0.0005642
25 H	1.0	-0.0001246	-0.0003049	-0.0004621
26 H	1.0	-0.0001563	0.0001933	-0.0005009
27 H	1.0	-0.0008260	0.0009578	-0.0003431
28 H	1.0	0.0005141	-0.0003174	0.0005285
29 H	1.0	-0.0000266	-0.0001028	0.0002296
30 H	1.0	0.0005264	0.0000967	-0.0000586
31 H	1.0	-0.0006581	0.0003603	-0.0002164
32 H	1.0	-0.0004324	0.0001790	0.0013528
33 H	1.0	0.0006870	-0.0002966	-0.0014264
34 H	1.0	-0.0005344	0.0001885	-0.0002445
35 H	1.0	0.0008962	0.0005605	0.0012090

MAXIMUM GRADIENT = 0.0014264 RMS GRADIENT = 0.0004808
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000944728
 PREDICTED ENERGY CHANGE WAS -0.0001409930 RATIO= 0.670
 GDIIS STEP HAS LENGTH = 0.169680
 RADIUS OF STEP TAKEN= 0.05927 CURRENT TRUST RADIUS= 0.05927

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 3899.6 SECONDS (65.0 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 3605.3 SECONDS (60.1 MIN)
 CPU UTILIZATION: STEP = 92.72% , TOTAL = 100.00%

INSERCH= 37

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1279229542	-1.7517149064	1.0238669266
C	6.0	4.9874899551	0.6834773621	0.4425633233
C	6.0	5.2168315840	-0.6793173630	0.2137856703
C	6.0	4.0883601245	-1.5487732961	0.0772885858
C	6.0	2.7718728335	-1.0600632845	0.1778411865
C	6.0	2.4740566067	0.3319554576	0.4915585141
C	6.0	3.6489098333	1.2076509435	0.5890556740
C	6.0	3.4920846043	2.6217819488	0.8233477721
C	6.0	2.2245299638	3.1910025646	1.0019604739
C	6.0	1.0713492605	2.3479977382	0.9781216439
C	6.0	1.1658241310	0.9612564035	0.7095383492
N	7.0	-0.0485655111	0.1515386487	0.7325306955
C	6.0	-1.2502562566	0.6953980745	0.5405484924

C	6.0	-2.5622483077	0.0487910714	0.5832861593
C	6.0	-2.8592408003	-1.3450398827	0.7632757813
C	6.0	-4.1704276098	-1.8536286341	0.7452428451
C	6.0	-5.2628146556	-0.9558932280	0.5460060176
C	6.0	-5.0246940745	0.4387115030	0.3847802367
C	6.0	-3.6961717327	0.9257209870	0.4054191640
O	8.0	-1.7602618150	-2.2872607011	0.9766943717
N	7.0	1.6923427251	-2.0694788661	-0.1375097470
H	1.0	5.8332830712	1.3911790455	0.5136789855
H	1.0	6.2395238248	-1.0833442818	0.1066370135
H	1.0	4.2597350040	-2.6213093799	-0.1457546775
H	1.0	4.4008566159	3.2490807691	0.8633137918
H	1.0	2.1077848690	4.2737786016	1.1863905947
H	1.0	0.0977860599	2.8157686817	1.2078458002
H	1.0	-1.2939296960	1.7717689695	0.2920701915
H	1.0	-4.3653647807	-2.9347707889	0.8841068331
H	1.0	-6.2929890343	-1.3552152730	0.5239229393
H	1.0	-5.8694346254	1.1369967887	0.2433699690
H	1.0	-3.5124261556	2.0099431313	0.2920219519
H	1.0	-2.0904353613	-3.2204500260	1.0300606815
H	1.0	1.3760542289	-1.9494996981	-1.1265097724
H	1.0	2.1186591667	-3.0169340806	-0.0774694385

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4665772	5.2633886	4.0770404
2 C	5.4665772	0.0000000	1.4007663 *	2.4340918 *
3 C	5.2633886	1.4007663 *	0.0000000	1.4310950 *
4 C	4.0770404	2.4340918 *	1.4310950 *	0.0000000
5 C	2.8608762 *	2.8317788 *	2.4746884 *	1.4078661 *
6 C	3.1826683	2.5383686 *	2.9364341 *	2.5129139 *
7 C	4.6199844	1.4449964 *	2.4819056 *	2.8377626 *
8 C	5.5213464	2.4775509 *	3.7740661	4.2785137
9 C	5.3690499	3.7728710	4.9552462	5.1763265
10 C	4.2071118	4.2887771	5.1897851	5.0098582
11 C	2.9216870 *	3.8410372	4.3986264	3.9039987
12 N	1.9334940 *	5.0723658	5.3557282	4.5204598
13 C	2.8497959 *	6.2385271	6.6196557	5.8096248
14 C	3.2669488	7.5776763	7.8218129	6.8584866
15 C	3.0259609	8.1110371	8.1220731	6.9843571
16 C	4.3085770	9.5076798	9.4753411	8.2913614
17 C	5.4700763	10.3810877	10.4885580	9.3816668
18 C	5.6352340	10.0153421	10.3037894	9.3323311

19	C	4.7090170	8.6871193	9.0583939	8.1749451
20	O	1.9632311 *	7.3920724	7.2005100	5.9632770
21	N	1.9741274 *	4.3328106	3.8049940	2.4613354 *
22	H	6.5336979	1.1051086 *	2.1810327 *	3.4465218
23	H	6.2160836	2.1913681 *	1.1048158 *	2.2011340 *
24	H	4.3813331	3.4347286	2.1946836 *	1.1088062 *
25	H	6.5796426	2.6652374 *	4.0644820	4.8718470
26	H	6.3445125	4.6622144	5.9283464	6.2493917
27	H	4.5712868	5.3890192	6.2776117	6.0209690
28	H	3.8693837	6.3767750	6.9572958	6.3278097
29	H	4.6485254	10.0380562	9.8668581	8.6044994
30	H	6.4525396	11.4635114	11.5338196	10.3927550
31	H	6.7023972	10.8682183	11.2341075	10.3149707
32	H	5.2856229	8.6041123	9.1344504	8.3953871
33	H	2.6605140 *	8.1044944	7.7794479	6.4714598
34	H	2.4942074 *	4.7367739	4.2616107	2.9943806 *
35	H	2.6032195 *	4.7110157	3.8920372	2.4615377 *

C C C C

1	CO	2.8608762 *	3.1826683	4.6199844	5.5213464
2	C	2.8317788 *	2.5383686 *	1.4449964 *	2.4775509 *
3	C	2.4746884 *	2.9364341 *	2.4819056 *	3.7740661
4	C	1.4078661 *	2.5129139 *	2.8377626 *	4.2785137
5	C	0.0000000	1.4576794 *	2.4659317 *	3.8067530
6	C	1.4576794 *	0.0000000	1.4685464 *	2.5277995 *
7	C	2.4659317 *	1.4685464 *	0.0000000	1.4419617 *
8	C	3.8067530	2.5277995 *	1.4419617 *	0.0000000
9	C	4.3646670	2.9149484 *	2.4764959 *	1.4009316 *
10	C	3.8919287	2.5037488 *	2.8452736 *	2.4410802 *
11	C	2.6358732 *	1.4679942 *	2.4981875 *	2.8603820 *
12	N	3.1193801	2.5405197 *	3.8480232	4.3181655
13	C	4.4034899	3.7423251	4.9261125	5.1264732
14	C	5.4632218	5.0450930	6.3183443	6.5827698
15	C	5.6686318	5.5973391	6.9930400	7.4885658
16	C	7.0105083	6.9993074	8.3986823	8.8740911
17	C	8.0437926	7.8435130	9.1706930	9.4617619
18	C	7.9420152	7.5002707	8.7100173	8.8030482
19	C	6.7698398	6.1993302	7.3527838	7.3974534
20	O	4.7628169	5.0025096	6.4516517	7.1909219
21	N	1.5112086 *	2.6026314 *	3.8853098	5.1156863
22	H	3.9361921	3.5223354	2.1933651 *	2.6629849 *
23	H	3.4684601	4.0410372	3.4918001	4.6679821
24	H	2.1808112 *	3.5094998	3.9463896	5.3868779
25	H	4.6574868	3.5157333	2.1927328 *	1.1049741 *
26	H	5.4688257	4.0193179	3.4832476	2.1856758 *

27 H	4.8201372	3.5112757	3.9470779	3.4215102
28 H	4.9561146	4.0386358	4.9837829	4.8898580
29 H	7.4130628	7.5896824	9.0263675	9.6238496
30 H	9.0762662	8.9279719	10.2671261	10.5666375
31 H	8.9164770	8.3859129	9.5248817	9.4962626
32 H	6.9950261	6.2204046	7.2122559	7.0512286
33 H	5.3884682	5.8089720	7.2624133	8.0832502
34 H	2.1073059 *	3.0047948	4.2516629	5.4014947
35 H	2.0787532 *	3.4154299	4.5423608	5.8730646

C C C N

1 CO	5.3690499	4.2071118	2.9216870 *	1.9334940 *
2 C	3.7728710	4.2887771	3.8410372	5.0723658
3 C	4.9552462	5.1897851	4.3986264	5.3557282
4 C	5.1763265	5.0098582	3.9039987	4.5204598
5 C	4.3646670	3.8919287	2.6358732 *	3.1193801
6 C	2.9149484 *	2.5037488 *	1.4679942 *	2.5405197 *
7 C	2.4764959 *	2.8452736 *	2.4981875 *	3.8480232
8 C	1.4009316 *	2.4410802 *	2.8603820 *	4.3181655
9 C	0.0000000	1.4286536 *	2.4855858 *	3.8049831
10 C	1.4286536 *	0.0000000	1.4156673 *	2.4776918 *
11 C	2.4855858 *	1.4156673 *	0.0000000	1.4597649 *
12 N	3.8049831	2.4776918 *	1.4597649 *	0.0000000
13 C	4.3029155	2.8831247 *	2.4365309 *	1.3329294 *
14 C	5.7412566	4.3180178	3.8401897	2.5202048 *
15 C	6.8174318	5.3976128	4.6392928	3.1844290
16 C	8.1492141	6.7219135	6.0332773	4.5837326
17 C	8.5711708	7.1570980	6.7104100	5.3338158
18 C	7.7786417	6.4155415	6.2210157	4.9965242
19 C	6.3672656	5.0080052	4.8716276	3.7431793
20 O	6.7742581	5.4317257	4.3802072	2.9895254 *
21 N	5.4087226	4.5983003	3.1906220	2.9530748 *
22 H	4.0621278	4.8792646	4.6913076	6.0150434
23 H	5.9322694	6.2644730	5.5033000	6.4386913
24 H	6.2643659	6.0102342	4.8102586	5.1982232
25 H	2.1815118 *	3.4511955	3.9652519	5.4230276
26 H	1.1045578 *	2.1968629 *	3.4767055	4.6742591
27 H	2.1693844 *	1.1042682 *	2.1973237 *	2.7102518 *
28 H	3.8597573	2.5292787 *	2.6232802 *	2.0904745 *
29 H	8.9980943	7.5811834	6.7678322	5.3087698
30 H	9.6666823	8.2555170	7.8124508	6.4270250
31 H	8.3849068	7.0838453	7.0528763	5.9239280
32 H	5.9001339	4.6471508	4.8124931	3.9555083
33 H	7.7282883	6.4036857	5.3096732	3.9532347
34 H	5.6280601	4.7948725	3.4478646	3.1464162

35 H	6.3019723	5.5671918	4.1657263	3.9232872
	C	C	C	C
1 CO	2.8497959 *	3.2669488	3.0259609	4.3085770
2 C	6.2385271	7.5776763	8.1110371	9.5076798
3 C	6.6196557	7.8218129	8.1220731	9.4753411
4 C	5.8096248	6.8584866	6.9843571	8.2913614
5 C	4.4034899	5.4632218	5.6686318	7.0105083
6 C	3.7423251	5.0450930	5.5973391	6.9993074
7 C	4.9261125	6.3183443	6.9930400	8.3986823
8 C	5.1264732	6.5827698	7.4885658	8.8740911
9 C	4.3029155	5.7412566	6.8174318	8.1492141
10 C	2.8831247 *	4.3180178	5.3976128	6.7219135
11 C	2.4365309 *	3.8401897	4.6392928	6.0332773
12 N	1.3329294 *	2.5202048 *	3.1844290	4.5837326
13 C	0.0000000	1.4633012 *	2.6080310 *	3.8816025
14 C	1.4633012 *	0.0000000	1.4364420 *	2.4963316 *
15 C	2.6080310 *	1.4364420 *	0.0000000	1.4064845 *
16 C	3.8816025	2.4963316 *	1.4064845 *	0.0000000
17 C	4.3390572	2.8816382 *	2.4445467 *	1.4279123 *
18 C	3.7863614	2.5010161 *	2.8309390 *	2.4727571 *
19 C	2.4604494 *	1.4444463 *	2.4463993 *	2.8399266 *
20 O	3.0572181	2.5010178 *	1.4632438 *	2.4597776 *
21 N	4.0942882	4.8070947	4.6960770	5.9327834
22 H	7.1176796	8.5024583	9.1164228	10.5193453
23 H	7.7103184	8.8870759	9.1261808	10.4579273
24 H	6.4677325	7.3620916	7.2893770	8.5118066
25 H	6.2097141	7.6684483	8.5921456	9.9758958
26 H	4.9495817	6.3264101	7.5114241	8.7838308
27 H	2.5997068 *	3.8887045	5.1238636	6.3431002
28 H	1.1055420 *	2.1591877 *	3.5194788	4.6500660
29 H	4.7958377	3.4990518	2.1932291 *	1.1073175 *
30 H	5.4437529	3.9866257	3.4420953	2.1914984 *
31 H	4.6497455	3.4981732	3.9359973	3.4759663
32 H	2.6281565 *	2.1985882 *	3.4503105	3.9453215
33 H	4.0347725	3.3331895	2.0443579 *	2.5051327 *
34 H	4.0831451	4.7356937	4.6770060	5.8545803
35 H	5.0510343	5.6343734	5.3180420	6.4484686
	C	C	C	O
1 CO	5.4700763	5.6352340	4.7090170	1.9632311 *
2 C	10.3810877	10.0153421	8.6871193	7.3920724
3 C	10.4885580	10.3037894	9.0583939	7.2005100
4 C	9.3816668	9.3323311	8.1749451	5.9632770

5 C	8.0437926	7.9420152	6.7698398	4.7628169
6 C	7.8435130	7.5002707	6.1993302	5.0025096
7 C	9.1706930	8.7100173	7.3527838	6.4516517
8 C	9.4617619	8.8030482	7.3974534	7.1909219
9 C	8.5711708	7.7786417	6.3672656	6.7742581
10 C	7.1570980	6.4155415	5.0080052	5.4317257
11 C	6.7104100	6.2210157	4.8716276	4.3802072
12 N	5.3338158	4.9965242	3.7431793	2.9895254 *
13 C	4.3390572	3.7863614	2.4604494 *	3.0572181
14 C	2.8816382 *	2.5010161 *	1.4444463 *	2.5010178 *
15 C	2.4445467 *	2.8309390 *	2.4463993 *	1.4632438 *
16 C	1.4279123 *	2.4727571 *	2.8399266 *	2.4597776 *
17 C	0.0000000	1.4239444 *	2.4524695 *	3.7717248
18 C	1.4239444 *	0.0000000	1.4151240 *	4.2939265
19 C	2.4524695 *	1.4151240 *	0.0000000	3.7943845
20 O	3.7717248	4.2939265	3.7943845	0.0000000
21 N	7.0768270	7.1890465	6.1888676	3.6344680
22 H	11.3416568	10.9004347	9.5414297	8.4502796
23 H	11.5114326	11.3699878	10.1411863	8.1365217
24 H	9.6918056	9.7900878	8.7282111	6.1328494
25 H	10.5436727	9.8472420	8.4362039	8.2839189
26 H	9.0600937	8.1377254	6.7457630	7.6192516
27 H	6.5878301	5.7068065	4.3139639	5.4356860
28 H	4.8225172	3.9628576	2.5493944 *	4.1426921
29 H	2.1990191 *	3.4733881	3.9471962	2.6859641 *
30 H	1.1050814 *	2.2013873 *	3.4583484	4.6496588
31 H	2.1999466 *	1.1050728 *	2.1895134 *	5.3989448
32 H	3.4531946	2.1827339 *	1.1055130 *	4.6909292
33 H	3.9276605	4.7345247	4.4899110	0.9913147 *
34 H	6.9180303	6.9969371	6.0283643	3.7913096
35 H	7.6891330	7.9487519	7.0420145	4.0853045

N H H H

1 CO	1.9741274 *	6.5336979	6.2160836	4.3813331
2 C	4.3328106	1.1051086 *	2.1913681 *	3.4347286
3 C	3.8049940	2.1810327 *	1.1048158 *	2.1946836 *
4 C	2.4613354 *	3.4465218	2.2011340 *	1.1088062 *
5 C	1.5112086 *	3.9361921	3.4684601	2.1808112 *
6 C	2.6026314 *	3.5223354	4.0410372	3.5094998
7 C	3.8853098	2.1933651 *	3.4918001	3.9463896
8 C	5.1156863	2.6629849 *	4.6679821	5.3868779
9 C	5.4087226	4.0621278	5.9322694	6.2643659
10 C	4.5983003	4.8792646	6.2644730	6.0102342
11 C	3.1906220	4.6913076	5.5033000	4.8102586
12 N	2.9530748 *	6.0150434	6.4386913	5.1982232

13 C	4.0942882	7.1176796	7.7103184	6.4677325
14 C	4.8070947	8.5024583	8.8870759	7.3620916
15 C	4.6960770	9.1164228	9.1261808	7.2893770
16 C	5.9327834	10.5193453	10.4579273	8.5118066
17 C	7.0768270	11.3416568	11.5114326	9.6918056
18 C	7.1890465	10.9004347	11.3699878	9.7900878
19 C	6.1888676	9.5414297	10.1411863	8.7282111
20 O	3.6344680	8.4502796	8.1365217	6.1328494
21 N	0.0000000	5.4357692	4.6592837	2.6260404 *
22 H	5.4357692	0.0000000	2.5404685 *	4.3601571
23 H	4.6592837	2.5404685 *	0.0000000	2.5196432 *
24 H	2.6260404 *	4.3601571	2.5196432 *	0.0000000
25 H	6.0518404	2.3718956 *	4.7668820	5.9581553
26 H	6.4932442	4.7582831	6.8509780	7.3449124
27 H	5.3120840	5.9503991	7.3577636	6.9796756
28 H	4.8844188	7.1408067	8.0584725	7.0946472
29 H	6.2038900	11.0843799	10.7933267	8.6920204
30 H	8.0444508	12.4333930	12.5424049	10.6494811
31 H	8.2223496	11.7085984	12.3115996	10.8109371
32 H	6.6268998	9.3687930	10.2324642	9.0579599
33 H	4.1227861	9.1825425	8.6491706	6.4858442
34 H	1.0452533 *	5.8066550	5.0915825	3.1191062
35 H	1.0406834 *	5.7947691	4.5556767	2.1783910 *

H H H H

1 CO	6.5796426	6.3445125	4.5712868	3.8693837
2 C	2.6652374 *	4.6622144	5.3890192	6.3767750
3 C	4.0644820	5.9283464	6.2776117	6.9572958
4 C	4.8718470	6.2493917	6.0209690	6.3278097
5 C	4.6574868	5.4688257	4.8201372	4.9561146
6 C	3.5157333	4.0193179	3.5112757	4.0386358
7 C	2.1927328 *	3.4832476	3.9470779	4.9837829
8 C	1.1049741 *	2.1856758 *	3.4215102	4.8898580
9 C	2.1815118 *	1.1045578 *	2.1693844 *	3.8597573
10 C	3.4511955	2.1968629 *	1.1042682 *	2.5292787 *
11 C	3.9652519	3.4767055	2.1973237 *	2.6232802 *
12 N	5.4230276	4.6742591	2.7102518 *	2.0904745 *
13 C	6.2097141	4.9495817	2.5997068 *	1.1055420 *
14 C	7.6684483	6.3264101	3.8887045	2.1591877 *
15 C	8.5921456	7.5114241	5.1238636	3.5194788
16 C	9.9758958	8.7838308	6.3431002	4.6500660
17 C	10.5436727	9.0600937	6.5878301	4.8225172
18 C	9.8472420	8.1377254	5.7068065	3.9628576
19 C	8.4362039	6.7457630	4.3139639	2.5493944 *
20 O	8.2839189	7.6192516	5.4356860	4.1426921

21 N	6.0518404	6.4932442	5.3120840	4.8844188
22 H	2.3718956 *	4.7582831	5.9503991	7.1408067
23 H	4.7668820	6.8509780	7.3577636	8.0584725
24 H	5.9581553	7.3449124	6.9796756	7.0946472
25 H	0.0000000	2.5323038 *	4.3385341	5.9109526
26 H	2.5323038 *	0.0000000	2.4832133 *	4.3164248
27 H	4.3385341	2.4832133 *	0.0000000	1.9660756 *
28 H	5.9109526	4.3164248	1.9660756 *	0.0000000
29 H	10.7278651	9.6931020	7.2865099	5.6511713
30 H	11.6478780	10.1339744	7.6620405	5.9010491
31 H	10.5035285	8.6234981	6.2734529	4.6195836
32 H	8.0300611	6.1246729	3.8107375	2.2312448 *
33 H	9.1662154	8.5914466	6.4230722	5.1089433
34 H	6.3351453	6.6793810	5.4581103	4.7946870
35 H	6.7347190	7.3994562	6.3052664	5.8918587

H H H H

1 CO	4.6485254	6.4525396	6.7023972	5.2856229
2 C	10.0380562	11.4635114	10.8682183	8.6041123
3 C	9.8668581	11.5338196	11.2341075	9.1344504
4 C	8.6044994	10.3927550	10.3149707	8.3953871
5 C	7.4130628	9.0762662	8.9164770	6.9950261
6 C	7.5896824	8.9279719	8.3859129	6.2204046
7 C	9.0263675	10.2671261	9.5248817	7.2122559
8 C	9.6238496	10.5666375	9.4962626	7.0512286
9 C	8.9980943	9.6666823	8.3849068	5.9001339
10 C	7.5811834	8.2555170	7.0838453	4.6471508
11 C	6.7678322	7.8124508	7.0528763	4.8124931
12 N	5.3087698	6.4270250	5.9239280	3.9555083
13 C	4.7958377	5.4437529	4.6497455	2.6281565 *
14 C	3.4990518	3.9866257	3.4981732	2.1985882 *
15 C	2.1932291 *	3.4420953	3.9359973	3.4503105
16 C	1.1073175 *	2.1914984 *	3.4759663	3.9453215
17 C	2.1990191 *	1.1050814 *	2.1999466 *	3.4531946
18 C	3.4733881	2.2013873 *	1.1050728 *	2.1827339 *
19 C	3.9471962	3.4583484	2.1895134 *	1.1055130 *
20 O	2.6859641 *	4.6496588	5.3989448	4.6909292
21 N	6.2038900	8.0444508	8.2223496	6.6268998
22 H	11.0843799	12.4333930	11.7085984	9.3687930
23 H	10.7933267	12.5424049	12.3115996	10.2324642
24 H	8.6920204	10.6494811	10.8109371	9.0579599
25 H	10.7278651	11.6478780	10.5035285	8.0300611
26 H	9.6931020	10.1339744	8.6234981	6.1246729
27 H	7.2865099	7.6620405	6.2734529	3.8107375
28 H	5.6511713	5.9010491	4.6195836	2.2312448 *

29 H	0.0000000	2.5180277 *	4.3877171	5.0525503
30 H	2.5180277 *	0.0000000	2.5434680 *	4.3714527
31 H	4.3877171	2.5434680 *	0.0000000	2.5139394 *
32 H	5.0525503	4.3714527	2.5139394 *	0.0000000
33 H	2.2974375 *	4.6256603	5.8212594	5.4702625
34 H	6.1625669	7.8671041	7.9937563	6.4487720
35 H	6.5554516	8.5952782	9.0093131	7.5574559

H H H

1 CO	2.6605140 *	2.4942074 *	2.6032195 *
2 C	8.1044944	4.7367739	4.7110157
3 C	7.7794479	4.2616107	3.8920372
4 C	6.4714598	2.9943806 *	2.4615377 *
5 C	5.3884682	2.1073059 *	2.0787532 *
6 C	5.8089720	3.0047948	3.4154299
7 C	7.2624133	4.2516629	4.5423608
8 C	8.0832502	5.4014947	5.8730646
9 C	7.7282883	5.6280601	6.3019723
10 C	6.4036857	4.7948725	5.5671918
11 C	5.3096732	3.4478646	4.1657263
12 N	3.9532347	3.1464162	3.9232872
13 C	4.0347725	4.0831451	5.0510343
14 C	3.3331895	4.7356937	5.6343734
15 C	2.0443579 *	4.6770060	5.3180420
16 C	2.5051327 *	5.8545803	6.4484686
17 C	3.9276605	6.9180303	7.6891330
18 C	4.7345247	6.9969371	7.9487519
19 C	4.4899110	6.0283643	7.0420145
20 O	0.9913147 *	3.7913096	4.0853045
21 N	4.1227861	1.0452533 *	1.0406834 *
22 H	9.1825425	5.8066550	5.7947691
23 H	8.6491706	5.0915825	4.5556767
24 H	6.4858442	3.1191062	2.1783910 *
25 H	9.1662154	6.3351453	6.7347190
26 H	8.5914466	6.6793810	7.3994562
27 H	6.4230722	5.4581103	6.3052664
28 H	5.1089433	4.7946870	5.8918587
29 H	2.2974375 *	6.1625669	6.5554516
30 H	4.6256603	7.8671041	8.5952782
31 H	5.8212594	7.9937563	9.0093131
32 H	5.4702625	6.4487720	7.5574559
33 H	0.0000000	4.2758228	4.3571227
34 H	4.2758228	0.0000000	1.6707375 *
35 H	4.3571227	1.6707375 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.81 , TOTAL = 3900.4 SECONDS (65.0 MIN)
WALL CLOCK TIME: STEP = 0.81 , TOTAL = 3606.1 SECONDS (60.1 MIN)
CPU UTILIZATION: STEP = 99.89%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.91 , TOTAL = 3901.3 SECONDS (65.0 MIN)
WALL CLOCK TIME: STEP = 0.92 , TOTAL = 3607.0 SECONDS (60.1 MIN)
CPU UTILIZATION: STEP = 99.42%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----
1 0 -284.633552994 -284.633552994 0.008606642 0.001052130 196758736
11422054
2 1 -284.633629942 -0.000076948 0.002982257 0.000144179 157330291
14780648
3 2 -284.633627983 0.000001959 0.001440119 0.000362473 143210583
15892806
4 3 -284.633631638 -0.000003655 0.000942832 0.000108192 137766372
16359975
5 4 -284.633631180 0.000000459 0.000623539 0.000165949 134200869
16623471
6 5 -284.633631896 -0.000000716 0.000149131 0.000030300 129278019
16992735
7 6 -284.633631898 -0.000000003 0.000122313 0.000022447 119194077
17755290
8 7 -284.633631947 -0.000000048 0.000268929 0.000021438 111754415
18359370
9 8 -284.633631984 -0.000000037 0.000295407 0.000021851 142263990
16055446
10 9 -284.633632018 -0.000000035 0.000192678 0.000020711 161139022
14588550
11 10 -284.633632044 -0.000000025 0.000335374 0.000017514 157363253
14839001

-----DISABLING FDIFF OPTION-----

12 11	-284.633632111	-0.000000067	0.000283918	0.000013782	196759940
11421832					
13 12	-284.633632128	-0.000000017	0.000251144	0.000008848	196759930
11421837					
14 13	-284.633632136	-0.000000008	0.000077839	0.000006725	196759828
11421839					
15 14	-284.633632139	-0.000000003	0.000054144	0.000003558	196759821
11421839					
16 15	-284.633632139	-0.000000001	0.000028735	0.000002972	196759815
11421840					
17 16	-284.633632140	-0.000000001	0.000054952	0.000002633	196759821
11421839					
18 17	-284.633632141	-0.000000001	0.000065262	0.000002255	196759787
11421845					
19 18	-284.633632142	-0.000000001	0.000052277	0.000002460	196759785
11421842					
20 19	-284.633632142	-0.000000001	0.000024680	0.000003093	196759788
11421839					
21 20	-284.633632143	0.000000000	0.000031729	0.000003007	196759782
11421840					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 70.7 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 22.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 1.9 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6336321427 AFTER 21 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6041980605
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000174914

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 73.50 , TOTAL = 3974.8 SECONDS (66.2 MIN)

WALL CLOCK TIME: STEP = 67.23 , TOTAL = 3674.2 SECONDS (61.2 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.64 , TOTAL = 3978.5 SECONDS (66.3 MIN)

WALL CLOCK TIME: STEP = 3.62 , TOTAL = 3677.8 SECONDS (61.3 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.85 , TOTAL = 3981.3 SECONDS (66.4 MIN)

WALL CLOCK TIME: STEP = 2.69 , TOTAL = 3680.5 SECONDS (61.3 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 37 ENERGY= -284.6336321

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0001155	-0.0007535	-0.0000375
2 C	6.0	-0.0003993	-0.0002694	0.0001207
3 C	6.0	0.0000902	-0.0003875	-0.0000695
4 C	6.0	0.0002557	0.0002077	0.0001651
5 C	6.0	0.0004661	0.0004838	-0.0000811
6 C	6.0	-0.0002658	0.0006943	0.0002145
7 C	6.0	-0.0001702	0.0001170	0.0003736
8 C	6.0	-0.0009473	-0.0010368	-0.0000067
9 C	6.0	-0.0002370	0.0001215	-0.0001108
10 C	6.0	-0.0005265	-0.0002189	-0.0000640
11 C	6.0	-0.0001092	-0.0001152	0.0001733
12 N	7.0	0.0000359	-0.0000899	0.0001716
13 C	6.0	0.0008017	-0.0001016	0.0002441
14 C	6.0	0.0000997	0.0001092	-0.0000974
15 C	6.0	0.0009284	-0.0001744	-0.0001076
16 C	6.0	0.0001167	0.0015515	-0.0003806
17 C	6.0	-0.0001574	-0.0004849	-0.0003120

18 C	6.0	-0.0003252	0.0006040	-0.0002840
19 C	6.0	0.0007649	-0.0000946	0.0002126
20 O	8.0	-0.0001178	-0.0006868	0.0006937
21 N	7.0	0.0000277	0.0003739	0.0002041
22 H	1.0	-0.0002324	0.0003804	-0.0003106
23 H	1.0	0.0003261	-0.0005078	-0.0006986
24 H	1.0	-0.0002027	-0.0006950	0.0004755
25 H	1.0	0.0001768	-0.0002960	-0.0004431
26 H	1.0	-0.0001389	0.0003612	-0.0005399
27 H	1.0	-0.0007921	0.0008681	-0.0002927
28 H	1.0	0.0004926	-0.0001247	0.0005933
29 H	1.0	-0.0000438	-0.0002191	0.0001165
30 H	1.0	0.0000475	0.0000863	-0.0001395
31 H	1.0	-0.0006048	0.0003284	-0.0001310
32 H	1.0	-0.0002818	-0.0000376	0.0012173
33 H	1.0	0.0004661	-0.0001512	-0.0014394
34 H	1.0	-0.0005138	0.0002132	-0.0005390
35 H	1.0	0.0010855	-0.0000556	0.0011088

MAXIMUM GRADIENT = 0.0015515 RMS GRADIENT = 0.0004777
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000869196
 PREDICTED ENERGY CHANGE WAS -0.0001485122 RATIO= 0.585
 GDIIS STEP HAS LENGTH = 0.191592
 RADIUS OF STEP TAKEN= 0.05927 CURRENT TRUST RADIUS= 0.05927

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 3981.3 SECONDS (66.4 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 3680.5 SECONDS (61.3 MIN)
 CPU UTILIZATION: STEP = 91.83% , TOTAL = 100.00%

INSERCH= 38

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1301658445	-1.7543095374	1.0241311405
C	6.0	4.9869273538	0.6849785907	0.4421220802
C	6.0	5.2154881794	-0.6777678582	0.2147775002
C	6.0	4.0879918413	-1.5483883568	0.0771327203
C	6.0	2.7713584104	-1.0597013615	0.1765702052
C	6.0	2.4742902661	0.3320079798	0.4906816239
C	6.0	3.6484459588	1.2090784870	0.5879116706
C	6.0	3.4910308377	2.6230473279	0.8236182478

C	6.0	2.2228310839	3.1903934306	1.0035452958
C	6.0	1.0709069286	2.3457505902	0.9804769975
C	6.0	1.1660677937	0.9594152259	0.7103928043
N	7.0	-0.0477092337	0.1492427906	0.7342684425
C	6.0	-1.2490000307	0.6931990656	0.5402778760
C	6.0	-2.5612530248	0.0472814961	0.5833047345
C	6.0	-2.8592103199	-1.3452175646	0.7681101993
C	6.0	-4.1711240906	-1.8527511917	0.7515258469
C	6.0	-5.2628198471	-0.9544107932	0.5493667492
C	6.0	-5.0225343458	0.4392375249	0.3818355952
C	6.0	-3.6935989217	0.9243792242	0.3997658761
O	8.0	-1.7600587739	-2.2880042213	0.9790225948
N	7.0	1.6923563304	-2.0687035839	-0.1426941431
H	1.0	5.8335356956	1.3920998025	0.5156538612
H	1.0	6.2378318631	-1.0832543191	0.1110077884
H	1.0	4.2575285878	-2.6210757750	-0.1460794587
H	1.0	4.3998801658	3.2504500306	0.8642361901
H	1.0	2.1049470232	4.2729725251	1.1885023662
H	1.0	0.0970531211	2.8109173775	1.2136881771
H	1.0	-1.2919465727	1.7693630601	0.2904103319
H	1.0	-4.3670019979	-2.9337649714	0.8913648360
H	1.0	-6.2941792446	-1.3518526523	0.5276637459
H	1.0	-5.8660034844	1.1384749793	0.2372917819
H	1.0	-3.5066808282	2.0074401861	0.2784969114
H	1.0	-2.0928249788	-3.2201325522	1.0356780821
H	1.0	1.3749880499	-1.9425578466	-1.1306565432
H	1.0	2.1183173596	-3.0167321098	-0.0905151282

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4659851	5.2606557	4.0747511
2 C	5.4659851	0.0000000	1.4003583 *	2.4350011 *
3 C	5.2606557	1.4003583 *	0.0000000	1.4311443 *
4 C	4.0747511	2.4350011 *	1.4311443 *	0.0000000
5 C	2.8594996 *	2.8325204 *	2.4740864 *	1.4079156 *
6 C	3.1831130	2.5377729 *	2.9342693 *	2.5121596 *
7 C	4.6206332	1.4448072 *	2.4809352 *	2.8386122 *
8 C	5.5223973	2.4777724 *	3.7735687	4.2795419
9 C	5.3693351	3.7726022	4.9538695	5.1762069
10 C	4.2068269	4.2875641	5.1870525	5.0083081
11 C	2.9216137 *	3.8400850	4.3958854	3.9022733
12 N	1.9336937 *	5.0714818	5.3530425	4.5186062
13 C	2.8507036 *	6.2367053	6.6162760	5.8071249

14 C	3.2686073	7.5763855	7.8191568	6.8567361
15 C	3.0280807	8.1110937	8.1211097	6.9844360
16 C	4.3110439	9.5081917	9.4750818	8.2921914
17 C	5.4726167	10.3805788	10.4872980	9.3815507
18 C	5.6368885	10.0126593	10.3001318	9.3298011
19 C	4.7102423	8.6839302	9.0538903	8.1714030
20 O	1.9646409 *	7.3924766	7.1996658	5.9632318
21 N	1.9750352 *	4.3334713	3.8045954	2.4613251 *
22 H	6.5335188	1.1055193 *	2.1810230 *	3.4475636
23 H	6.2118994	2.1911290 *	1.1047054 *	2.1998430 *
24 H	4.3767339	3.4362769	2.1964403 *	1.1087041 *
25 H	6.5805505	2.6654171 *	4.0642230	4.8729515
26 H	6.3446755	4.6622521	5.9273465	6.2494681
27 H	4.5692806	5.3875597	6.2743226	6.0185461
28 H	3.8700153	6.3736304	6.9527604	6.3242944
29 H	4.6511569	10.0395776	9.8676953	8.6063444
30 H	6.4560562	11.4638285	11.5336348	10.3938001
31 H	6.7038321	10.8643326	11.2293679	10.3114940
32 H	5.2852044	8.5975030	9.1263703	8.3882964
33 H	2.6627915 *	8.1071015	7.7813198	6.4742594
34 H	2.4956221 *	4.7353654	4.2613763	2.9957493 *
35 H	2.6055505 *	4.7133096	3.8931253	2.4624696 *

C C C C

1 CO	2.8594996 *	3.1831130	4.6206332	5.5223973
2 C	2.8325204 *	2.5377729 *	1.4448072 *	2.4777724 *
3 C	2.4740864 *	2.9342693 *	2.4809352 *	3.7735687
4 C	1.4079156 *	2.5121596 *	2.8386122 *	4.2795419
5 C	0.0000000	1.4573161 *	2.4669508 *	3.8077864
6 C	1.4573161 *	0.0000000	1.4687913 *	2.5285311 *
7 C	2.4669508 *	1.4687913 *	0.0000000	1.4420974 *
8 C	3.8077864	2.5285311 *	1.4420974 *	0.0000000
9 C	4.3644101	2.9148976 *	2.4760327 *	1.4009233 *
10 C	3.8903604	2.5029070 *	2.8442641 *	2.4410035 *
11 C	2.6341519 *	1.4674328 *	2.4979061 *	2.8611090 *
12 N	3.1176459	2.5403187 *	3.8478871	4.3186078
13 C	4.4009346	3.7410974	4.9247719	5.1256696
14 C	5.4614640	5.0444370	6.3174485	6.5819800
15 C	5.6687515	5.5978818	6.9933175	7.4883757
16 C	7.0112456	7.0001960	8.3992408	8.8739274
17 C	8.0435119	7.8435445	9.1702143	9.4606196
18 C	7.9393776	7.4983815	8.7075267	8.8002835
19 C	6.7662446	6.1969369	7.3499711	7.3948650
20 O	4.7630242	5.0032642	6.4524785	7.1914199
21 N	1.5113771 *	2.6030754 *	3.8863771	5.1167877

22 H	3.9374149	3.5226337	2.1939314 *	2.6640951 *
23 H	3.4671734	4.0387331	3.4910094	4.6679119
24 H	2.1796088 *	3.5080062	3.9471263	5.3878251
25 H	4.6585805	3.5163537	2.1927623 *	1.1051204 *
26 H	5.4685941	4.0192748	3.4828932	2.1855484 *
27 H	4.8175940	3.5098414	3.9458681	3.4214813
28 H	4.9524754	4.0361663	4.9809541	4.8877357
29 H	7.4147984	7.5913833	9.0278814	9.6245225
30 H	9.0770365	8.9287632	10.2673168	10.5658769
31 H	8.9128944	8.3830242	9.5211694	9.4921981
32 H	6.9879556	6.2148299	7.2061750	7.0458568
33 H	5.3912716	5.8114770	7.2650256	8.0849964
34 H	2.1066864 *	3.0018082	4.2491057	5.3982940
35 H	2.0803285 *	3.4173918	4.5452207	5.8759760

C C C N

1 CO	5.3693351	4.2068269	2.9216137 *	1.9336937 *
2 C	3.7726022	4.2875641	3.8400850	5.0714818
3 C	4.9538695	5.1870525	4.3958854	5.3530425
4 C	5.1762069	5.0083081	3.9022733	4.5186062
5 C	4.3644101	3.8903604	2.6341519 *	3.1176459
6 C	2.9148976 *	2.5029070 *	1.4674328 *	2.5403187 *
7 C	2.4760327 *	2.8442641 *	2.4979061 *	3.8478871
8 C	1.4009233 *	2.4410035 *	2.8611090 *	4.3186078
9 C	0.0000000	1.4285947 *	2.4859507 *	3.8047944
10 C	1.4285947 *	0.0000000	1.4156012 *	2.4772096 *
11 C	2.4859507 *	1.4156012 *	0.0000000	1.4595219 *
12 N	3.8047944	2.4772096 *	1.4595219 *	0.0000000
13 C	4.3016517	2.8821294 *	2.4356442 *	1.3328992 *
14 C	5.7396181	4.3166297	3.8394088	2.5201366 *
15 C	6.8157422	5.3957545	4.6386989	3.1841946
16 C	8.1473606	6.7200242	6.0328757	4.5837570
17 C	8.5685851	7.1549295	6.7096390	5.3338184
18 C	7.7750050	6.4127366	6.2191102	4.9957172
19 C	6.3642371	5.0058004	4.8697102	3.7423576
20 O	6.7732454	5.4301061	4.3795104	2.9886817 *
21 N	5.4086384	4.5972947	3.1897085	2.9523173 *
22 H	4.0631374	4.8793589	4.6915238	6.0151083
23 H	5.9313506	6.2618819	5.5004138	6.4354899
24 H	6.2637693	6.0077493	4.8073475	5.1946848
25 H	2.1823282 *	3.4516743	3.9661128	5.4235993
26 H	1.1045738 *	2.1969747 *	3.4770311	4.6739068
27 H	2.1695838 *	1.1041553 *	2.1963968 *	2.7083779 *
28 H	3.8576613	2.5281399 *	2.6218763 *	2.0904369 *
29 H	8.9968773	7.5797150	6.7678995	5.3090400

30 H	9.6642603	8.2535934	7.8122106	6.4276248
31 H	8.3801407	7.0802941	7.0502421	5.9226780
32 H	5.8951150	4.6434405	4.8082710	3.9528610
33 H	7.7279210	6.4024450	5.3098787	3.9529782
34 H	5.6232414	4.7894613	3.4430449	3.1428717
35 H	6.3036734	5.5677925	4.1662910	3.9236891

C C C C

1 CO	2.8507036 *	3.2686073	3.0280807	4.3110439
2 C	6.2367053	7.5763855	8.1110937	9.5081917
3 C	6.6162760	7.8191568	8.1211097	9.4750818
4 C	5.8071249	6.8567361	6.9844360	8.2921914
5 C	4.4009346	5.4614640	5.6687515	7.0112456
6 C	3.7410974	5.0444370	5.5978818	7.0001960
7 C	4.9247719	6.3174485	6.9933175	8.3992408
8 C	5.1256696	6.5819800	7.4883757	8.8739274
9 C	4.3016517	5.7396181	6.8157422	8.1473606
10 C	2.8821294 *	4.3166297	5.3957545	6.7200242
11 C	2.4356442 *	3.8394088	4.6386989	6.0328757
12 N	1.3328992 *	2.5201366 *	3.1841946	4.5837570
13 C	0.0000000	1.4632391 *	2.6076478 *	3.8814041
14 C	1.4632391 *	0.0000000	1.4359614 *	2.4960183 *
15 C	2.6076478 *	1.4359614 *	0.0000000	1.4067634 *
16 C	3.8814041	2.4960183 *	1.4067634 *	0.0000000
17 C	4.3388305	2.8814931 *	2.4449780 *	1.4281748 *
18 C	3.7853879	2.5004250 *	2.8308053 *	2.4728086 *
19 C	2.4595226 *	1.4440201 *	2.4460072 *	2.8397568 *
20 O	3.0563460	2.5004128 *	1.4633745 *	2.4605763 *
21 N	4.0922041	4.8060025	4.6978458	5.9352058
22 H	7.1169784	8.5020933	9.1170430	10.5203570
23 H	7.7066667	8.8839783	9.1245046	10.4569954
24 H	6.4635409	7.3585267	7.2877657	8.5110636
25 H	6.2092132	7.6678932	8.5920775	9.9758448
26 H	4.9481243	6.3242511	7.5089046	8.7809173
27 H	2.5980899 *	3.8860852	5.1197159	6.3388276
28 H	1.1056252 *	2.1592802 *	3.5192507	4.6499465
29 H	4.7958385	3.4988953	2.1936523 *	1.1074809 *
30 H	5.4439167	3.9869049	3.4433806	2.1928011 *
31 H	4.6483107	3.4973996	3.9358991	3.4762749
32 H	2.6254298 *	2.1974903 *	3.4495294	3.9454174
33 H	4.0338104	3.3316754	2.0430970 *	2.5039572 *
34 H	4.0773214	4.7319254	4.6787356	5.8574769
35 H	5.0497837	5.6338789	5.3204304	6.4514307

C C C O

1 CO	5.4726167	5.6368885	4.7102423	1.9646409 *
2 C	10.3805788	10.0126593	8.6839302	7.3924766
3 C	10.4872980	10.3001318	9.0538903	7.1996658
4 C	9.3815507	9.3298011	8.1714030	5.9632318
5 C	8.0435119	7.9393776	6.7662446	4.7630242
6 C	7.8435445	7.4983815	6.1969369	5.0032642
7 C	9.1702143	8.7075267	7.3499711	6.4524785
8 C	9.4606196	8.8002835	7.3948650	7.1914199
9 C	8.5685851	7.7750050	6.3642371	6.7732454
10 C	7.1549295	6.4127366	5.0058004	5.4301061
11 C	6.7096390	6.2191102	4.8697102	4.3795104
12 N	5.3338184	4.9957172	3.7423576	2.9886817 *
13 C	4.3388305	3.7853879	2.4595226 *	3.0563460
14 C	2.8814931 *	2.5004250 *	1.4440201 *	2.5004128 *
15 C	2.4449780 *	2.8308053 *	2.4460072 *	1.4633745 *
16 C	1.4281748 *	2.4728086 *	2.8397568 *	2.4605763 *
17 C	0.0000000	1.4240995 *	2.4524858 *	3.7725867
18 C	1.4240995 *	0.0000000	1.4148333 *	4.2939756
19 C	2.4524858 *	1.4148333 *	0.0000000	3.7938797
20 O	3.7725867	4.2939756	3.7938797	0.0000000
21 N	7.0777873	7.1871174	6.1855737	3.6366896
22 H	11.3417968	10.8986288	9.5393127	8.4510682
23 H	11.5097241	11.3660537	10.1364338	8.1345637
24 H	9.6901214	9.7858970	8.7228795	6.1309175
25 H	10.5426642	9.8446697	8.4339043	8.2844734
26 H	9.0563800	8.1332174	6.7422784	7.6176484
27 H	6.5838634	5.7032464	4.3116747	5.4316603
28 H	4.8222232	3.9616761	2.5483113 *	4.1419253
29 H	2.1993852 *	3.4736852	3.9472038	2.6871628 *
30 H	1.1055014 *	2.2014428 *	3.4584111	4.6517043
31 H	2.2003164 *	1.1051091 *	2.1889670 *	5.3990468
32 H	3.4539768	2.1835179 *	1.1057421 *	4.6895914
33 H	3.9266858	4.7330430	4.4881889	0.9913659 *
34 H	6.9180493	6.9920580	6.0209713	3.7945484
35 H	7.6905009	7.9472388	7.0392546	4.0886131

N H H H

1 CO	1.9750352 *	6.5335188	6.2118994	4.3767339
2 C	4.3334713	1.1055193 *	2.1911290 *	3.4362769
3 C	3.8045954	2.1810230 *	1.1047054 *	2.1964403 *
4 C	2.4613251 *	3.4475636	2.1998430 *	1.1087041 *
5 C	1.5113771 *	3.9374149	3.4671734	2.1796088 *
6 C	2.6030754 *	3.5226337	4.0387331	3.5080062
7 C	3.8863771	2.1939314 *	3.4910094	3.9471263

8 C	5.1167877	2.6640951 *	4.6679119	5.3878251
9 C	5.4086384	4.0631374	5.9313506	6.2637693
10 C	4.5972947	4.8793589	6.2618819	6.0077493
11 C	3.1897085	4.6915238	5.5004138	4.8073475
12 N	2.9523173 *	6.0151083	6.4354899	5.1946848
13 C	4.0922041	7.1169784	7.7066667	6.4635409
14 C	4.8060025	8.5020933	8.8839783	7.3585267
15 C	4.6978458	9.1170430	9.1245046	7.2877657
16 C	5.9352058	10.5203570	10.4569954	8.5110636
17 C	7.0777873	11.3417968	11.5097241	9.6901214
18 C	7.1871174	10.8986288	11.3660537	9.7858970
19 C	6.1855737	9.5393127	10.1364338	8.7228795
20 O	3.6366896	8.4510682	8.1345637	6.1309175
21 N	0.0000000	5.4369062	4.6579848	2.6239732 *
22 H	5.4369062	0.0000000	2.5405849 *	4.3620256
23 H	4.6579848	2.5405849 *	0.0000000	2.5204344 *
24 H	2.6239732 *	4.3620256	2.5204344 *	0.0000000
25 H	6.0529323	2.3728345 *	4.7672228	5.9595148
26 H	6.4930094	4.7596771	6.8506129	7.3445638
27 H	5.3099403	5.9504225	7.3545660	6.9760357
28 H	4.8810244	7.1390167	8.0540160	7.0896510
29 H	6.2075303	11.0862633	10.7933242	8.6923296
30 H	8.0466145	12.4342627	12.5418121	10.6491030
31 H	8.2194396	11.7055981	12.3066998	10.8058825
32 H	6.6198442	9.3634679	10.2242835	9.0491090
33 H	4.1281894	9.1853310	8.6499195	6.4870957
34 H	1.0453253 *	5.8059389	5.0918938	3.1207080
35 H	1.0406361 *	5.7972482	4.5551452	2.1762022 *

H H H H

1 CO	6.5805505	6.3446755	4.5692806	3.8700153
2 C	2.6654171 *	4.6622521	5.3875597	6.3736304
3 C	4.0642230	5.9273465	6.2743226	6.9527604
4 C	4.8729515	6.2494681	6.0185461	6.3242944
5 C	4.6585805	5.4685941	4.8175940	4.9524754
6 C	3.5163537	4.0192748	3.5098414	4.0361663
7 C	2.1927623 *	3.4828932	3.9458681	4.9809541
8 C	1.1051204 *	2.1855484 *	3.4214813	4.8877357
9 C	2.1823282 *	1.1045738 *	2.1695838 *	3.8576613
10 C	3.4516743	2.1969747 *	1.1041553 *	2.5281399 *
11 C	3.9661128	3.4770311	2.1963968 *	2.6218763 *
12 N	5.4235993	4.6739068	2.7083779 *	2.0904369 *
13 C	6.2092132	4.9481243	2.5980899 *	1.1056252 *
14 C	7.6678932	6.3242511	3.8860852	2.1592802 *
15 C	8.5920775	7.5089046	5.1197159	3.5192507

16 C	9.9758448	8.7809173	6.3388276	4.6499465
17 C	10.5426642	9.0563800	6.5838634	4.8222232
18 C	9.8446697	8.1332174	5.7032464	3.9616761
19 C	8.4339043	6.7422784	4.3116747	2.5483113 *
20 O	8.2844734	7.6176484	5.4316603	4.1419253
21 N	6.0529323	6.4930094	5.3099403	4.8810244
22 H	2.3728345 *	4.7596771	5.9504225	7.1390167
23 H	4.7672228	6.8506129	7.3545660	8.0540160
24 H	5.9595148	7.3445638	6.9760357	7.0896510
25 H	0.0000000	2.5332625 *	4.3393117	5.9092966
26 H	2.5332625 *	0.0000000	2.4839238 *	4.3143384
27 H	4.3393117	2.4839238 *	0.0000000	1.9663666 *
28 H	5.9092966	4.3143384	1.9663666 *	0.0000000
29 H	10.7286287	9.6907936	7.2823798	5.6512411
30 H	11.6472047	10.1301870	7.6581417	5.9008989
31 H	10.4996126	8.6177682	6.2696457	4.6176659
32 H	8.0250776	6.1197315	3.8088130	2.2275256 *
33 H	9.1680451	8.5901844	6.4187863	5.1080228
34 H	6.3322113	6.6741408	5.4520268	4.7864735
35 H	6.7375553	7.4010714	6.3045978	5.8891180

H H H H

1 CO	4.6511569	6.4560562	6.7038321	5.2852044
2 C	10.0395776	11.4638285	10.8643326	8.5975030
3 C	9.8676953	11.5336348	11.2293679	9.1263703
4 C	8.6063444	10.3938001	10.3114940	8.3882964
5 C	7.4147984	9.0770365	8.9128944	6.9879556
6 C	7.5913833	8.9287632	8.3830242	6.2148299
7 C	9.0278814	10.2673168	9.5211694	7.2061750
8 C	9.6245225	10.5658769	9.4921981	7.0458568
9 C	8.9968773	9.6642603	8.3801407	5.8951150
10 C	7.5797150	8.2535934	7.0802941	4.6434405
11 C	6.7678995	7.8122106	7.0502421	4.8082710
12 N	5.3090400	6.4276248	5.9226780	3.9528610
13 C	4.7958385	5.4439167	4.6483107	2.6254298 *
14 C	3.4988953	3.9869049	3.4973996	2.1974903 *
15 C	2.1936523 *	3.4433806	3.9358991	3.4495294
16 C	1.1074809 *	2.1928011 *	3.4762749	3.9454174
17 C	2.1993852 *	1.1055014 *	2.2003164 *	3.4539768
18 C	3.4736852	2.2014428 *	1.1051091 *	2.1835179 *
19 C	3.9472038	3.4584111	2.1889670 *	1.1057421 *
20 O	2.6871628 *	4.6517043	5.3990468	4.6895914
21 N	6.2075303	8.0466145	8.2194396	6.6198442
22 H	11.0862633	12.4342627	11.7055981	9.3634679
23 H	10.7933242	12.5418121	12.3066998	10.2242835

24 H	8.6923296	10.6491030	10.8058825	9.0491090
25 H	10.7286287	11.6472047	10.4996126	8.0250776
26 H	9.6907936	10.1301870	8.6177682	6.1197315
27 H	7.2823798	7.6581417	6.2696457	3.8088130
28 H	5.6512411	5.9008989	4.6176659	2.2275256 *
29 H	0.0000000	2.5196701 *	4.3883887	5.0528475
30 H	2.5196701 *	0.0000000	2.5434980 *	4.3723083
31 H	4.3883887	2.5434980 *	0.0000000	2.5145977 *
32 H	5.0528475	4.3723083	2.5145977 *	0.0000000
33 H	2.2966745 *	4.6260054	5.8199447	5.4680736
34 H	6.1677801	7.8686140	7.9872401	6.4357508
35 H	6.5597514	8.5979107	9.0068076	7.5510980

H H H

1 CO	2.6627915 *	2.4956221 *	2.6055505 *
2 C	8.1071015	4.7353654	4.7133096
3 C	7.7813198	4.2613763	3.8931253
4 C	6.4742594	2.9957493 *	2.4624696 *
5 C	5.3912716	2.1066864 *	2.0803285 *
6 C	5.8114770	3.0018082	3.4173918
7 C	7.2650256	4.2491057	4.5452207
8 C	8.0849964	5.3982940	5.8759760
9 C	7.7279210	5.6232414	6.3036734
10 C	6.4024450	4.7894613	5.5677925
11 C	5.3098787	3.4430449	4.1662910
12 N	3.9529782	3.1428717	3.9236891
13 C	4.0338104	4.0773214	5.0497837
14 C	3.3316754	4.7319254	5.6338789
15 C	2.0430970 *	4.6787356	5.3204304
16 C	2.5039572 *	5.8574769	6.4514307
17 C	3.9266858	6.9180493	7.6905009
18 C	4.7330430	6.9920580	7.9472388
19 C	4.4881889	6.0209713	7.0392546
20 O	0.9913659 *	3.7945484	4.0886131
21 N	4.1281894	1.0453253 *	1.0406361 *
22 H	9.1853310	5.8059389	5.7972482
23 H	8.6499195	5.0918938	4.5551452
24 H	6.4870957	3.1207080	2.1762022 *
25 H	9.1680451	6.3322113	6.7375553
26 H	8.5901844	6.6741408	7.4010714
27 H	6.4187863	5.4520268	6.3045978
28 H	5.1080228	4.7864735	5.8891180
29 H	2.2966745 *	6.1677801	6.5597514
30 H	4.6260054	7.8686140	8.5979107
31 H	5.8199447	7.9872401	9.0068076

32 H	5.4680736	6.4357508	7.5510980
33 H	0.0000000	4.2837986	4.3638747
34 H	4.2837986	0.0000000	1.6698153 *
35 H	4.3638747	1.6698153 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.81 , TOTAL = 3982.2 SECONDS (66.4 MIN)
WALL CLOCK TIME: STEP = 0.80 , TOTAL = 3681.3 SECONDS (61.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.94 , TOTAL = 3983.1 SECONDS (66.4 MIN)
WALL CLOCK TIME: STEP = 0.94 , TOTAL = 3682.3 SECONDS (61.4 MIN)

CPU UTILIZATION: STEP = 99.70%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.633634885	-284.633634885	0.007967857	0.001033354	196784916
11418803					
2 1	-284.633707672	-0.000072787	0.001589859	0.000131201	156482477
14852606					
3 2	-284.633706834	0.000000838	0.000940587	0.000329260	140062308
16176675					
4 3	-284.633708866	-0.000002031	0.000617060	0.000085723	133917322
16694401					
5 4	-284.633708637	0.000000229	0.000433962	0.000105096	131636505
16830959					
6 5	-284.633709062	-0.000000425	0.000174065	0.000024651	126141682
17233524					
7 6	-284.633709100	-0.000000038	0.000136967	0.000020005	117630153
17864485					
8 7	-284.633709137	-0.000000037	0.000373658	0.000020497	110201722
18486426					
9 8	-284.633709176	-0.000000039	0.000311480	0.000022838	143304292
16001084					

10	9	-284.633709206	-0.000000030	0.000160403	0.000020357	141410373
16150161						
11	10	-284.633709231	-0.000000025	0.000294574	0.000017482	136223556
16513910						
12	11	-284.633709258	-0.000000027	0.000279921	0.000009682	160833048
14595464						
13	12	-284.633709272	-0.000000014	0.000190653	0.000010379	159137337
14753075						
14	13	-284.633709276	-0.000000004	0.000063532	0.000004904	157568155
14826499						
15	14	-284.633709279	-0.000000003	0.000041224	0.000002756	152153161
15239286						
16	15	-284.633709279	-0.000000001	0.000020186	0.000002704	146770706
15661912						
17	16	-284.633709280	-0.000000001	0.000052429	0.000002709	141093081
16136943						
-----DISABLING FDIFF OPTION-----						
18	17	-284.633709274	0.000000006	0.000065082	0.000001989	196785138
11418598						
19	18	-284.633709275	-0.000000001	0.000052786	0.000002314	196785183
11418598						
20	19	-284.633709275	-0.000000001	0.000034837	0.000002770	196785166
11418598						
21	20	-284.633709276	0.000000000	0.000032296	0.000002736	196785178
11418597						

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 69.8 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 22.8 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.6 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6337092755 AFTER 21 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6042709343
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000183369

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 73.52 , TOTAL = 4056.6 SECONDS (67.6 MIN)
WALL CLOCK TIME: STEP = 67.64 , TOTAL = 3749.9 SECONDS (62.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.86 , TOTAL = 4060.5 SECONDS (67.7 MIN)
WALL CLOCK TIME: STEP = 3.83 , TOTAL = 3753.8 SECONDS (62.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84 , TOTAL = 4063.3 SECONDS (67.7 MIN)
WALL CLOCK TIME: STEP = 2.68 , TOTAL = 3756.4 SECONDS (62.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 38 ENERGY= -284.6337093

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000681	-0.0006377	0.0001629
2 C	6.0	-0.0005126	-0.0005858	-0.0001249
3 C	6.0	-0.0002401	0.0004312	-0.0000332
4 C	6.0	0.0006352	-0.0001122	0.0001420
5 C	6.0	0.0000735	0.0008772	0.0001041
6 C	6.0	-0.0001535	0.0005376	0.0001773
7 C	6.0	-0.0000956	0.0002328	0.0002603
8 C	6.0	-0.0009280	-0.0007985	0.0000597
9 C	6.0	-0.0003295	0.0000013	-0.0000896
10 C	6.0	-0.0003811	-0.0002137	-0.0001518
11 C	6.0	-0.0001383	-0.0004646	0.0001296
12 N	7.0	-0.0000022	-0.0000432	0.0002516

13 C	6.0	0.0008468	-0.0000255	0.0002360
14 C	6.0	-0.0001854	-0.0000356	-0.0000319
15 C	6.0	0.0009727	0.0000865	0.0001402
16 C	6.0	0.0001308	0.0015698	-0.0002847
17 C	6.0	-0.0001456	-0.0004961	-0.0002745
18 C	6.0	-0.0000780	0.0005964	-0.0002756
19 C	6.0	0.0006596	-0.0004632	0.0001840
20 O	8.0	0.0000528	-0.0006812	0.0004521
21 N	7.0	0.0003064	0.0000275	0.0002864
22 H	1.0	0.0000034	0.0005383	-0.0001756
23 H	1.0	0.0001821	-0.0006111	-0.0005997
24 H	1.0	-0.0005276	-0.0007038	0.0004596
25 H	1.0	0.0003133	-0.0002937	-0.0004052
26 H	1.0	-0.0001075	0.0003788	-0.0005917
27 H	1.0	-0.0007583	0.0007176	-0.0002525
28 H	1.0	0.0004763	-0.0000454	0.0006478
29 H	1.0	-0.0000594	-0.0003291	0.0000369
30 H	1.0	-0.0002618	0.0000785	-0.0002174
31 H	1.0	-0.0005813	0.0003992	-0.0000845
32 H	1.0	-0.0000559	0.0000849	0.0010464
33 H	1.0	0.0002450	-0.0000929	-0.0014375
34 H	1.0	-0.0003792	0.0001955	-0.0006188
35 H	1.0	0.0009548	-0.0001197	0.0008723

MAXIMUM GRADIENT = 0.0015698 RMS GRADIENT = 0.0004657
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000771328
 PREDICTED ENERGY CHANGE WAS -0.0000889693 RATIO= 0.867
 GDIIS STEP HAS LENGTH = 0.197835
 RADIUS OF STEP TAKEN= 0.08382 CURRENT TRUST RADIUS= 0.08382

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 4063.3 SECONDS (67.7 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 3756.5 SECONDS (62.6 MIN)
 CPU UTILIZATION: STEP = 91.60%, TOTAL = 100.00%

INSERCH= 39

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1330678987	-1.7577435099	1.0241427426
C	6.0	4.9861617605	0.6873554681	0.4417650491
C	6.0	5.2138934493	-0.6762863552	0.2162192963

C	6.0	4.0869756818	-1.5475586271	0.0768085189
C	6.0	2.7706596126	-1.0596411939	0.1744893524
C	6.0	2.4744424357	0.3322388753	0.4893407867
C	6.0	3.6477476182	1.2109007635	0.5862570225
C	6.0	3.4895654622	2.6246331709	0.8239082328
C	6.0	2.2207751001	3.1894582906	1.0057824614
C	6.0	1.0702851532	2.3424860104	0.9838936299
C	6.0	1.1665785102	0.9572767083	0.7115062310
N	7.0	-0.0466685118	0.1460997928	0.7364852330
C	6.0	-1.2474409394	0.6900012697	0.5397898963
C	6.0	-2.5596050467	0.0453456476	0.5831927546
C	6.0	-2.8593956822	-1.3456443453	0.7746072717
C	6.0	-4.1720517316	-1.8517057731	0.7601873732
C	6.0	-5.2625703583	-0.9522780839	0.5542528862
C	6.0	-5.0196288277	0.4397692167	0.3778583286
C	6.0	-3.6898691098	0.9228570315	0.3916802718
O	8.0	-1.7598949955	-2.2888855924	0.9824839700
N	7.0	1.6918920430	-2.0672214406	-0.1502031034
H	1.0	5.8336867919	1.3930120845	0.5184410092
H	1.0	6.2353660881	-1.0828903599	0.1173904482
H	1.0	4.2548190859	-2.6205333282	-0.1467045668
H	1.0	4.3983408263	3.2525669480	0.8657557814
H	1.0	2.1009578499	4.2717812302	1.1918746511
H	1.0	0.0962393026	2.8040650337	1.2220570407
H	1.0	-1.2892892350	1.7659110137	0.2878414017
H	1.0	-4.3691939471	-2.9323683331	0.9014378199
H	1.0	-6.2953922732	-1.3471827877	0.5332686048
H	1.0	-5.8608940516	1.1402495545	0.2289348516
H	1.0	-3.4987704168	2.0038472759	0.2589072277
H	1.0	-2.0959208814	-3.2194697783	1.0443799289
H	1.0	1.3734534340	-1.9330220180	-1.1362617020
H	1.0	2.1176749038	-3.0163188594	-0.1088837021

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4653630	5.2570979	4.0712414
2 C	5.4653630	0.0000000	1.4008039 *	2.4365077 *
3 C	5.2570979	1.4008039 *	0.0000000	1.4312562 *
4 C	4.0712414	2.4365077 *	1.4312562 *	0.0000000
5 C	2.8576472 *	2.8340578 *	2.4734781 *	1.4072288 *
6 C	3.1837202	2.5371451 *	2.9319465 *	2.5107937 *
7 C	4.6214247	1.4444134 *	2.4801645 *	2.8392882 *
8 C	5.5237121	2.4776761 *	3.7734152	4.2804487

9 C	5.3696987	3.7717367	4.9523882	5.1754252
10 C	4.2061715	4.2857263	5.1838017	5.0055641
11 C	2.9218522 *	3.8385979	4.3925614	3.8994565
12 N	1.9338230 *	5.0704239	5.3498138	4.5156026
13 C	2.8516411 *	6.2343739	6.6121314	5.8031911
14 C	3.2704824	7.5743498	7.8155423	6.8535250
15 C	3.0309952	8.1115130	8.1202115	6.9842514
16 C	4.3142272	9.5090010	9.4748868	8.2928310
17 C	5.4756263	10.3796706	10.4855487	9.3806355
18 C	5.6388855	10.0090573	10.2954692	9.3257894
19 C	4.7117380	8.6793710	9.0479298	8.1658688
20 O	1.9665086 *	7.3932178	7.1987057	5.9628609
21 N	1.9760560 *	4.3347818	3.8044000	2.4613024 *
22 H	6.5329971	1.1054995 *	2.1811643 *	3.4486222
23 H	6.2060994	2.1907763 *	1.1038570 *	2.1984415 *
24 H	4.3708263	3.4385007	2.1980977 *	1.1087850 *
25 H	6.5818577	2.6656353 *	4.0648385	4.8744837
26 H	6.3447532	4.6620997	5.9266891	6.2491884
27 H	4.5662483	5.3852258	6.2701626	6.0144991
28 H	3.8705789	6.3693218	6.9470024	6.3188480
29 H	4.6545850	10.0417319	9.8688902	8.6083980
30 H	6.4602336	11.4639077	11.5331817	10.3943288
31 H	6.7050950	10.8585924	11.2227841	10.3057056
32 H	5.2844489	8.5884027	9.1156706	8.3778988
33 H	2.6656039 *	8.1106302	7.7837663	6.4776301
34 H	2.4973238 *	4.7337309	4.2611699	2.9972194 *
35 H	2.6089128 *	4.7168458	3.8946134	2.4637134 *

C C C C

1 CO	2.8576472 *	3.1837202	4.6214247	5.5237121
2 C	2.8340578 *	2.5371451 *	1.4444134 *	2.4776761 *
3 C	2.4734781 *	2.9319465 *	2.4801645 *	3.7734152
4 C	1.4072288 *	2.5107937 *	2.8392882 *	4.2804487
5 C	0.0000000	1.4574657 *	2.4686427 *	3.8095207
6 C	1.4574657 *	0.0000000	1.4690420 *	2.5293244 *
7 C	2.4686427 *	1.4690420 *	0.0000000	1.4422687 *
8 C	3.8095207	2.5293244 *	1.4422687 *	0.0000000
9 C	4.3644321	2.9145775 *	2.4752661 *	1.4006908 *
10 C	3.8885573	2.5014663 *	2.8428705 *	2.4409260 *
11 C	2.6323794 *	1.4664712 *	2.4972410 *	2.8616394 *
12 N	3.1156040	2.5400253 *	3.8477370	4.3192269
13 C	4.3977068	3.7393789	4.9230444	5.1247198
14 C	5.4589153	5.0430893	6.3158337	6.5805115
15 C	5.6691677	5.5987943	6.9938768	7.4883137
16 C	7.0122499	7.0013468	8.3999448	8.8736717

17 C	8.0429181	7.8431859	9.1691948	9.4586939
18 C	7.9358796	7.4956718	8.7041076	8.7965322
19 C	6.7613536	6.1933112	7.3458457	7.3910178
20 O	4.7633835	5.0043079	6.4535338	7.1919850
21 N	1.5114174 *	2.6036150 *	3.8876509	5.1180096
22 H	3.9390286	3.5228695	2.1945600 *	2.6655404 *
23 H	3.4652549	4.0355278	3.4895677	4.6673675
24 H	2.1776775 *	3.5061601	3.9478672	5.3888286
25 H	4.6607225	3.5172986	2.1931508 *	1.1054070 *
26 H	5.4687877	4.0190843	3.4825738	2.1855725 *
27 H	4.8143689	3.5075131	3.9440620	3.4213127
28 H	4.9477044	4.0325791	4.9770896	4.8848975
29 H	7.4170796	7.5936054	9.0298045	9.6252987
30 H	9.0777034	8.9292994	10.2670653	10.5643358
31 H	8.9076485	8.3784561	9.5156154	9.4862259
32 H	6.9783838	6.2069837	7.1978220	7.0385680
33 H	5.3949212	5.8147161	7.2682727	8.0870146
34 H	2.1054803 *	2.9976936 *	4.2454370	5.3937387
35 H	2.0821328 *	3.4202331	4.5490360	5.8798405

C C C N

1 CO	5.3696987	4.2061715	2.9218522 *	1.9338230 *
2 C	3.7717367	4.2857263	3.8385979	5.0704239
3 C	4.9523882	5.1838017	4.3925614	5.3498138
4 C	5.1754252	5.0055641	3.8994565	4.5156026
5 C	4.3644321	3.8885573	2.6323794 *	3.1156040
6 C	2.9145775 *	2.5014663 *	1.4664712 *	2.5400253 *
7 C	2.4752661 *	2.8428705 *	2.4972410 *	3.8477370
8 C	1.4006908 *	2.4409260 *	2.8616394 *	4.3192269
9 C	0.0000000	1.4287996 *	2.4860739 *	3.8047145
10 C	1.4287996 *	0.0000000	1.4150166 *	2.4764710 *
11 C	2.4860739 *	1.4150166 *	0.0000000	1.4596576 *
12 N	3.8047145	2.4764710 *	1.4596576 *	0.0000000
13 C	4.3003438	2.8809353 *	2.4348332 *	1.3328062 *
14 C	5.7372520	4.3143386	3.8382973	2.5196230 *
15 C	6.8138633	5.3933754	4.6385230	3.1840521
16 C	8.1450529	6.7173942	6.0327212	4.5837294
17 C	8.5649471	7.1515817	6.7085828	5.3334112
18 C	7.7703621	6.4089517	6.2167754	4.9945159
19 C	6.3600564	5.0025125	4.8670892	3.7410096
20 O	6.7718926	5.4276629	4.3789549	2.9874428 *
21 N	5.4082069	4.5954423	3.1884301	2.9508643 *
22 H	4.0642160	4.8793588	4.6913792	6.0150571
23 H	5.9295147	6.2579623	5.4961680	6.4309917
24 H	6.2627122	6.0042543	4.8035904	5.1900943

25 H	2.1829756 *	3.4522686	3.9669179	5.4244776
26 H	1.1047214 *	2.1972079 *	3.4770330	4.6734276
27 H	2.1700127 *	1.1038760 *	2.1947472 *	2.7057313 *
28 H	3.8551884	2.5267605 *	2.6200511 *	2.0902574 *
29 H	8.9952955	7.5775207	6.7683225	5.3092750
30 H	9.6607188	8.2504498	7.8117418	6.4278876
31 H	8.3735372	7.0750675	7.0463980	5.9204020
32 H	5.8886923	4.6385936	4.8026697	3.9492169
33 H	7.7272060	6.4003024	5.3103595	3.9523781
34 H	5.6165925	4.7819388	3.4366947	3.1379412
35 H	6.3059322	5.5684807	4.1673836	3.9242735

C C C C

1 CO	2.8516411 *	3.2704824	3.0309952	4.3142272
2 C	6.2343739	7.5743498	8.1115130	9.5090010
3 C	6.6121314	7.8155423	8.1202115	9.4748868
4 C	5.8031911	6.8535250	6.9842514	8.2928310
5 C	4.3977068	5.4589153	5.6691677	7.0122499
6 C	3.7393789	5.0430893	5.5987943	7.0013468
7 C	4.9230444	6.3158337	6.9938768	8.3999448
8 C	5.1247198	6.5805115	7.4883137	8.8736717
9 C	4.3003438	5.7372520	6.8138633	8.1450529
10 C	2.8809353 *	4.3143386	5.3933754	6.7173942
11 C	2.4348332 *	3.8382973	4.6385230	6.0327212
12 N	1.3328062 *	2.5196230 *	3.1840521	4.5837294
13 C	0.0000000	1.4626139 *	2.6071805 *	3.8810048
14 C	1.4626139 *	0.0000000	1.4357462 *	2.4960199 *
15 C	2.6071805 *	1.4357462 *	0.0000000	1.4069016 *
16 C	3.8810048	2.4960199 *	1.4069016 *	0.0000000
17 C	4.3380358	2.8813386 *	2.4451056 *	1.4284992 *
18 C	3.7839449	2.4998898 *	2.8304979 *	2.4729375 *
19 C	2.4579694 *	1.4436759 *	2.4458981 *	2.8401578 *
20 O	3.0548902	2.4995210 *	1.4634953 *	2.4615122 *
21 N	4.0887707	4.8037524	4.7000178	5.9381053
22 H	7.1159715	8.5010438	9.1178694	10.5214751
23 H	7.7015561	8.8792683	9.1222621	10.4555541
24 H	6.4580012	7.3536411	7.2860284	8.5103291
25 H	6.2086914	7.6667543	8.5922404	9.9757894
26 H	4.9463256	6.3209254	7.5056438	8.7769070
27 H	2.5961954 *	3.8822918	5.1143013	6.3330746
28 H	1.1058079 *	2.1589997 *	3.5190840	4.6497937
29 H	4.7955910	3.4989531	2.1939165 *	1.1075416 *
30 H	5.4435259	3.9871963	3.4444621	2.1942221 *
31 H	4.6457835	3.4961153	3.9352788	3.4765233
32 H	2.6217496 *	2.1961151 *	3.4487448	3.9458686

33 H	4.0321822	3.3296721	2.0412968 *	2.5023715 *
34 H	4.0692121	4.7264586	4.6811798	5.8613786
35 H	5.0479294	5.6329128	5.3238089	6.4554062

C C C O

1 CO	5.4756263	5.6388855	4.7117380	1.9665086 *
2 C	10.3796706	10.0090573	8.6793710	7.3932178
3 C	10.4855487	10.2954692	9.0479298	7.1987057
4 C	9.3806355	9.3257894	8.1658688	5.9628609
5 C	8.0429181	7.9358796	6.7613536	4.7633835
6 C	7.8431859	7.4956718	6.1933112	5.0043079
7 C	9.1691948	8.7041076	7.3458457	6.4535338
8 C	9.4586939	8.7965322	7.3910178	7.1919850
9 C	8.5649471	7.7703621	6.3600564	6.7718926
10 C	7.1515817	6.4089517	5.0025125	5.4276629
11 C	6.7085828	6.2167754	4.8670892	4.3789549
12 N	5.3334112	4.9945159	3.7410096	2.9874428 *
13 C	4.3380358	3.7839449	2.4579694 *	3.0548902
14 C	2.8813386 *	2.4998898 *	1.4436759 *	2.4995210 *
15 C	2.4451056 *	2.8304979 *	2.4458981 *	1.4634953 *
16 C	1.4284992 *	2.4729375 *	2.8401578 *	2.4615122 *
17 C	0.0000000	1.4240545 *	2.4527435 *	3.7734117
18 C	1.4240545 *	0.0000000	1.4148589 *	4.2938321
19 C	2.4527435 *	1.4148589 *	0.0000000	3.7933020
20 O	3.7734117	4.2938321	3.7933020	0.0000000
21 N	7.0784111	7.1838961	6.1804175	3.6396358
22 H	11.3414545	10.8960036	9.5359966	8.4518750
23 H	11.5069740	11.3605126	10.1295879	8.1318516
24 H	9.6878852	9.7803886	8.7157067	6.1287717
25 H	10.5409184	9.8411395	8.4303876	8.2852393
26 H	9.0509063	8.1270962	6.7371568	7.6152727
27 H	6.5782153	5.6986554	4.3084900	5.4259355
28 H	4.8214614	3.9600743	2.5464301 *	4.1406972
29 H	2.1998673 *	3.4739765	3.9476699	2.6886948 *
30 H	1.1059436 *	2.2011184 *	3.4585949	4.6539590
31 H	2.2005670 *	1.1047978 *	2.1879431 *	5.3986107
32 H	3.4549814	2.1848341 *	1.1057519 *	4.6877294
33 H	3.9253091	4.7309988	4.4861519	0.9913281 *
34 H	6.9178400	6.9852844	6.0106478	3.7991571
35 H	7.6920761	7.9449712	7.0352852	4.0933838

N H H H

1 CO	1.9760560 *	6.5329971	6.2060994	4.3708263
2 C	4.3347818	1.1054995 *	2.1907763 *	3.4385007

3 C	3.8044000	2.1811643 *	1.1038570 *	2.1980977 *
4 C	2.4613024 *	3.4486222	2.1984415 *	1.1087850 *
5 C	1.5114174 *	3.9390286	3.4652549	2.1776775 *
6 C	2.6036150 *	3.5228695	4.0355278	3.5061601
7 C	3.8876509	2.1945600 *	3.4895677	3.9478672
8 C	5.1180096	2.6655404 *	4.6673675	5.3888286
9 C	5.4082069	4.0642160	5.9295147	6.2627122
10 C	4.5954423	4.8793588	6.2579623	6.0042543
11 C	3.1884301	4.6913792	5.4961680	4.8035904
12 N	2.9508643 *	6.0150571	6.4309917	5.1900943
13 C	4.0887707	7.1159715	7.7015561	6.4580012
14 C	4.8037524	8.5010438	8.8792683	7.3536411
15 C	4.7000178	9.1178694	9.1222621	7.2860284
16 C	5.9381053	10.5214751	10.4555541	8.5103291
17 C	7.0784111	11.3414545	11.5069740	9.6878852
18 C	7.1838961	10.8960036	11.3605126	9.7803886
19 C	6.1804175	9.5359966	10.1295879	8.7157067
20 O	3.6396358	8.4518750	8.1318516	6.1287717
21 N	0.0000000	5.4382685	4.6565728	2.6219766 *
22 H	5.4382685	0.0000000	2.5401340 *	4.3639190
23 H	4.6565728	2.5401340 *	0.0000000	2.5212415 *
24 H	2.6219766 *	4.3639190	2.5212415 *	0.0000000
25 H	6.0545178	2.3746136 *	4.7676936	5.9614580
26 H	6.4924158	4.7617318	6.8498435	7.3440393
27 H	5.3064713	5.9501638	7.3496659	6.9709082
28 H	4.8756773	7.1364569	8.0476804	7.0828569
29 H	6.2121809	11.0884795	10.7931456	8.6930688
30 H	8.0487452	12.4347677	12.5404430	10.6485090
31 H	8.2143894	11.7008941	12.2993619	10.7987150
32 H	6.6093834	9.3560267	10.2128052	9.0370110
33 H	4.1354844	9.1885950	8.6507008	6.4891683
34 H	1.0448561 *	5.8046727	5.0924024	3.1231656
35 H	1.0410496 *	5.8003862	4.5546379	2.1738127 *

H H H H

1 CO	6.5818577	6.3447532	4.5662483	3.8705789
2 C	2.6656353 *	4.6620997	5.3852258	6.3693218
3 C	4.0648385	5.9266891	6.2701626	6.9470024
4 C	4.8744837	6.2491884	6.0144991	6.3188480
5 C	4.6607225	5.4687877	4.8143689	4.9477044
6 C	3.5172986	4.0190843	3.5075131	4.0325791
7 C	2.1931508 *	3.4825738	3.9440620	4.9770896
8 C	1.1054070 *	2.1855725 *	3.4213127	4.8848975
9 C	2.1829756 *	1.1047214 *	2.1700127 *	3.8551884
10 C	3.4522686	2.1972079 *	1.1038760 *	2.5267605 *

11 C	3.9669179	3.4770330	2.1947472 *	2.6200511 *
12 N	5.4244776	4.6734276	2.7057313 *	2.0902574 *
13 C	6.2086914	4.9463256	2.5961954 *	1.1058079 *
14 C	7.6667543	6.3209254	3.8822918	2.1589997 *
15 C	8.5922404	7.5056438	5.1143013	3.5190840
16 C	9.9757894	8.7769070	6.3330746	4.6497937
17 C	10.5409184	9.0509063	6.5782153	4.8214614
18 C	9.8411395	8.1270962	5.6986554	3.9600743
19 C	8.4303876	6.7371568	4.3084900	2.5464301 *
20 O	8.2852393	7.6152727	5.4259355	4.1406972
21 N	6.0545178	6.4924158	5.3064713	4.8756773
22 H	2.3746136 *	4.7617318	5.9501638	7.1364569
23 H	4.7676936	6.8498435	7.3496659	8.0476804
24 H	5.9614580	7.3440393	6.9709082	7.0828569
25 H	0.0000000	2.5343875 *	4.3400671	5.9070523
26 H	2.5343875 *	0.0000000	2.4847532 *	4.3116629
27 H	4.3400671	2.4847532 *	0.0000000	1.9672854 *
28 H	5.9070523	4.3116629	1.9672854 *	0.0000000
29 H	10.7296022	9.6874655	7.2766447	5.6512072
30 H	11.6457792	10.1244859	7.6524664	5.9002250
31 H	10.4937756	8.6095778	6.2643445	4.6145956
32 H	8.0182250	6.1131751	3.8068492	2.2224441 *
33 H	9.1703109	8.5880375	6.4124962	5.1065670
34 H	6.3283766	6.6670132	5.4436143	4.7749737
35 H	6.7416829	7.4032867	6.3035287	5.8851099

H H H H

1 CO	4.6545850	6.4602336	6.7050950	5.2844489
2 C	10.0417319	11.4639077	10.8585924	8.5884027
3 C	9.8688902	11.5331817	11.2227841	9.1156706
4 C	8.6083980	10.3943288	10.3057056	8.3778988
5 C	7.4170796	9.0777034	8.9076485	6.9783838
6 C	7.5936054	8.9292994	8.3784561	6.2069837
7 C	9.0298045	10.2670653	9.5156154	7.1978220
8 C	9.6252987	10.5643358	9.4862259	7.0385680
9 C	8.9952955	9.6607188	8.3735372	5.8886923
10 C	7.5775207	8.2504498	7.0750675	4.6385936
11 C	6.7683225	7.8117418	7.0463980	4.8026697
12 N	5.3092750	6.4278876	5.9204020	3.9492169
13 C	4.7955910	5.4435259	4.6457835	2.6217496 *
14 C	3.4989531	3.9871963	3.4961153	2.1961151 *
15 C	2.1939165 *	3.4444621	3.9352788	3.4487448
16 C	1.1075416 *	2.1942221 *	3.4765233	3.9458686
17 C	2.1998673 *	1.1059436 *	2.2005670 *	3.4549814
18 C	3.4739765	2.2011184 *	1.1047978 *	2.1848341 *

19 C	3.9476699	3.4585949	2.1879431 *	1.1057519 *
20 O	2.6886948 *	4.6539590	5.3986107	4.6877294
21 N	6.2121809	8.0487452	8.2143894	6.6093834
22 H	11.0884795	12.4347677	11.7008941	9.3560267
23 H	10.7931456	12.5404430	12.2993619	10.2128052
24 H	8.6930688	10.6485090	10.7987150	9.0370110
25 H	10.7296022	11.6457792	10.4937756	8.0182250
26 H	9.6874655	10.1244859	8.6095778	6.1131751
27 H	7.2766447	7.6524664	6.2643445	3.8068492
28 H	5.6512072	5.9002250	4.6145956	2.2224441 *
29 H	0.0000000	2.5216268 *	4.3890370	5.0533857
30 H	2.5216268 *	0.0000000	2.5433693 *	4.3733020
31 H	4.3890370	2.5433693 *	0.0000000	2.5152192 *
32 H	5.0533857	4.3733020	2.5152192 *	0.0000000
33 H	2.2957853 *	4.6262569	5.8178283	5.4651620
34 H	6.1748612	7.8703071	7.9777530	6.4174763
35 H	6.5656123	8.6010508	9.0027076	7.5420021

H H H

1 CO	2.6656039 *	2.4973238 *	2.6089128 *
2 C	8.1106302	4.7337309	4.7168458
3 C	7.7837663	4.2611699	3.8946134
4 C	6.4776301	2.9972194 *	2.4637134 *
5 C	5.3949212	2.1054803 *	2.0821328 *
6 C	5.8147161	2.9976936 *	3.4202331
7 C	7.2682727	4.2454370	4.5490360
8 C	8.0870146	5.3937387	5.8798405
9 C	7.7272060	5.6165925	6.3059322
10 C	6.4003024	4.7819388	5.5684807
11 C	5.3103595	3.4366947	4.1673836
12 N	3.9523781	3.1379412	3.9242735
13 C	4.0321822	4.0692121	5.0479294
14 C	3.3296721	4.7264586	5.6329128
15 C	2.0412968 *	4.6811798	5.3238089
16 C	2.5023715 *	5.8613786	6.4554062
17 C	3.9253091	6.9178400	7.6920761
18 C	4.7309988	6.9852844	7.9449712
19 C	4.4861519	6.0106478	7.0352852
20 O	0.9913281 *	3.7991571	4.0933838
21 N	4.1354844	1.0448561 *	1.0410496 *
22 H	9.1885950	5.8046727	5.8003862
23 H	8.6507008	5.0924024	4.5546379
24 H	6.4891683	3.1231656	2.1738127 *
25 H	9.1703109	6.3283766	6.7416829
26 H	8.5880375	6.6670132	7.4032867

27 H	6.4124962	5.4436143	6.3035287
28 H	5.1065670	4.7749737	5.8851099
29 H	2.2957853 *	6.1748612	6.5656123
30 H	4.6262569	7.8703071	8.6010508
31 H	5.8178283	7.9777530	9.0027076
32 H	5.4651620	6.4174763	7.5420021
33 H	0.0000000	4.2949626	4.3732913
34 H	4.2949626	0.0000000	1.6682036 *
35 H	4.3732913	1.6682036 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.83 , TOTAL = 4064.2 SECONDS (67.7 MIN)
WALL CLOCK TIME: STEP = 0.84 , TOTAL = 3757.3 SECONDS (62.6 MIN)
CPU UTILIZATION: STEP = 99.38% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.19 , TOTAL = 4065.4 SECONDS (67.8 MIN)
WALL CLOCK TIME: STEP = 1.19 , TOTAL = 3758.5 SECONDS (62.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.633649479	-284.633649479	0.012375587	0.001442312	196827866
11413466						
2	1	-284.633792007	-0.000142527	0.001694106	0.000169991	159510333
14596260						
3	2	-284.633791188	0.000000819	0.001506599	0.000430159	142911203
15962432						
4	3	-284.633794129	-0.000002941	0.000844902	0.000125089	136455184
16521497						
5	4	-284.633793873	0.000000256	0.000708746	0.000106232	135745709
16513520						
6	5	-284.633794549	-0.000000676	0.000302979	0.000034210	129817177
16947995						

7 6	-284.633794592	-0.000000043	0.000151561	0.000028464	123076793
17453452					
8 7	-284.633794682	-0.000000090	0.000422609	0.000029176	114094908
18163913					
9 8	-284.633794758	-0.000000076	0.000453450	0.000029898	145833725
15779242					
10 9	-284.633794830	-0.000000072	0.000300790	0.000027185	164580815
14310222					
11 10	-284.633794883	-0.000000053	0.000443092	0.000027659	161692487
14517526					
-----DISABLING FDIFF OPTION-----					
12 11	-284.633794941	-0.000000057	0.000330128	0.000021548	196828851
11413208					
13 12	-284.633794969	-0.000000029	0.000294039	0.000013618	196828890
11413199					
14 13	-284.633794982	-0.000000013	0.000099190	0.000010169	196828878
11413208					
15 14	-284.633794987	-0.000000005	0.000053133	0.000005002	196828774
11413208					
16 15	-284.633794989	-0.000000002	0.000030019	0.000004059	196828816
11413205					
17 16	-284.633794990	-0.000000001	0.000067304	0.000004079	196828777
11413208					
18 17	-284.633794992	-0.000000002	0.000122911	0.000003324	196828764
11413211					
19 18	-284.633794994	-0.000000002	0.000076628	0.000003890	196828783
11413206					
20 19	-284.633794995	-0.000000001	0.000041359	0.000004387	196828818
11413202					
21 20	-284.633794996	-0.000000001	0.000051151	0.000004276	196828819
11413201					
22 21	-284.633794997	-0.000000001	0.000061384	0.000003533	196828809
11413201					
23 22	-284.633794998	-0.000000001	0.000055091	0.000002602	196828811
11413201					
24 23	-284.633794999	-0.000000001	0.000049316	0.000001597	196828889
11413199					
25 24	-284.633794999	0.000000000	0.000012774	0.000001209	196828893
11413200					
26 25	-284.633794999	0.000000000	0.000008253	0.000000587	196828886
11413202					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 87.9 SECONDS (3.4 SEC/ITER)

OF THE ABOVE TIME, DFT PART= 28.1 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6337949994 AFTER 26 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6048355523
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000192606

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 91.64 , TOTAL = 4157.0 SECONDS (69.3 MIN)
WALL CLOCK TIME: STEP = 83.80 , TOTAL = 3842.3 SECONDS (64.0
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.83 , TOTAL = 4160.8 SECONDS (69.3 MIN)
WALL CLOCK TIME: STEP = 3.80 , TOTAL = 3846.1 SECONDS (64.1
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.81 , TOTAL = 4163.6 SECONDS (69.4 MIN)
WALL CLOCK TIME: STEP = 2.63 , TOTAL = 3848.7 SECONDS (64.1
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 39 ENERGY= -284.6337950

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0003149	-0.0004885	0.0004053
2 C	6.0	-0.0006049	0.0002150	-0.0002364
3 C	6.0	0.0000678	0.0002845	-0.0002093
4 C	6.0	0.0003840	0.0000454	0.0002136
5 C	6.0	0.0001898	0.0005693	0.0002009
6 C	6.0	-0.0002563	0.0007130	0.0002282
7 C	6.0	0.0000165	0.0003015	0.0000858
8 C	6.0	-0.0010416	-0.0006083	0.0001093
9 C	6.0	-0.0000917	-0.0002000	-0.0001211
10 C	6.0	-0.0004015	-0.0005954	-0.0002935
11 C	6.0	0.0001178	-0.0004607	0.0001258
12 N	7.0	-0.0002465	-0.0000378	0.0003258
13 C	6.0	0.0006209	-0.0001650	0.0002775
14 C	6.0	-0.0000040	0.0000083	0.0000744
15 C	6.0	0.0007537	0.0001174	0.0004580
16 C	6.0	0.0001537	0.0014934	-0.0001511
17 C	6.0	-0.0000411	-0.0004129	-0.0002119
18 C	6.0	-0.0002808	0.0004095	-0.0002631
19 C	6.0	0.0006954	-0.0004181	0.0001127
20 O	8.0	0.0002452	-0.0007016	0.0001259
21 N	7.0	0.0002501	0.0001244	0.0000576
22 H	1.0	0.0000550	0.0004682	-0.0000374
23 H	1.0	-0.0003999	-0.0004864	-0.0004087
24 H	1.0	-0.0008572	-0.0008080	0.0004213
25 H	1.0	0.0005111	-0.0002097	-0.0003261
26 H	1.0	-0.0001180	0.0004819	-0.0006327
27 H	1.0	-0.0006359	0.0004809	-0.0002114
28 H	1.0	0.0004567	0.0000918	0.0006996
29 H	1.0	-0.0000468	-0.0003851	-0.0000814
30 H	1.0	-0.0005864	0.0000863	-0.0003223
31 H	1.0	-0.0003287	0.0003768	0.0000042
32 H	1.0	0.0002210	0.0000480	0.0008054
33 H	1.0	-0.0000203	0.0000797	-0.0014344
34 H	1.0	-0.0000557	0.0000657	-0.0003340
35 H	1.0	0.0009638	-0.0004835	0.0005436

MAXIMUM GRADIENT = 0.0014934 RMS GRADIENT = 0.0004406

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0000857238

PREDICTED ENERGY CHANGE WAS -0.0000925103 RATIO= 0.927

GDIIS STEP HAS LENGTH = 0.157144

RADIUS OF STEP TAKEN= 0.15714 CURRENT TRUST RADIUS= 0.16764

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 4163.7 SECONDS (69.4 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 3848.7 SECONDS (64.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 40

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1376147000	-1.7638103266	1.0233214068
C	6.0	4.9849595459	0.6905131126	0.4415581098
C	6.0	5.2103392655	-0.6737180244	0.2194056161
C	6.0	4.0852880220	-1.5459666107	0.0758831315
C	6.0	2.7692073193	-1.0596512056	0.1701719438
C	6.0	2.4748555039	0.3322841206	0.4865771155
C	6.0	3.6466081445	1.2139989289	0.5832891956
C	6.0	3.4876219585	2.6273816490	0.8242033391
C	6.0	2.2175987524	3.1881061877	1.0100749510
C	6.0	1.0692606916	2.3367240913	0.9906462120
C	6.0	1.1671934387	0.9534328130	0.7133540486
N	7.0	-0.0443285266	0.1407859114	0.7401337752
C	6.0	-1.2446972222	0.6840237239	0.5385125915
C	6.0	-2.5572712567	0.0418858496	0.5827256562
C	6.0	-2.8602993246	-1.3465567676	0.7859323718
C	6.0	-4.1739412804	-1.8509577345	0.7761777512
C	6.0	-5.2620805989	-0.9484567826	0.5635578158
C	6.0	-5.0137160621	0.4409750240	0.3707082541
C	6.0	-3.6833760457	0.9204587359	0.3765450014
O	8.0	-1.7602887214	-2.2900215478	0.9898077276
N	7.0	1.6905905044	-2.0644246839	-0.1636877907
H	1.0	5.8342219054	1.3943137414	0.5235268006
H	1.0	6.2320123921	-1.0818221560	0.1295683136
H	1.0	4.2514543982	-2.6186482037	-0.1483936996
H	1.0	4.3949503301	3.2569433885	0.8689321350
H	1.0	2.0938182458	4.2690061315	1.1990596016
H	1.0	0.0953858735	2.7912896978	1.2379407671
H	1.0	-1.2848373706	1.7592168133	0.2820286476
H	1.0	-4.3735177506	-2.9296216614	0.9204546676
H	1.0	-6.2967803356	-1.3386872805	0.5442763274
H	1.0	-5.8513260212	1.1429633865	0.2133501434
H	1.0	-3.4849535666	1.9971710671	0.2215730252
H	1.0	-2.1012557982	-3.2182655382	1.0620348899

H 1.0 1.3700308695 -1.9151313718 -1.1470201847
H 1.0 2.1156550201 -3.0146294786 -0.1433426586

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4643302	5.2504396	4.0656143
2 C	5.4643302	0.0000000	1.4004550 *	2.4382306 *
3 C	5.2504396	1.4004550 *	0.0000000	1.4307888 *
4 C	4.0656143	2.4382306 *	1.4307888 *	0.0000000
5 C	2.8546425 *	2.8365972 *	2.4719413 *	1.4062224 *
6 C	3.1850276	2.5359371 *	2.9268229 *	2.5079849 *
7 C	4.6232036	1.4440601 *	2.4781327 *	2.8403012 *
8 C	5.5267317	2.4778815 *	3.7723725	4.2818248
9 C	5.3710321	3.7708710	4.9492767	5.1742075
10 C	4.2051652	4.2830136	5.1774613	5.0008499
11 C	2.9222461 *	3.8364486	4.3861866	3.8946942
12 N	1.9341110 *	5.0680456	5.3428558	4.5099995
13 C	2.8526685 *	6.2304146	6.6039979	5.7961734
14 C	3.2736942	7.5713863	7.8089605	6.8484859
15 C	3.0361065	8.1127267	8.1184279	6.9846344
16 C	4.3195127	9.5108627	9.4742076	8.2944741
17 C	5.4802275	10.3780026	10.4816745	9.3791335
18 C	5.6412047	10.0020399	10.2857542	9.3180864
19 C	4.7141903	8.6716287	9.0368282	8.1563345
20 O	1.9697865 *	7.3947643	7.1969168	5.9631907
21 N	1.9776485 *	4.3369197	3.8038739	2.4618630 *
22 H	6.5326010	1.1060293 *	2.1813928 *	3.4502758
23 H	6.1972240	2.1894407 *	1.1038277 *	2.1969838 *
24 H	4.3620341	3.4404392	2.1994295 *	1.1084030 *
25 H	6.5845813	2.6678313 *	4.0665517	4.8777825
26 H	6.3444851	4.6624156	5.9247740	6.2483106
27 H	4.5603488	5.3810239	6.2615047	6.0067869
28 H	3.8709954	6.3622269	6.9361670	6.3091188
29 H	4.6604735	10.0456864	9.8707085	8.6127346
30 H	6.4661931	11.4632395	11.5308944	10.3946958
31 H	6.7061761	10.8481277	11.2098531	10.2949279
32 H	5.2830656	8.5729328	9.0962504	8.3596416
33 H	2.6701086 *	8.1165257	7.7874366	6.4840114
34 H	2.5004260 *	4.7308217	4.2610087	3.0007327
35 H	2.6150138 *	4.7226157	3.8972456	2.4666748 *

C C C C

1 CO	2.8546425 *	3.1850276	4.6232036	5.5267317
2 C	2.8365972 *	2.5359371 *	1.4440601 *	2.4778815 *
3 C	2.4719413 *	2.9268229 *	2.4781327 *	3.7723725
4 C	1.4062224 *	2.5079849 *	2.8403012 *	4.2818248
5 C	0.0000000	1.4574770 *	2.4718380 *	3.8128845
6 C	1.4574770 *	0.0000000	1.4696185 *	2.5312369 *
7 C	2.4718380 *	1.4696185 *	0.0000000	1.4425557 *
8 C	3.8128845	2.5312369 *	1.4425557 *	0.0000000
9 C	4.3649916	2.9147814 *	2.4741288 *	1.4006853 *
10 C	3.8856610	2.4995124 *	2.8406287 *	2.4414455 *
11 C	2.6294491 *	1.4653442 *	2.4964593 *	2.8633513 *
12 N	3.1115735	2.5391437 *	3.8469988	4.3202894
13 C	4.3917544	3.7365078	4.9201369	5.1237783
14 C	5.4548106	5.0414160	6.3136336	6.5790451
15 C	5.6703457	5.6010711	6.9955239	7.4893094
16 C	7.0143226	7.0040640	8.4019140	8.8745356
17 C	8.0416853	7.8426018	9.1674063	9.4557840
18 C	7.9288076	7.4902566	8.6973543	8.7896974
19 C	6.7527222	6.1872346	7.3387722	7.3849303
20 O	4.7646562	5.0066131	6.4558462	7.1936670
21 N	1.5114385 *	2.6042521 *	3.8899924	5.1203806
22 H	3.9422225	3.5234379	2.1958458 *	2.6678445 *
23 H	3.4631141	4.0303076	3.4872586	4.6660893
24 H	2.1746292 *	3.5024981	3.9484659	5.3898251
25 H	4.6652219	3.5194590	2.1943632 *	1.1052572 *
26 H	5.4689441	4.0187810	3.4818671	2.1858950 *
27 H	4.8082426	3.5033029	3.9405069	3.4213024
28 H	4.9390087	4.0265702	4.9706313	4.8809867
29 H	7.4214712	7.5979270	9.0335869	9.6274123
30 H	9.0779925	8.9295616	10.2659000	10.5613725
31 H	8.8975823	8.3700151	9.5054013	9.4758951
32 H	6.9614174	6.1936580	7.1835485	7.0268868
33 H	5.4015226	5.8205111	7.2740708	8.0909647
34 H	2.1034581 *	2.9900090 *	4.2388950	5.3855676
35 H	2.0850329 *	3.4245663	4.5555581	5.8864869

C C C N

1 CO	5.3710321	4.2051652	2.9222461 *	1.9341110 *
2 C	3.7708710	4.2830136	3.8364486	5.0680456
3 C	4.9492767	5.1774613	4.3861866	5.3428558
4 C	5.1742075	5.0008499	3.8946942	4.5099995
5 C	4.3649916	3.8856610	2.6294491 *	3.1115735
6 C	2.9147814 *	2.4995124 *	1.4653442 *	2.5391437 *
7 C	2.4741288 *	2.8406287 *	2.4964593 *	3.8469988
8 C	1.4006853 *	2.4414455 *	2.8633513 *	4.3202894

9 C	0.0000000	1.4296535 *	2.4869981 *	3.8046477
10 C	1.4296535 *	0.0000000	1.4142053 *	2.4748701 *
11 C	2.4869981 *	1.4142053 *	0.0000000	1.4590742 *
12 N	3.8046477	2.4748701 *	1.4590742 *	0.0000000
13 C	4.2988712	2.8792785 *	2.4331805 *	1.3329079 *
14 C	5.7341707	4.3109646	3.8366156	2.5198095 *
15 C	6.8116413	5.3897966	4.6385254	3.1849611
16 C	8.1423987	6.7137056	6.0329324	4.5849802
17 C	8.5589797	7.1456770	6.7063543	5.3331572
18 C	7.7619220	6.4016243	6.2115748	4.9921339
19 C	6.3533526	4.9970475	4.8623607	3.7393520
20 O	6.7700726	5.4233869	4.3779647	2.9859138 *
21 N	5.4078219	4.5922378	3.1860023	2.9478452 *
22 H	4.0662493	4.8796714	4.6916484	6.0146160
23 H	5.9264742	6.2515533	5.4895774	6.4233960
24 H	6.2607519	5.9982900	4.7973990	5.1824423
25 H	2.1830070 *	3.4528002	3.9684733	5.4253316
26 H	1.1042561 *	2.1970135 *	3.4767183	4.6716685
27 H	2.1709845 *	1.1028221 *	2.1912737 *	2.7004633 *
28 H	3.8521209	2.5253576 *	2.6168272 *	2.0899859 *
29 H	8.9931887	7.5738472	6.7690829	5.3105365
30 H	9.6541949	8.2441771	7.8098211	6.4280911
31 H	8.3621126	7.0656758	7.0388594	5.9163401
32 H	5.8787043	4.6311594	4.7930898	3.9437256
33 H	7.7263706	6.3964976	5.3110645	3.9519358
34 H	5.6048608	4.7684751	3.4250249	3.1286672
35 H	6.3098886	5.5693677	4.1688160	3.9246281

C C C C

1 CO	2.8526685 *	3.2736942	3.0361065	4.3195127
2 C	6.2304146	7.5713863	8.1127267	9.5108627
3 C	6.6039979	7.8089605	8.1184279	9.4742076
4 C	5.7961734	6.8484859	6.9846344	8.2944741
5 C	4.3917544	5.4548106	5.6703457	7.0143226
6 C	3.7365078	5.0414160	5.6010711	7.0040640
7 C	4.9201369	6.3136336	6.9955239	8.4019140
8 C	5.1237783	6.5790451	7.4893094	8.8745356
9 C	4.2988712	5.7341707	6.8116413	8.1423987
10 C	2.8792785 *	4.3109646	5.3897966	6.7137056
11 C	2.4331805 *	3.8366156	4.6385254	6.0329324
12 N	1.3329079 *	2.5198095 *	3.1849611	4.5849802
13 C	0.0000000	1.4618982 *	2.6066538 *	3.8811192
14 C	1.4618982 *	0.0000000	1.4355807 *	2.4967784 *
15 C	2.6066538 *	1.4355807 *	0.0000000	1.4071854 *
16 C	3.8811192	2.4967784 *	1.4071854 *	0.0000000

17 C	4.3364720	2.8804756 *	2.4446855 *	1.4296022 *
18 C	3.7805732	2.4976678 *	2.8292905 *	2.4743854 *
19 C	2.4554611 *	1.4430914 *	2.4463059 *	2.8427293 *
20 O	3.0519579	2.4977368 *	1.4634597 *	2.4625461 *
21 N	4.0820299	4.7997924	4.7040101	5.9432019
22 H	7.1144805	8.4999837	9.1200837	10.5242078
23 H	7.6932850	8.8724054	9.1198153	10.4543553
24 H	6.4488111	7.3465449	7.2847939	8.5106682
25 H	6.2076338	7.6649784	8.5928895	9.9762298
26 H	4.9430868	6.3151443	7.4999001	8.7702677
27 H	2.5933747 *	3.8762247	5.1051112	6.3238312
28 H	1.1060902 *	2.1584097 *	3.5187823	4.6502113
29 H	4.7951883	3.4989526	2.1940877 *	1.1064188 *
30 H	5.4419608	3.9864005	3.4449762	2.1960521 *
31 H	4.6408388	3.4927936	3.9334211	3.4776369
32 H	2.6160189 *	2.1941208 *	3.4480734	3.9484663
33 H	4.0293461	3.3266010	2.0385469 *	2.4994539 *
34 H	4.0538168	4.7165283	4.6856458	5.8684270
35 H	5.0435037	5.6307816	5.3297411	6.4620950

C C C O

1 CO	5.4802275	5.6412047	4.7141903	1.9697865 *
2 C	10.3780026	10.0020399	8.6716287	7.3947643
3 C	10.4816745	10.2857542	9.0368282	7.1969168
4 C	9.3791335	9.3180864	8.1563345	5.9631907
5 C	8.0416853	7.9288076	6.7527222	4.7646562
6 C	7.8426018	7.4902566	6.1872346	5.0066131
7 C	9.1674063	8.6973543	7.3387722	6.4558462
8 C	9.4557840	8.7896974	7.3849303	7.1936670
9 C	8.5589797	7.7619220	6.3533526	6.7700726
10 C	7.1456770	6.4016243	4.9970475	5.4233869
11 C	6.7063543	6.2115748	4.8623607	4.3779647
12 N	5.3331572	4.9921339	3.7393520	2.9859138 *
13 C	4.3364720	3.7805732	2.4554611 *	3.0519579
14 C	2.8804756 *	2.4976678 *	1.4430914 *	2.4977368 *
15 C	2.4446855 *	2.8292905 *	2.4463059 *	1.4634597 *
16 C	1.4296022 *	2.4743854 *	2.8427293 *	2.4625461 *
17 C	0.0000000	1.4245689 *	2.4535947 *	3.7741266
18 C	1.4245689 *	0.0000000	1.4141228 *	4.2926001
19 C	2.4535947 *	1.4141228 *	0.0000000	3.7923001
20 O	3.7741266	4.2926001	3.7923001	0.0000000
21 N	7.0791176	7.1770700	6.1709721	3.6455470
22 H	11.3409923	10.8908203	9.5305201	8.4538947
23 H	11.5030564	11.3509237	10.1185500	8.1287536
24 H	9.6852343	9.7710872	8.7041584	6.1273610

25 H	10.5374044	9.8336620	8.4238330	8.2867604
26 H	9.0407428	8.1152346	6.7279472	7.6104383
27 H	6.5683288	5.6902543	4.3036093	5.4152398
28 H	4.8196700	3.9560285	2.5427222 *	4.1380353
29 H	2.2004394 *	3.4746219	3.9490825	2.6912570 *
30 H	1.1060087 *	2.2008130 *	3.4585772	4.6565321
31 H	2.2008848 *	1.1041466 *	2.1854400 *	5.3967451
32 H	3.4571459	2.1865732 *	1.1057564 *	4.6845143
33 H	3.9231779	4.7276208	4.4835298	0.9915202 *
34 H	6.9170398	6.9718693	5.9915560	3.8086056
35 H	7.6941381	7.9393566	7.0273725	4.1026853

N H H H

1 CO	1.9776485 *	6.5326010	6.1972240	4.3620341
2 C	4.3369197	1.1060293 *	2.1894407 *	3.4404392
3 C	3.8038739	2.1813928 *	1.1038277 *	2.1994295 *
4 C	2.4618630 *	3.4502758	2.1969838 *	1.1084030 *
5 C	1.5114385 *	3.9422225	3.4631141	2.1746292 *
6 C	2.6042521 *	3.5234379	4.0303076	3.5024981
7 C	3.8899924	2.1958458 *	3.4872586	3.9484659
8 C	5.1203806	2.6678445 *	4.6660893	5.3898251
9 C	5.4078219	4.0662493	5.9264742	6.2607519
10 C	4.5922378	4.8796714	6.2515533	5.9982900
11 C	3.1860023	4.6916484	5.4895774	4.7973990
12 N	2.9478452 *	6.0146160	6.4233960	5.1824423
13 C	4.0820299	7.1144805	7.6932850	6.4488111
14 C	4.7997924	8.4999837	8.8724054	7.3465449
15 C	4.7040101	9.1200837	9.1198153	7.2847939
16 C	5.9432019	10.5242078	10.4543553	8.5106682
17 C	7.0791176	11.3409923	11.5030564	9.6852343
18 C	7.1770700	10.8908203	11.3509237	9.7710872
19 C	6.1709721	9.5305201	10.1185500	8.7041584
20 O	3.6455470	8.4538947	8.1287536	6.1273610
21 N	0.0000000	5.4410308	4.6557512	2.6201949 *
22 H	5.4410308	0.0000000	2.5386393 *	4.3658325
23 H	4.6557512	2.5386393 *	0.0000000	2.5222425 *
24 H	2.6201949 *	4.3658325	2.5222425 *	0.0000000
25 H	6.0577904	2.3791168 *	4.7693126	5.9647397
26 H	6.4909182	4.7655871	6.8483447	7.3423979
27 H	5.2997361	5.9494679	7.3408222	6.9614838
28 H	4.8653950	7.1324947	8.0372742	7.0711733
29 H	6.2207186	11.0928769	10.7943103	8.6965100
30 H	8.0514596	12.4350690	12.5382858	10.6481617
31 H	8.2042672	11.6923658	12.2867309	10.7864152
32 H	6.5902384	9.3435349	10.1935319	9.0163558

33 H	4.1487158	9.1944377	8.6531638	6.4947367
34 H	1.0449830 *	5.8027714	5.0953848	3.1296633
35 H	1.0411450 *	5.8061377	4.5557242	2.1722030 *

H H H H

1 CO	6.5845813	6.3444851	4.5603488	3.8709954
2 C	2.6678313 *	4.6624156	5.3810239	6.3622269
3 C	4.0665517	5.9247740	6.2615047	6.9361670
4 C	4.8777825	6.2483106	6.0067869	6.3091188
5 C	4.6652219	5.4689441	4.8082426	4.9390087
6 C	3.5194590	4.0187810	3.5033029	4.0265702
7 C	2.1943632 *	3.4818671	3.9405069	4.9706313
8 C	1.1052572 *	2.1858950 *	3.4213024	4.8809867
9 C	2.1830070 *	1.1042561 *	2.1709845 *	3.8521209
10 C	3.4528002	2.1970135 *	1.1028221 *	2.5253576 *
11 C	3.9684733	3.4767183	2.1912737 *	2.6168272 *
12 N	5.4253316	4.6716685	2.7004633 *	2.0899859 *
13 C	6.2076338	4.9430868	2.5933747 *	1.1060902 *
14 C	7.6649784	6.3151443	3.8762247	2.1584097 *
15 C	8.5928895	7.4999001	5.1051112	3.5187823
16 C	9.9762298	8.7702677	6.3238312	4.6502113
17 C	10.5374044	9.0407428	6.5683288	4.8196700
18 C	9.8336620	8.1152346	5.6902543	3.9560285
19 C	8.4238330	6.7279472	4.3036093	2.5427222 *
20 O	8.2867604	7.6104383	5.4152398	4.1380353
21 N	6.0577904	6.4909182	5.2997361	4.8653950
22 H	2.3791168 *	4.7655871	5.9494679	7.1324947
23 H	4.7693126	6.8483447	7.3408222	8.0372742
24 H	5.9647397	7.3423979	6.9614838	7.0711733
25 H	0.0000000	2.5354416 *	4.3404211	5.9031880
26 H	2.5354416 *	0.0000000	2.4857372 *	4.3075866
27 H	4.3404211	2.4857372 *	0.0000000	1.9707761 *
28 H	5.9031880	4.3075866	1.9707761 *	0.0000000
29 H	10.7313687	9.6811310	7.2664107	5.6509062
30 H	11.6420929	10.1132147	7.6418368	5.8979111
31 H	10.4825988	8.5947125	6.2554095	4.6083949
32 H	8.0061842	6.1024101	3.8055825	2.2137724 *
33 H	9.1742200	8.5835109	6.4008540	5.1039474
34 H	6.3217528	6.6536843	5.4279976	4.7530349
35 H	6.7492602	7.4063397	6.3006451	5.8765549

H H H H

1 CO	4.6604735	6.4661931	6.7061761	5.2830656
2 C	10.0456864	11.4632395	10.8481277	8.5729328

3 C	9.8707085	11.5308944	11.2098531	9.0962504
4 C	8.6127346	10.3946958	10.2949279	8.3596416
5 C	7.4214712	9.0779925	8.8975823	6.9614174
6 C	7.5979270	8.9295616	8.3700151	6.1936580
7 C	9.0335869	10.2659000	9.5054013	7.1835485
8 C	9.6274123	10.5613725	9.4758951	7.0268868
9 C	8.9931887	9.6541949	8.3621126	5.8787043
10 C	7.5738472	8.2441771	7.0656758	4.6311594
11 C	6.7690829	7.8098211	7.0388594	4.7930898
12 N	5.3105365	6.4280911	5.9163401	3.9437256
13 C	4.7951883	5.4419608	4.6408388	2.6160189 *
14 C	3.4989526	3.9864005	3.4927936	2.1941208 *
15 C	2.1940877 *	3.4449762	3.9334211	3.4480734
16 C	1.1064188 *	2.1960521 *	3.4776369	3.9484663
17 C	2.2004394 *	1.1060087 *	2.2008848 *	3.4571459
18 C	3.4746219	2.2008130 *	1.1041466 *	2.1865732 *
19 C	3.9490825	3.4585772	2.1854400 *	1.1057564 *
20 O	2.6912570 *	4.6565321	5.3967451	4.6845143
21 N	6.2207186	8.0514596	8.2042672	6.5902384
22 H	11.0928769	12.4350690	11.6923658	9.3435349
23 H	10.7943103	12.5382858	12.2867309	10.1935319
24 H	8.6965100	10.6481617	10.7864152	9.0163558
25 H	10.7313687	11.6420929	10.4825988	8.0061842
26 H	9.6811310	10.1132147	8.5947125	6.1024101
27 H	7.2664107	7.6418368	6.2554095	3.8055825
28 H	5.6509062	5.8979111	4.6083949	2.2137724 *
29 H	0.0000000	2.5241873 *	4.3897452	5.0548263
30 H	2.5241873 *	0.0000000	2.5429376 *	4.3747523
31 H	4.3897452	2.5429376 *	0.0000000	2.5158412 *
32 H	5.0548263	4.3747523	2.5158412 *	0.0000000
33 H	2.2948932 *	4.6263716	5.8140872	5.4609317
34 H	6.1880525	7.8722783	7.9593056	6.3835751
35 H	6.5763405	8.6052699	8.9936419	7.5245016

H H H

1 CO	2.6701086 *	2.5004260 *	2.6150138 *
2 C	8.1165257	4.7308217	4.7226157
3 C	7.7874366	4.2610087	3.8972456
4 C	6.4840114	3.0007327	2.4666748 *
5 C	5.4015226	2.1034581 *	2.0850329 *
6 C	5.8205111	2.9900090 *	3.4245663
7 C	7.2740708	4.2388950	4.5555581
8 C	8.0909647	5.3855676	5.8864869
9 C	7.7263706	5.6048608	6.3098886
10 C	6.3964976	4.7684751	5.5693677

11	C	5.3110645	3.4250249	4.1688160
12	N	3.9519358	3.1286672	3.9246281
13	C	4.0293461	4.0538168	5.0435037
14	C	3.3266010	4.7165283	5.6307816
15	C	2.0385469 *	4.6856458	5.3297411
16	C	2.4994539 *	5.8684270	6.4620950
17	C	3.9231779	6.9170398	7.6941381
18	C	4.7276208	6.9718693	7.9393566
19	C	4.4835298	5.9915560	7.0273725
20	O	0.9915202 *	3.8086056	4.1026853
21	N	4.1487158	1.0449830 *	1.0411450 *
22	H	9.1944377	5.8027714	5.8061377
23	H	8.6531638	5.0953848	4.5557242
24	H	6.4947367	3.1296633	2.1722030 *
25	H	9.1742200	6.3217528	6.7492602
26	H	8.5835109	6.6536843	7.4063397
27	H	6.4008540	5.4279976	6.3006451
28	H	5.1039474	4.7530349	5.8765549
29	H	2.2948932 *	6.1880525	6.5763405
30	H	4.6263716	7.8722783	8.6052699
31	H	5.8140872	7.9593056	8.9936419
32	H	5.4609317	6.3835751	7.5245016
33	H	0.0000000	4.3160067	4.3905284
34	H	4.3160067	0.0000000	1.6649985 *
35	H	4.3905284	1.6649985 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.75 , TOTAL = 4164.4 SECONDS (69.4 MIN)
WALL CLOCK TIME: STEP = 0.75 , TOTAL = 3849.5 SECONDS (64.2 MIN)

CPU UTILIZATION: STEP = 99.35%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.98 , TOTAL = 4165.4 SECONDS (69.4 MIN)
WALL CLOCK TIME: STEP = 0.98 , TOTAL = 3850.5 SECONDS (64.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.633392414	-284.633392414	0.018983761	0.002608895	196894572
11405753						
2	1	-284.633878548	-0.000486134	0.003933713	0.000287864	164411543
14189530						
3	2	-284.633875086	0.000003462	0.002017653	0.000726449	149501033
15424566						
4	3	-284.633886311	-0.000011225	0.001578457	0.000239243	142760666
15986526						
5	4	-284.633884859	0.000001453	0.001187732	0.000292182	141619581
16056908						
6	5	-284.633887549	-0.000002690	0.000433884	0.000057104	135806087
16488955						
7	6	-284.633887658	-0.000000109	0.000270548	0.000046638	128205763
17057524						
8	7	-284.633887935	-0.000000277	0.000877442	0.000049573	119447312
17782253						
9	8	-284.633888242	-0.000000306	0.000956770	0.000053446	151469313
15349037						
10	9	-284.633888438	-0.000000196	0.000416332	0.000052339	170752277
13796654						
11	10	-284.633888630	-0.000000192	0.000755263	0.000047535	165578766
14177482						

-----DISABLING FDIFF OPTION-----

12	11	-284.633888807	-0.000000177	0.000613999	0.000030189	196890107
11405550						
13	12	-284.633888901	-0.000000094	0.000565165	0.000028313	196890502
11405546						
14	13	-284.633888937	-0.000000036	0.000184488	0.000014320	196890192
11405545						
15	14	-284.633888958	-0.000000021	0.000116372	0.000006890	196890052
11405546						
16	15	-284.633888962	-0.000000004	0.000056081	0.000007095	196890291
11405543						
17	16	-284.633888966	-0.000000004	0.000135854	0.000007180	196890039
11405551						
18	17	-284.633888972	-0.000000006	0.000204590	0.000006008	196890046
11405552						
19	18	-284.633888980	-0.000000008	0.000245571	0.000006214	196890201
11405549						
20	19	-284.633888988	-0.000000008	0.000139643	0.000005353	196890282
11405540						
21	20	-284.633888992	-0.000000005	0.000072496	0.000004002	196890213
11405546						

22 21	-284.633888995	-0.000000003	0.000057005	0.000003286	196890240
11405542					
23 22	-284.633888997	-0.000000002	0.000034797	0.000003099	196890286
11405539					
24 23	-284.633888998	-0.000000001	0.000053156	0.000001896	196890286
11405539					
25 24	-284.633888998	0.000000000	0.000017233	0.000001228	196890247
11405544					
26 25	-284.633888998	0.000000000	0.000007368	0.000000721	196890274
11405540					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 88.3 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 28.1 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6338889981 AFTER 26 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6060835511
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000222077

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 92.15 , TOTAL = 4257.6 SECONDS (71.0 MIN)
WALL CLOCK TIME: STEP = 84.57 , TOTAL = 3935.1 SECONDS (65.6 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.65 , TOTAL = 4261.2 SECONDS (71.0 MIN)
WALL CLOCK TIME: STEP = 3.64 , TOTAL = 3938.7 SECONDS (65.6 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.82 , TOTAL = 4264.0 SECONDS (71.1 MIN)
WALL CLOCK TIME: STEP = 2.68 , TOTAL = 3941.4 SECONDS (65.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 40 ENERGY= -284.6338890

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0007373	-0.0002533	0.0007596
2 C	6.0	-0.0005864	0.0001524	-0.0006005
3 C	6.0	-0.0010437	0.0008786	-0.0002919
4 C	6.0	0.0004583	0.0003763	0.0003054
5 C	6.0	0.0001563	0.0001483	0.0003263
6 C	6.0	-0.0001422	0.0005548	0.0002056
7 C	6.0	0.0000121	0.0006123	-0.0001578
8 C	6.0	-0.0003974	-0.0002813	0.0000608
9 C	6.0	0.0004369	0.0004088	-0.0000937
10 C	6.0	-0.0010611	-0.0011346	-0.0003545
11 C	6.0	-0.0000160	-0.0006204	0.0001193
12 N	7.0	-0.0000890	0.0001794	0.0004587
13 C	6.0	0.0002619	-0.0003355	0.0003902
14 C	6.0	-0.0000641	0.0001688	0.0002782
15 C	6.0	0.0004160	0.0001353	0.0008709
16 C	6.0	0.0003665	-0.0001318	0.0003048
17 C	6.0	-0.0006765	-0.0004016	-0.0001100
18 C	6.0	0.0001156	0.0007162	-0.0002406
19 C	6.0	0.0002798	-0.0002718	0.0000217
20 O	8.0	0.0003787	-0.0004424	-0.0004354
21 N	7.0	0.0004494	-0.0002275	0.0005674
22 H	1.0	0.0003911	0.0006485	0.0001994
23 H	1.0	-0.0004578	-0.0004979	-0.0001497
24 H	1.0	-0.0013547	-0.0006317	0.0004130
25 H	1.0	0.0003883	-0.0001668	-0.0001426
26 H	1.0	-0.0001678	0.0001647	-0.0007517
27 H	1.0	-0.0000799	-0.0001284	-0.0002397

28 H	1.0	0.0003960	0.0002796	0.0007620
29 H	1.0	0.0000938	0.0002905	-0.0003824
30 H	1.0	-0.0006602	0.0001772	-0.0004897
31 H	1.0	0.0001792	0.0002771	0.0001503
32 H	1.0	0.0006696	-0.0000328	0.0003100
33 H	1.0	-0.0005011	0.0001369	-0.0014050
34 H	1.0	0.0003579	-0.0000922	-0.0004897
35 H	1.0	0.0007532	-0.0006559	-0.0001688

MAXIMUM GRADIENT = 0.0014050 RMS GRADIENT = 0.0004743
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000939988
 PREDICTED ENERGY CHANGE WAS -0.0000745588 RATIO= 1.261
 GDIIS STEP HAS LENGTH = 0.047006
 RADIUS OF STEP TAKEN= 0.04701 CURRENT TRUST RADIUS= 0.22223

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 4264.1 SECONDS (71.1 MIN)
 WALL CLOCK TIME: STEP = 0.03 , TOTAL = 3941.4 SECONDS (65.7 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

INSERCH= 41

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1384590868	-1.7650928782	1.0225300372
C	6.0	4.9847069000	0.6910715176	0.4418267526
C	6.0	5.2095624356	-0.6732969630	0.2205954756
C	6.0	4.0846102946	-1.5456780645	0.0752463493
C	6.0	2.7684198457	-1.0595534605	0.1685004678
C	6.0	2.4749324293	0.3320771510	0.4853465696
C	6.0	3.6464732773	1.2146246343	0.5823086225
C	6.0	3.4872407985	2.6282589542	0.8242606969
C	6.0	2.2168424508	3.1875990019	1.0114859401
C	6.0	1.0696146949	2.3355550445	0.9927501708
C	6.0	1.1673267888	0.9526195538	0.7135505641
N	7.0	-0.0436686878	0.1395704663	0.7406990030
C	6.0	-1.2440096580	0.6825509828	0.5377325142
C	6.0	-2.5569048073	0.0408294542	0.5822662164
C	6.0	-2.8607704846	-1.3466573074	0.7886261635
C	6.0	-4.1744905742	-1.8507017186	0.7803592565
C	6.0	-5.2614244980	-0.9473581401	0.5665428684
C	6.0	-5.0118722601	0.4409311618	0.3690870611

C	6.0	-3.6817042176	0.9197630465	0.3719363598
O	8.0	-1.7605692416	-2.2899517730	0.9924005800
N	7.0	1.6898485377	-2.0636232540	-0.1677648211
H	1.0	5.8343611149	1.3941486276	0.5251383796
H	1.0	6.2312477924	-1.0813341861	0.1335854430
H	1.0	4.2512454865	-2.6177413555	-0.1493856829
H	1.0	4.3939097342	3.2584682283	0.8703172715
H	1.0	2.0920158641	4.2680868466	1.2020522692
H	1.0	0.0953810889	2.7876564151	1.2428980166
H	1.0	-1.2840046599	1.7572819660	0.2797143064
H	1.0	-4.3746491836	-2.9292678106	0.9254986291
H	1.0	-6.2967724220	-1.3365158645	0.5480932630
H	1.0	-5.8486453485	1.1432816576	0.2093746237
H	1.0	-3.4814696600	1.9951992671	0.2096254395
H	1.0	-2.1024453485	-3.2175963956	1.0689283486
H	1.0	1.3687613708	-1.9103598703	-1.1500605382
H	1.0	2.1144380598	-3.0137399353	-0.1531796173

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4640715	5.2489243	4.0641849
2 C	5.4640715	0.0000000	1.4003588 *	2.4387710 *
3 C	5.2489243	1.4003588 *	0.0000000	1.4309761 *
4 C	4.0641849	2.4387710 *	1.4309761 *	0.0000000
5 C	2.8537424 *	2.8374854 *	2.4720609 *	1.4061902 *
6 C	3.1852466	2.5356930 *	2.9255891 *	2.5070320 *
7 C	4.6237079	1.4438533 *	2.4775658 *	2.8404836 *
8 C	5.5276749	2.4781759 *	3.7724097	4.2824786
9 C	5.3711224	3.7707075	4.9485754	5.1738780
10 C	4.2051458	4.2820310	5.1757686	4.9995982
11 C	2.9223275 *	3.8359656	4.3847780	3.8935159
12 N	1.9339963 *	5.0673503	5.3411327	4.5083896
13 C	2.8525793 *	6.2294607	6.6020824	5.7942289
14 C	3.2741677	7.5708946	7.8076114	6.8471745
15 C	3.0372977	8.1132068	8.1182724	6.9847573
16 C	4.3205914	9.5113676	9.4741790	8.2947556
17 C	5.4804523	10.3770523	10.4802842	9.3780449
18 C	5.6408725	9.9999728	10.2830580	9.3155222
19 C	4.7143792	8.6697097	9.0341224	8.1536535
20 O	1.9704551 *	7.3951593	7.1966653	5.9633245
21 N	1.9780626 *	4.3377456	3.8042367	2.4621546 *
22 H	6.5323430	1.1059704 *	2.1811582 *	3.4505959
23 H	6.1951451	2.1886751 *	1.1035878 *	2.1970597 *

24 H	4.3606660	3.4403111	2.1991183 *	1.1079470 *
25 H	6.5854533	2.6691143 *	4.0677027	4.8793058
26 H	6.3441209	4.6626862	5.9244939	6.2481987
27 H	4.5582830	5.3798597	6.2592453	6.0045939
28 H	3.8706980	6.3608042	6.9338029	6.3066139
29 H	4.6618521	10.0468075	9.8713426	8.6137286
30 H	6.4669137	11.4627300	11.5300848	10.3942503
31 H	6.7056158	10.8452777	11.2064287	10.2916501
32 H	5.2824705	8.5691780	9.0914813	8.3547254
33 H	2.6708748 *	8.1177995	7.7883622	6.4855510
34 H	2.5009790 *	4.7303924	4.2615461	3.0017004
35 H	2.6164681 *	4.7242040	3.8983556	2.4675824 *

C C C C

1 CO	2.8537424 *	3.1852466	4.6237079	5.5276749
2 C	2.8374854 *	2.5356930 *	1.4438533 *	2.4781759 *
3 C	2.4720609 *	2.9255891 *	2.4775658 *	3.7724097
4 C	1.4061902 *	2.5070320 *	2.8404836 *	4.2824786
5 C	0.0000000	1.4571074 *	2.4726708 *	3.8140117
6 C	1.4571074 *	0.0000000	1.4699659 *	2.5322089 *
7 C	2.4726708 *	1.4699659 *	0.0000000	1.4430030 *
8 C	3.8140117	2.5322089 *	1.4430030 *	0.0000000
9 C	4.3649933	2.9150366 *	2.4739978 *	1.4006522 *
10 C	3.8848537	2.4992599 *	2.8399203 *	2.4411023 *
11 C	2.6285773 *	1.4652585 *	2.4964051 *	2.8639178 *
12 N	3.1101690	2.5388216 *	3.8468138	4.3206336
13 C	4.3898577	3.7357873	4.9195440	5.1237300
14 C	5.4535426	5.0411908	6.3134535	6.5791374
15 C	5.6705175	5.6017724	6.9962099	7.4898916
16 C	7.0145771	7.0047400	8.4025547	8.8749729
17 C	8.0404867	7.8418599	9.1665185	9.4546603
18 C	7.9261992	7.4884985	8.6954593	8.7878614
19 C	6.7500504	6.1856618	7.3371238	7.3835851
20 O	4.7649170	5.0071563	6.4564960	7.1942045
21 N	1.5114717 *	2.6042833 *	3.8907454	5.1213760
22 H	3.9430750	3.5235409	2.1959851 *	2.6686094 *
23 H	3.4630725	4.0288178	3.4862356	4.6655855
24 H	2.1743443 *	3.5013715	3.9481838	5.3900102
25 H	4.6669128	3.5205740	2.1952009 *	1.1051396 *
26 H	5.4689581	4.0190129	3.4819609	2.1859585 *
27 H	4.8062969	3.5022876	3.9396780	3.4213122
28 H	4.9365043	4.0253076	4.9694721	4.8805650
29 H	7.4224196	7.5991363	9.0348232	9.6283782
30 H	9.0773625	8.9292187	10.2653604	10.5604272
31 H	8.8942659	8.3675660	9.5027074	9.4732261

32 H	6.9566029	6.1903734	7.1802340	7.0243481
33 H	5.4030776	5.8217813	7.2754002	8.0918773
34 H	2.1027407 *	2.9877575 *	4.2372872	5.3837682
35 H	2.0856690 *	3.4252246	4.5570980	5.8883044

C C C N

1 CO	5.3711224	4.2051458	2.9223275 *	1.9339963 *
2 C	3.7707075	4.2820310	3.8359656	5.0673503
3 C	4.9485754	5.1757686	4.3847780	5.3411327
4 C	5.1738780	4.9995982	3.8935159	4.5083896
5 C	4.3649933	3.8848537	2.6285773 *	3.1101690
6 C	2.9150366 *	2.4992599 *	1.4652585 *	2.5388216 *
7 C	2.4739978 *	2.8399203 *	2.4964051 *	3.8468138
8 C	1.4006522 *	2.4411023 *	2.8639178 *	4.3206336
9 C	0.0000000	1.4291471 *	2.4870428 *	3.8044335
10 C	1.4291471 *	0.0000000	1.4142173 *	2.4749299 *
11 C	2.4870428 *	1.4142173 *	0.0000000	1.4588680 *
12 N	3.8044335	2.4749299 *	1.4588680 *	0.0000000
13 C	4.2985120	2.8796391 *	2.4327746 *	1.3329823 *
14 C	5.7336769	4.3111375	3.8364694	2.5201600 *
15 C	6.8111159	5.3896458	4.6387367	3.1854721
16 C	8.1416848	6.7134563	6.0330827	4.5854603
17 C	8.5568874	7.1443144	6.7052494	5.3326091
18 C	7.7595861	6.4002374	6.2099099	4.9911883
19 C	6.3517680	4.9964896	4.8611605	3.7389823
20 O	6.7693228	5.4226612	4.3777393	2.9855786 *
21 N	5.4077435	4.5917594	3.1855088	2.9469393 *
22 H	4.0668710	4.8793150	4.6916582	6.0142886
23 H	5.9253650	6.2494602	5.4878614	6.4213528
24 H	6.2600635	5.9968654	4.7961120	5.1808597
25 H	2.1827902 *	3.4522016	3.9689232	5.4255347
26 H	1.1042424 *	2.1963130 *	3.4764935	4.6710430
27 H	2.1711987 *	1.1027696 *	2.1901225 *	2.6988697 *
28 H	3.8519121	2.5263301 *	2.6162418 *	2.0899595 *
29 H	8.9928425	7.5738294	6.7695989	5.3112439
30 H	9.6521493	8.2429051	7.8089880	6.4278483
31 H	8.3591094	7.0638173	7.0366477	5.9150229
32 H	5.8766962	4.6304962	4.7908477	3.9425719
33 H	7.7256763	6.3957219	5.3111585	3.9518180
34 H	5.6018487	4.7653877	3.4220277	3.1260430
35 H	6.3105893	5.5695393	4.1689625	3.9242592

C C C C

1 CO	2.8525793 *	3.2741677	3.0372977	4.3205914
------	-------------	-----------	-----------	-----------

2 C	6.2294607	7.5708946	8.1132068	9.5113676
3 C	6.6020824	7.8076114	8.1182724	9.4741790
4 C	5.7942289	6.8471745	6.9847573	8.2947556
5 C	4.3898577	5.4535426	5.6705175	7.0145771
6 C	3.7357873	5.0411908	5.6017724	7.0047400
7 C	4.9195440	6.3134535	6.9962099	8.4025547
8 C	5.1237300	6.5791374	7.4898916	8.8749729
9 C	4.2985120	5.7336769	6.8111159	8.1416848
10 C	2.8796391 *	4.3111375	5.3896458	6.7134563
11 C	2.4327746 *	3.8364694	4.6387367	6.0330827
12 N	1.3329823 *	2.5201600 *	3.1854721	4.5854603
13 C	0.0000000	1.4620135 *	2.6066357 *	3.8812312
14 C	1.4620135 *	0.0000000	1.4352833 *	2.4967408 *
15 C	2.6066357 *	1.4352833 *	0.0000000	1.4071210 *
16 C	3.8812312	2.4967408 *	1.4071210 *	0.0000000
17 C	4.3355571	2.8794424 *	2.4437472 *	1.4293958 *
18 C	3.7793664	2.4964759 *	2.8282016 *	2.4742543 *
19 C	2.4548142 *	1.4428918 *	2.4462673 *	2.8434350 *
20 O	3.0511194	2.4969785 *	1.4634792 *	2.4627055 *
21 N	4.0800396	4.7985604	4.7049822	5.9443038
22 H	7.1140609	8.4998871	9.1206774	10.5247947
23 H	7.6911702	8.8708620	9.1194447	10.4541682
24 H	6.4468512	7.3453539	7.2853478	8.5115101
25 H	6.2074228	7.6648546	8.5932671	9.9764319
26 H	4.9423127	6.3139768	7.4984242	8.7684948
27 H	2.5928160 *	3.8750630	5.1027194	6.3214011
28 H	1.1059926 *	2.1582450 *	3.5184685	4.6500646
29 H	4.7954668	3.4990686	2.1943607 *	1.1065413 *
30 H	5.4412452	3.9855812	3.4444257	2.1959997 *
31 H	4.6392630	3.4914187	3.9322671	3.4774637
32 H	2.6147518 *	2.1939104 *	3.4479725	3.9492999
33 H	4.0286760	3.3257649	2.0381461 *	2.4990087 *
34 H	4.0494944	4.7136982	4.6867053	5.8700700
35 H	5.0417355	5.6296287	5.3309345	6.4633409

C C C O

1 CO	5.4804523	5.6408725	4.7143792	1.9704551 *
2 C	10.3770523	9.9999728	8.6697097	7.3951593
3 C	10.4802842	10.2830580	9.0341224	7.1966653
4 C	9.3780449	9.3155222	8.1536535	5.9633245
5 C	8.0404867	7.9261992	6.7500504	4.7649170
6 C	7.8418599	7.4884985	6.1856618	5.0071563
7 C	9.1665185	8.6954593	7.3371238	6.4564960
8 C	9.4546603	8.7878614	7.3835851	7.1942045
9 C	8.5568874	7.7595861	6.3517680	6.7693228

10 C	7.1443144	6.4002374	4.9964896	5.4226612
11 C	6.7052494	6.2099099	4.8611605	4.3777393
12 N	5.3326091	4.9911883	3.7389823	2.9855786 *
13 C	4.3355571	3.7793664	2.4548142 *	3.0511194
14 C	2.8794424 *	2.4964759 *	1.4428918 *	2.4969785 *
15 C	2.4437472 *	2.8282016 *	2.4462673 *	1.4634792 *
16 C	1.4293958 *	2.4742543 *	2.8434350 *	2.4627055 *
17 C	0.0000000	1.4242936 *	2.4534729 *	3.7735792
18 C	1.4242936 *	0.0000000	1.4137309 *	4.2915280
19 C	2.4534729 *	1.4137309 *	0.0000000	3.7918339
20 O	3.7735792	4.2915280	3.7918339	0.0000000
21 N	7.0785205	7.1745428	6.1680994	3.6472717
22 H	11.3402304	10.8891576	9.5291139	8.4542236
23 H	11.5016050	11.3481497	10.1157214	8.1281892
24 H	9.6847108	9.7688096	8.7015749	6.1280534
25 H	10.5359733	9.8315046	8.4222008	8.2871877
26 H	9.0375784	8.1121007	6.7257868	7.6088262
27 H	6.5652994	5.6881194	4.3027867	5.4119687
28 H	4.8184248	3.9544612	2.5414378 *	4.1370444
29 H	2.2007239 *	3.4747501	3.9498914	2.6919537 *
30 H	1.1062231 *	2.2005294 *	3.4583822	4.6565640
31 H	2.2007208 *	1.1040804 *	2.1844955 *	5.3956082
32 H	3.4574952	2.1870778 *	1.1058941 *	4.6836689
33 H	3.9224383	4.7264539	4.4830346	0.9915948 *
34 H	6.9161741	6.9677015	5.9860900	3.8114223
35 H	7.6935871	7.9367382	7.0244899	4.1051072

N H H H

1 CO	1.9780626 *	6.5323430	6.1951451	4.3606660
2 C	4.3377456	1.1059704 *	2.1886751 *	3.4403111
3 C	3.8042367	2.1811582 *	1.1035878 *	2.1991183 *
4 C	2.4621546 *	3.4505959	2.1970597 *	1.1079470 *
5 C	1.5114717 *	3.9430750	3.4630725	2.1743443 *
6 C	2.6042833 *	3.5235409	4.0288178	3.5013715
7 C	3.8907454	2.1959851 *	3.4862356	3.9481838
8 C	5.1213760	2.6686094 *	4.6655855	5.3900102
9 C	5.4077435	4.0668710	5.9253650	6.2600635
10 C	4.5917594	4.8793150	6.2494602	5.9968654
11 C	3.1855088	4.6916582	5.4878614	4.7961120
12 N	2.9469393 *	6.0142886	6.4213528	5.1808597
13 C	4.0800396	7.1140609	7.6911702	6.4468512
14 C	4.7985604	8.4998871	8.8708620	7.3453539
15 C	4.7049822	9.1206774	9.1194447	7.2853478
16 C	5.9443038	10.5247947	10.4541682	8.5115101
17 C	7.0785205	11.3402304	11.5016050	9.6847108

18 C	7.1745428	10.8891576	11.3481497	9.7688096
19 C	6.1680994	9.5291139	10.1157214	8.7015749
20 O	3.6472717	8.4542236	8.1281892	6.1280534
21 N	0.0000000	5.4418090	4.6561799	2.6207135 *
22 H	5.4418090	0.0000000	2.5374885 *	4.3653750
23 H	4.6561799	2.5374885 *	0.0000000	2.5221080 *
24 H	2.6207135 *	4.3653750	2.5221080 *	0.0000000
25 H	6.0592260	2.3811208 *	4.7699549	5.9657343
26 H	6.4906618	4.7668523	6.8477126	7.3418858
27 H	5.2978496	5.9491961	7.3381553	6.9590220
28 H	4.8624435	7.1318462	8.0348065	7.0685182
29 H	6.2227565	11.0939672	10.7947689	8.6981885
30 H	8.0515373	12.4346876	12.5374728	10.6484129
31 H	8.2009367	11.6899650	12.2832601	10.7834038
32 H	6.5847548	9.3405307	10.1886074	9.0112704
33 H	4.1524158	9.1954770	8.6538387	6.4971919
34 H	1.0447447 *	5.8023830	5.0969407	3.1321643
35 H	1.0407741 *	5.8075317	4.5568134	2.1731947 *

H H H H

1 CO	6.5854533	6.3441209	4.5582830	3.8706980
2 C	2.6691143 *	4.6626862	5.3798597	6.3608042
3 C	4.0677027	5.9244939	6.2592453	6.9338029
4 C	4.8793058	6.2481987	6.0045939	6.3066139
5 C	4.6669128	5.4689581	4.8062969	4.9365043
6 C	3.5205740	4.0190129	3.5022876	4.0253076
7 C	2.1952009 *	3.4819609	3.9396780	4.9694721
8 C	1.1051396 *	2.1859585 *	3.4213122	4.8805650
9 C	2.1827902 *	1.1042424 *	2.1711987 *	3.8519121
10 C	3.4522016	2.1963130 *	1.1027696 *	2.5263301 *
11 C	3.9689232	3.4764935	2.1901225 *	2.6162418 *
12 N	5.4255347	4.6710430	2.6988697 *	2.0899595 *
13 C	6.2074228	4.9423127	2.5928160 *	1.1059926 *
14 C	7.6648546	6.3139768	3.8750630	2.1582450 *
15 C	8.5932671	7.4984242	5.1027194	3.5184685
16 C	9.9764319	8.7684948	6.3214011	4.6500646
17 C	10.5359733	9.0375784	6.5652994	4.8184248
18 C	9.8315046	8.1121007	5.6881194	3.9544612
19 C	8.4222008	6.7257868	4.3027867	2.5414378 *
20 O	8.2871877	7.6088262	5.4119687	4.1370444
21 N	6.0592260	6.4906618	5.2978496	4.8624435
22 H	2.3811208 *	4.7668523	5.9491961	7.1318462
23 H	4.7699549	6.8477126	7.3381553	8.0348065
24 H	5.9657343	7.3418858	6.9590220	7.0685182
25 H	0.0000000	2.5353685 *	4.3402568	5.9026336

26 H	2.5353685 *	0.0000000	2.4859391 *	4.3072454
27 H	4.3402568	2.4859391 *	0.0000000	1.9728404 *
28 H	5.9026336	4.3072454	1.9728404 *	0.0000000
29 H	10.7321362	9.6796773	7.2639614	5.6509176
30 H	11.6408072	10.1099457	7.6387942	5.8967324
31 H	10.4795417	8.5909206	6.2532863	4.6062879
32 H	8.0033720	6.1003828	3.8065078	2.2114180 *
33 H	9.1750471	8.5817644	6.3971687	5.1031479
34 H	6.3206197	6.6504688	5.4239381	4.7468959
35 H	6.7516022	7.4068993	6.2993510	5.8736241

H H H H

1 CO	4.6618521	6.4669137	6.7056158	5.2824705
2 C	10.0468075	11.4627300	10.8452777	8.5691780
3 C	9.8713426	11.5300848	11.2064287	9.0914813
4 C	8.6137286	10.3942503	10.2916501	8.3547254
5 C	7.4224196	9.0773625	8.8942659	6.9566029
6 C	7.5991363	8.9292187	8.3675660	6.1903734
7 C	9.0348232	10.2653604	9.5027074	7.1802340
8 C	9.6283782	10.5604272	9.4732261	7.0243481
9 C	8.9928425	9.6521493	8.3591094	5.8766962
10 C	7.5738294	8.2429051	7.0638173	4.6304962
11 C	6.7695989	7.8089880	7.0366477	4.7908477
12 N	5.3112439	6.4278483	5.9150229	3.9425719
13 C	4.7954668	5.4412452	4.6392630	2.6147518 *
14 C	3.4990686	3.9855812	3.4914187	2.1939104 *
15 C	2.1943607 *	3.4444257	3.9322671	3.4479725
16 C	1.1065413 *	2.1959997 *	3.4774637	3.9492999
17 C	2.2007239 *	1.1062231 *	2.2007208 *	3.4574952
18 C	3.4747501	2.2005294 *	1.1040804 *	2.1870778 *
19 C	3.9498914	3.4583822	2.1844955 *	1.1058941 *
20 O	2.6919537 *	4.6565640	5.3956082	4.6836689
21 N	6.2227565	8.0515373	8.2009367	6.5847548
22 H	11.0939672	12.4346876	11.6899650	9.3405307
23 H	10.7947689	12.5374728	12.2832601	10.1886074
24 H	8.6981885	10.6484129	10.7834038	9.0112704
25 H	10.7321362	11.6408072	10.4795417	8.0033720
26 H	9.6796773	10.1099457	8.5909206	6.1003828
27 H	7.2639614	7.6387942	6.2532863	3.8065078
28 H	5.6509176	5.8967324	4.6062879	2.2114180 *
29 H	0.0000000	2.5246488 *	4.3898926	5.0557512
30 H	2.5246488 *	0.0000000	2.5426254 *	4.3750218
31 H	4.3898926	2.5426254 *	0.0000000	2.5158069 *
32 H	5.0557512	4.3750218	2.5158069 *	0.0000000
33 H	2.2949108 *	4.6262418	5.8129256	5.4601601

34 H	6.1913556	7.8723206	7.9538513	6.3739218
35 H	6.5786728	8.6054242	8.9901597	7.5189948

H H H

1 CO	2.6708748 *	2.5009790 *	2.6164681 *
2 C	8.1177995	4.7303924	4.7242040
3 C	7.7883622	4.2615461	3.8983556
4 C	6.4855510	3.0017004	2.4675824 *
5 C	5.4030776	2.1027407 *	2.0856690 *
6 C	5.8217813	2.9877575 *	3.4252246
7 C	7.2754002	4.2372872	4.5570980
8 C	8.0918773	5.3837682	5.8883044
9 C	7.7256763	5.6018487	6.3105893
10 C	6.3957219	4.7653877	5.5695393
11 C	5.3111585	3.4220277	4.1689625
12 N	3.9518180	3.1260430	3.9242592
13 C	4.0286760	4.0494944	5.0417355
14 C	3.3257649	4.7136982	5.6296287
15 C	2.0381461 *	4.6867053	5.3309345
16 C	2.4990087 *	5.8700700	6.4633409
17 C	3.9224383	6.9161741	7.6935871
18 C	4.7264539	6.9677015	7.9367382
19 C	4.4830346	5.9860900	7.0244899
20 O	0.9915948 *	3.8114223	4.1051072
21 N	4.1524158	1.0447447 *	1.0407741 *
22 H	9.1954770	5.8023830	5.8075317
23 H	8.6538387	5.0969407	4.5568134
24 H	6.4971919	3.1321643	2.1731947 *
25 H	9.1750471	6.3206197	6.7516022
26 H	8.5817644	6.6504688	7.4068993
27 H	6.3971687	5.4239381	6.2993510
28 H	5.1031479	4.7468959	5.8736241
29 H	2.2949108 *	6.1913556	6.5786728
30 H	4.6262418	7.8723206	8.6054242
31 H	5.8129256	7.9538513	8.9901597
32 H	5.4601601	6.3739218	7.5189948
33 H	0.0000000	4.3222743	4.3951349
34 H	4.3222743	0.0000000	1.6635062 *
35 H	4.3951349	1.6635062 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 4264.8 SECONDS (71.1 MIN)
WALL CLOCK TIME: STEP = 0.78 , TOTAL = 3942.2 SECONDS (65.7 MIN)

CPU UTILIZATION: STEP = 99.82%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.87 , TOTAL = 4265.7 SECONDS (71.1 MIN)
WALL CLOCK TIME: STEP = 0.87 , TOTAL = 3943.1 SECONDS (65.7 MIN)

CPU UTILIZATION: STEP = 99.77%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.633877045	-284.633877045	0.006682267	0.000709738	196912404
11403372						
2	1	-284.633919884	-0.000042839	0.000943773	0.000062860	153634924
15066388						
3	2	-284.633919753	0.000000131	0.000561111	0.000140078	137509205
16333850						
4	3	-284.633920565	-0.000000812	0.000348685	0.000055460	131438084
16821311						
5	4	-284.633920490	0.000000075	0.000198088	0.000084751	127059065
17153894						
6	5	-284.633920657	-0.000000167	0.000195629	0.000016045	121422632
17584773						
7	6	-284.633920646	0.000000012	0.000108839	0.000017501	116865594
17865566						
8	7	-284.633920669	-0.000000024	0.000133207	0.000012791	134367814
16584088						
9	8	-284.633920685	-0.000000015	0.000251679	0.000013752	156618392
14887828						

-----DISABLING FDIFF OPTION-----

10	9	-284.633920697	-0.000000012	0.000180592	0.000014485	196911864
11403310						
11	10	-284.633920714	-0.000000017	0.000214159	0.000014393	196911856
11403305						
12	11	-284.633920725	-0.000000012	0.000133938	0.000010536	196911823
11403315						
13	12	-284.633920731	-0.000000006	0.000090223	0.000006718	196911836
11403316						

14 13 -284.633920737 -0.000000005 0.000085248 0.000003058 196911814
11403313
15 14 -284.633920737 -0.000000001 0.000032057 0.000002892 196911920
11403309
16 15 -284.633920738 -0.000000001 0.000018192 0.000001936 196911834
11403312

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 52.7 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 17.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.6 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6339207383 AFTER 16 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6069655844
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000233701

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 55.31 , TOTAL = 4321.0 SECONDS (72.0 MIN)
WALL CLOCK TIME: STEP = 51.45 , TOTAL = 3994.5 SECONDS (66.6
MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 4.10 , TOTAL = 4325.1 SECONDS (72.1 MIN)
WALL CLOCK TIME: STEP = 4.07 , TOTAL = 3998.6 SECONDS (66.6
MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.83 , TOTAL = 4327.9 SECONDS (72.1 MIN)

WALL CLOCK TIME: STEP = 2.65 , TOTAL = 4001.2 SECONDS (66.7 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 41 ENERGY= -284.6339207

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0008106	-0.0001433	0.0008303
2 C	6.0	-0.0005362	0.0001920	-0.0006427
3 C	6.0	-0.0009218	0.0010224	-0.0002975
4 C	6.0	0.0003224	0.0000764	0.0002272
5 C	6.0	-0.0001456	0.0003463	0.0004297
6 C	6.0	-0.0000179	0.0001361	0.0001048
7 C	6.0	0.0001279	0.0004589	-0.0002683
8 C	6.0	-0.0002344	0.0001465	0.0000617
9 C	6.0	0.0002342	0.0001393	-0.0001481
10 C	6.0	-0.0005298	-0.0007706	-0.0003368
11 C	6.0	-0.0002524	-0.0006618	0.0001175
12 N	7.0	0.0000252	0.0000851	0.0004957
13 C	6.0	0.0002725	-0.0001592	0.0004119
14 C	6.0	-0.0003497	-0.0000548	0.0003898
15 C	6.0	0.0001778	0.0002959	0.0008625
16 C	6.0	0.0002680	-0.0000812	0.0003244
17 C	6.0	-0.0002822	-0.0001670	-0.0000539
18 C	6.0	0.0004116	0.0003928	-0.0001269
19 C	6.0	0.0000508	-0.0002904	0.0000393
20 O	8.0	0.0003812	-0.0003384	-0.0005705
21 N	7.0	0.0005625	-0.0005688	0.0005726
22 H	1.0	0.0003850	0.0005984	0.0002263
23 H	1.0	-0.0005901	-0.0003808	-0.0000562
24 H	1.0	-0.0014002	-0.0003357	0.0004554
25 H	1.0	0.0002876	-0.0001451	-0.0000676
26 H	1.0	-0.0002051	0.0001453	-0.0007496
27 H	1.0	-0.0000775	-0.0002893	-0.0002179
28 H	1.0	0.0003525	0.0002055	0.0007852
29 H	1.0	0.0000923	0.0001832	-0.0004268
30 H	1.0	-0.0007894	0.0001213	-0.0005330
31 H	1.0	0.0002761	0.0003121	0.0001685

32 H	1.0	0.0007940	0.0000346	0.0001098
33 H	1.0	-0.0005924	0.0001083	-0.0013785
34 H	1.0	0.0005368	-0.0001848	-0.0003400
35 H	1.0	0.0005557	-0.0004293	-0.0003983

MAXIMUM GRADIENT = 0.0014002 RMS GRADIENT = 0.0004457
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000317402
 PREDICTED ENERGY CHANGE WAS -0.0000052035 RATIO= 6.100
 GDIIS STEP HAS LENGTH = 0.136490
 RADIUS OF STEP TAKEN= 0.05000 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 4328.0 SECONDS (72.1 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4001.2 SECONDS (66.7 MIN)
 CPU UTILIZATION: STEP = 90.62% , TOTAL = 100.00%

INSERCH= 42

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1378716732	-1.7652456119	1.0202269797
C	6.0	4.9848458569	0.6901794272	0.4429626973
C	6.0	5.2091392675	-0.6736785920	0.2224533916
C	6.0	4.0840043218	-1.5454980634	0.0739213905
C	6.0	2.7673556401	-1.0598791634	0.1657238660
C	6.0	2.4747551827	0.3322150192	0.4835033025
C	6.0	3.6463835379	1.2148412506	0.5814838085
C	6.0	3.4874220795	2.6285466357	0.8242680023
C	6.0	2.2167564753	3.1875062889	1.0133447127
C	6.0	1.0702595090	2.3352223172	0.9950928119
C	6.0	1.1679987607	0.9528160931	0.7129414438
N	7.0	-0.0433533307	0.1393511236	0.7398700237
C	6.0	-1.2439765736	0.6814976457	0.5358788121
C	6.0	-2.5564491736	0.0403258929	0.5807010323
C	6.0	-2.8612766364	-1.3468339357	0.7895168831
C	6.0	-4.1748397858	-1.8513231861	0.7830701644
C	6.0	-5.2607360173	-0.9466743258	0.5697388195
C	6.0	-5.0105716256	0.4406312416	0.3683871457
C	6.0	-3.6804073749	0.9192616582	0.3671814130
O	8.0	-1.7612527933	-2.2890656703	0.9961587658
N	7.0	1.6880767293	-2.0622384720	-0.1720769416
H	1.0	5.8344823270	1.3927726094	0.5268038637

H	1.0	6.2315625028	-1.0807157330	0.1381128705
H	1.0	4.2531867336	-2.6164908993	-0.1516361212
H	1.0	4.3928143737	3.2603872062	0.8724627342
H	1.0	2.0911189299	4.2670296436	1.2070229705
H	1.0	0.0960730258	2.7848346302	1.2481696227
H	1.0	-1.2842920856	1.7556922956	0.2759389252
H	1.0	-4.3753323210	-2.9293918913	0.9292275396
H	1.0	-6.2952479916	-1.3351021840	0.5532592463
H	1.0	-5.8466211615	1.1423698519	0.2068954373
H	1.0	-3.4798508481	1.9932831250	0.1967544116
H	1.0	-2.1024283287	-3.2163176293	1.0796176007
H	1.0	1.3665377458	-1.9068384557	-1.1527611187
H	1.0	2.1119883752	-3.0123651430	-0.1613295069

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4640191	5.2484013	4.0639570
2 C	5.4640191	0.0000000	1.3996573 *	2.4384341 *
3 C	5.2484013	1.3996573 *	0.0000000	1.4311043 *
4 C	4.0639570	2.4384341 *	1.4311043 *	0.0000000
5 C	2.8534021 *	2.8384554 *	2.4727872 *	1.4063489 *
6 C	3.1856613	2.5358110 *	2.9252052 *	2.5066405 *
7 C	4.6241830	1.4442782 *	2.4774211 *	2.8405289 *
8 C	5.5284083	2.4788988 *	3.7724239	4.2827070
9 C	5.3713649	3.7715111	4.9485970	5.1740179
10 C	4.2052130	4.2819388	5.1750152	4.9991204
11 C	2.9229173 *	3.8353863	4.3837062	3.8926866
12 N	1.9336316 *	5.0669866	5.3401700	4.5074700
13 C	2.8514295 *	6.2295215	6.6013212	5.7931248
14 C	3.2730164	7.5704962	7.8065682	6.8459686
15 C	3.0369699	8.1136405	8.1182703	6.9848745
16 C	4.3200848	9.5118216	9.4741860	8.2948735
17 C	5.4788652	10.3762860	10.4791900	9.3770249
18 C	5.6389056	9.9988103	10.2813167	9.3135778
19 C	4.7129930	8.6686121	9.0323001	8.1515110
20 O	1.9701879 *	7.3953887	7.1968369	5.9640964
21 N	1.9781125 *	4.3385210	3.8054742	2.4633321 *
22 H	6.5320685	1.1056892 *	2.1803449 *	3.4500305
23 H	6.1951412	2.1870769 *	1.1036946 *	2.1982150 *
24 H	4.3627629	3.4384504	2.1973411 *	1.1074857 *
25 H	6.5866044	2.6722537 *	4.0701071	4.8815536
26 H	6.3433755	4.6638290	5.9246963	6.2482789
27 H	4.5559780	5.3792228	6.2575438	6.0028523

28 H	3.8695631	6.3612346	6.9332066	6.3053370
29 H	4.6618159	10.0474218	9.8716700	8.6143536
30 H	6.4643724	11.4609968	11.5281325	10.3924448
31 H	6.7029762	10.8434718	11.2039329	10.2888113
32 H	5.2813409	8.5679512	9.0891086	8.3516445
33 H	2.6698467 *	8.1176046	7.7883737	6.4865254
34 H	2.5003092 *	4.7310665	4.2635061	3.0033217
35 H	2.6169676 *	4.7251789	3.8998830	2.4689854 *

C C C C

1 CO	2.8534021 *	3.1856613	4.6241830	5.5284083
2 C	2.8384554 *	2.5358110 *	1.4442782 *	2.4788988 *
3 C	2.4727872 *	2.9252052 *	2.4774211 *	3.7724239
4 C	1.4063489 *	2.5066405 *	2.8405289 *	4.2827070
5 C	0.0000000	1.4575750 *	2.4738430 *	3.8153192
6 C	1.4575750 *	0.0000000	1.4701504 *	2.5327364 *
7 C	2.4738430 *	1.4701504 *	0.0000000	1.4431825 *
8 C	3.8153192	2.5327364 *	1.4431825 *	0.0000000
9 C	4.3659940	2.9154731 *	2.4742160 *	1.4009914 *
10 C	3.8851901	2.4992739 *	2.8394966 *	2.4408800 *
11 C	2.6283705 *	1.4647184 *	2.4956621 *	2.8635976 *
12 N	3.1093218	2.5384623 *	3.8465469	4.3208324
13 C	4.3886438	3.7354662	4.9195688	5.1244806
14 C	5.4521147	5.0406015	6.3130516	6.5792546
15 C	5.6703582	5.6023286	6.9967920	7.4907165
16 C	7.0143836	7.0053332	8.4031860	8.8758767
17 C	8.0390484	7.8409705	9.1656460	9.4539547
18 C	7.9239357	7.4869969	8.6941178	8.7869618
19 C	6.7476834	6.1841880	7.3358815	7.3829779
20 O	4.7653768	5.0077631	6.4569226	7.1945149
21 N	1.5111838 *	2.6042381 *	3.8912814	5.1218953
22 H	3.9437477	3.5234108	2.1960022 *	2.6691411 *
23 H	3.4643796	4.0285567	3.4855860	4.6647340
24 H	2.1751900 *	3.5015836	3.9477565	5.3897313
25 H	4.6697213	3.5219927	2.1968354 *	1.1051156 *
26 H	5.4696944	4.0191322	3.4822408	2.1865019 *
27 H	4.8051289	3.5011693	3.9387884	3.4213107
28 H	4.9351230	4.0248984	4.9696519	4.8817820
29 H	7.4226685	7.6000295	9.0356803	9.6293616
30 H	9.0750601	8.9273607	10.2634812	10.5586264
31 H	8.8911300	8.3652954	9.5006688	9.4717598
32 H	6.9534417	6.1885948	7.1789418	7.0242598
33 H	5.4037232	5.8222028	7.2754480	8.0916049
34 H	2.1019119 *	2.9864473 *	4.2367660	5.3829836
35 H	2.0853469 *	3.4254380	4.5580055	5.8892365

	C	C	C	N
1 CO	5.3713649	4.2052130	2.9229173 *	1.9336316 *
2 C	3.7715111	4.2819388	3.8353863	5.0669866
3 C	4.9485970	5.1750152	4.3837062	5.3401700
4 C	5.1740179	4.9991204	3.8926866	4.5074700
5 C	4.3659940	3.8851901	2.6283705 *	3.1093218
6 C	2.9154731 *	2.4992739 *	1.4647184 *	2.5384623 *
7 C	2.4742160 *	2.8394966 *	2.4956621 *	3.8465469
8 C	1.4009914 *	2.4408800 *	2.8635976 *	4.3208324
9 C	0.0000000	1.4286974 *	2.4867600 *	3.8044888
10 C	1.4286974 *	0.0000000	1.4142876 *	2.4753025 *
11 C	2.4867600 *	1.4142876 *	0.0000000	1.4593918 *
12 N	3.8044888	2.4753025 *	1.4593918 *	0.0000000
13 C	4.2993867	2.8812101 *	2.4336372 *	1.3330534 *
14 C	5.7337088	4.3117614	3.8368787	2.5200777 *
15 C	6.8115168	5.3904338	4.6399692	3.1862050
16 C	8.1421945	6.7144012	6.0344046	4.5862655
17 C	8.5557659	7.1437578	6.7050132	5.3319300
18 C	7.7585800	6.3999018	6.2093303	4.9901931
19 C	6.3512993	4.9968043	4.8608351	3.7383578
20 O	6.7688768	5.4223152	4.3784157	2.9856441 *
21 N	5.4078227	4.5914752	3.1850106	2.9455889 *
22 H	4.0676444	4.8790701	4.6908718	6.0137688
23 H	5.9247293	6.2483675	5.4868349	6.4206887
24 H	6.2602406	5.9971224	4.7964395	5.1816701
25 H	2.1818312 *	3.4511359	3.9685976	5.4256825
26 H	1.1039324 *	2.1952102 *	3.4756696	4.6703248
27 H	2.1713096 *	1.1023785 *	2.1890148 *	2.6974787 *
28 H	3.8537254	2.5292194 *	2.6171190 *	2.0899091 *
29 H	8.9932838	7.5746268	6.7710293	5.3121636
30 H	9.6498646	8.2411892	7.8076962	6.4261204
31 H	8.3576912	7.0631006	7.0354037	5.9133769
32 H	5.8774419	4.6322533	4.7907752	3.9422777
33 H	7.7245524	6.3947391	5.3114801	3.9516745
34 H	5.6006459	4.7640463	3.4202175	3.1235776
35 H	6.3110412	5.5694886	4.1687082	3.9231332

	C	C	C	C
1 CO	2.8514295 *	3.2730164	3.0369699	4.3200848
2 C	6.2295215	7.5704962	8.1136405	9.5118216
3 C	6.6013212	7.8065682	8.1182703	9.4741860
4 C	5.7931248	6.8459686	6.9848745	8.2948735
5 C	4.3886438	5.4521147	5.6703582	7.0143836

6 C	3.7354662	5.0406015	5.6023286	7.0053332
7 C	4.9195688	6.3130516	6.9967920	8.4031860
8 C	5.1244806	6.5792546	7.4907165	8.8758767
9 C	4.2993867	5.7337088	6.8115168	8.1421945
10 C	2.8812101 *	4.3117614	5.3904338	6.7144012
11 C	2.4336372 *	3.8368787	4.6399692	6.0344046
12 N	1.3330534 *	2.5200777 *	3.1862050	4.5862655
13 C	0.0000000	1.4614016 *	2.6065534 *	3.8815260
14 C	1.4614016 *	0.0000000	1.4355265 *	2.4976945 *
15 C	2.6065534 *	1.4355265 *	0.0000000	1.4071244 *
16 C	3.8815260	2.4976945 *	1.4071244 *	0.0000000
17 C	4.3343335	2.8787944 *	2.4425060 *	1.4293602 *
18 C	3.7780032	2.4956038 *	2.8269862 *	2.4745636 *
19 C	2.4538104 *	1.4427060 *	2.4463302 *	2.8449195 *
20 O	3.0501932	2.4961986 *	1.4630632 *	2.4621997 *
21 N	4.0775269	4.7961914	4.7045810	5.9439533
22 H	7.1141110	8.4993969	9.1208928	10.5250349
23 H	7.6907281	8.8702744	9.1200258	10.4548082
24 H	6.4473413	7.3461646	7.2878932	8.5141522
25 H	6.2078476	7.6646059	8.5939050	9.9770873
26 H	4.9426042	6.3132553	7.4977328	8.7679083
27 H	2.5936688 *	3.8747537	5.1016629	6.3206782
28 H	1.1059332 *	2.1572542 *	3.5179982	4.6500547
29 H	4.7956892	3.4998615	2.1946237 *	1.1062510 *
30 H	5.4389631	3.9838640	3.4421090	2.1944084 *
31 H	4.6373452	3.4899088	3.9303772	3.4769280
32 H	2.6143680 *	2.1941120 *	3.4482435	3.9506675
33 H	4.0280957	3.3257751	2.0383764 *	2.4992078 *
34 H	4.0454633	4.7102194	4.6861992	5.8700417
35 H	5.0391688	5.6270633	5.3302409	6.4625163

C C C O

1 CO	5.4788652	5.6389056	4.7129930	1.9701879 *
2 C	10.3762860	9.9988103	8.6686121	7.3953887
3 C	10.4791900	10.2813167	9.0323001	7.1968369
4 C	9.3770249	9.3135778	8.1515110	5.9640964
5 C	8.0390484	7.9239357	6.7476834	4.7653768
6 C	7.8409705	7.4869969	6.1841880	5.0077631
7 C	9.1656460	8.6941178	7.3358815	6.4569226
8 C	9.4539547	8.7869618	7.3829779	7.1945149
9 C	8.5557659	7.7585800	6.3512993	6.7688768
10 C	7.1437578	6.3999018	4.9968043	5.4223152
11 C	6.7050132	6.2093303	4.8608351	4.3784157
12 N	5.3319300	4.9901931	3.7383578	2.9856441 *
13 C	4.3343335	3.7780032	2.4538104 *	3.0501932

14 C	2.8787944 *	2.4956038 *	1.4427060 *	2.4961986 *
15 C	2.4425060 *	2.8269862 *	2.4463302 *	1.4630632 *
16 C	1.4293602 *	2.4745636 *	2.8449195 *	2.4621997 *
17 C	0.0000000	1.4239879 *	2.4536066 *	3.7722979
18 C	1.4239879 *	0.0000000	1.4136568 *	4.2899202
19 C	2.4536066 *	1.4136568 *	0.0000000	3.7910594
20 O	3.7722979	4.2899202	3.7910594	0.0000000
21 N	7.0767770	7.1713561	6.1644760	3.6488491
22 H	11.3392559	10.8879229	9.5280018	8.4540771
23 H	11.5011823	11.3469424	10.1143230	8.1290497
24 H	9.6862477	9.7690142	8.7013007	6.1317308
25 H	10.5348015	9.8299941	8.4209909	8.2875974
26 H	9.0354088	8.1104034	6.7248346	7.6070768
27 H	6.5635227	5.6874534	4.3032902	5.4090325
28 H	4.8167634	3.9526057	2.5395491 *	4.1359733
29 H	2.2009863 *	3.4749283	3.9510696	2.6921941 *
30 H	1.1051528 *	2.1995000 *	3.4574807	4.6543870
31 H	2.1997778 *	1.1034018 *	2.1835638 *	5.3933219
32 H	3.4574585	2.1870738 *	1.1057985 *	4.6830693
33 H	3.9225202	4.7261423	4.4833692	0.9915454 *
34 H	6.9144543	6.9636219	5.9806958	3.8140566
35 H	7.6914631	7.9331359	7.0206027	4.1066943

N H H H

1 CO	1.9781125 *	6.5320685	6.1951412	4.3627629
2 C	4.3385210	1.1056892 *	2.1870769 *	3.4384504
3 C	3.8054742	2.1803449 *	1.1036946 *	2.1973411 *
4 C	2.4633321 *	3.4500305	2.1982150 *	1.1074857 *
5 C	1.5111838 *	3.9437477	3.4643796	2.1751900 *
6 C	2.6042381 *	3.5234108	4.0285567	3.5015836
7 C	3.8912814	2.1960022 *	3.4855860	3.9477565
8 C	5.1218953	2.6691411 *	4.6647340	5.3897313
9 C	5.4078227	4.0676444	5.9247293	6.2602406
10 C	4.5914752	4.8790701	6.2483675	5.9971224
11 C	3.1850106	4.6908718	5.4868349	4.7964395
12 N	2.9455889 *	6.0137688	6.4206887	5.1816701
13 C	4.0775269	7.1141110	7.6907281	6.4473413
14 C	4.7961914	8.4993969	8.8702744	7.3461646
15 C	4.7045810	9.1208928	9.1200258	7.2878932
16 C	5.9439533	10.5250349	10.4548082	8.5141522
17 C	7.0767770	11.3392559	11.5011823	9.6862477
18 C	7.1713561	10.8879229	11.3469424	9.7690142
19 C	6.1644760	9.5280018	10.1143230	8.7013007
20 O	3.6488491	8.4540771	8.1290497	6.1317308
21 N	0.0000000	5.4422620	4.6586337	2.6243862 *

22 H	5.4422620	0.0000000	2.5351327 *	4.3629085
23 H	4.6586337	2.5351327 *	0.0000000	2.5212161 *
24 H	2.6243862 *	4.3629085	2.5212161 *	0.0000000
25 H	6.0611066	2.3845064 *	4.7713142	5.9670739
26 H	6.4903000	4.7683143	6.8472054	7.3418899
27 H	5.2958185	5.9487433	7.3361391	6.9581153
28 H	4.8592479	7.1324325	8.0344431	7.0684141
29 H	6.2233235	11.0942943	10.7958179	8.7015811
30 H	8.0491188	12.4327132	12.5362690	10.6493338
31 H	8.1966339	11.6881659	12.2812606	10.7825646
32 H	6.5795720	9.3395047	10.1864840	9.0095096
33 H	4.1553058	9.1947739	8.6546305	6.5015091
34 H	1.0436848 *	5.8026632	5.1007157	3.1366543
35 H	1.0404601 *	5.8082465	4.5598055	2.1775079 *

H H H H

1 CO	6.5866044	6.3433755	4.5559780	3.8695631
2 C	2.6722537 *	4.6638290	5.3792228	6.3612346
3 C	4.0701071	5.9246963	6.2575438	6.9332066
4 C	4.8815536	6.2482789	6.0028523	6.3053370
5 C	4.6697213	5.4696944	4.8051289	4.9351230
6 C	3.5219927	4.0191322	3.5011693	4.0248984
7 C	2.1968354 *	3.4822408	3.9387884	4.9696519
8 C	1.1051156 *	2.1865019 *	3.4213107	4.8817820
9 C	2.1818312 *	1.1039324 *	2.1713096 *	3.8537254
10 C	3.4511359	2.1952102 *	1.1023785 *	2.5292194 *
11 C	3.9685976	3.4756696	2.1890148 *	2.6171190 *
12 N	5.4256825	4.6703248	2.6974787 *	2.0899091 *
13 C	6.2078476	4.9426042	2.5936688 *	1.1059332 *
14 C	7.6646059	6.3132553	3.8747537	2.1572542 *
15 C	8.5939050	7.4977328	5.1016629	3.5179982
16 C	9.9770873	8.7679083	6.3206782	4.6500547
17 C	10.5348015	9.0354088	6.5635227	4.8167634
18 C	9.8299941	8.1104034	5.6874534	3.9526057
19 C	8.4209909	6.7248346	4.3032902	2.5395491 *
20 O	8.2875974	7.6070768	5.4090325	4.1359733
21 N	6.0611066	6.4903000	5.2958185	4.8592479
22 H	2.3845064 *	4.7683143	5.9487433	7.1324325
23 H	4.7713142	6.8472054	7.3361391	8.0344431
24 H	5.9670739	7.3418899	6.9581153	7.0684141
25 H	0.0000000	2.5343760 *	4.3392732	5.9033453
26 H	2.5343760 *	0.0000000	2.4857199 *	4.3089595
27 H	4.3392732	2.4857199 *	0.0000000	1.9773149 *
28 H	5.9033453	4.3089595	1.9773149 *	0.0000000
29 H	10.7329858	9.6788762	7.2627525	5.6507813

30 H	11.6385175	10.1065542	7.6358211	5.8940306
31 H	10.4773574	8.5890321	6.2528039	4.6038873
32 H	8.0025616	6.1013335	3.8104146	2.2097959 *
33 H	9.1749003	8.5791933	6.3934065	5.1025610
34 H	6.3214004	6.6490786	5.4212863	4.7415413
35 H	6.7541332	7.4069165	6.2974699	5.8702893

H H H H

1 CO	4.6618159	6.4643724	6.7029762	5.2813409
2 C	10.0474218	11.4609968	10.8434718	8.5679512
3 C	9.8716700	11.5281325	11.2039329	9.0891086
4 C	8.6143536	10.3924448	10.2888113	8.3516445
5 C	7.4226685	9.0750601	8.8911300	6.9534417
6 C	7.6000295	8.9273607	8.3652954	6.1885948
7 C	9.0356803	10.2634812	9.5006688	7.1789418
8 C	9.6293616	10.5586264	9.4717598	7.0242598
9 C	8.9932838	9.6498646	8.3576912	5.8774419
10 C	7.5746268	8.2411892	7.0631006	4.6322533
11 C	6.7710293	7.8076962	7.0354037	4.7907752
12 N	5.3121636	6.4261204	5.9133769	3.9422777
13 C	4.7956892	5.4389631	4.6373452	2.6143680 *
14 C	3.4998615	3.9838640	3.4899088	2.1941120 *
15 C	2.1946237 *	3.4421090	3.9303772	3.4482435
16 C	1.1062510 *	2.1944084 *	3.4769280	3.9506675
17 C	2.2009863 *	1.1051528 *	2.1997778 *	3.4574585
18 C	3.4749283	2.1995000 *	1.1034018 *	2.1870738 *
19 C	3.9510696	3.4574807	2.1835638 *	1.1057985 *
20 O	2.6921941 *	4.6543870	5.3933219	4.6830693
21 N	6.2233235	8.0491188	8.1966339	6.5795720
22 H	11.0942943	12.4327132	11.6881659	9.3395047
23 H	10.7958179	12.5362690	12.2812606	10.1864840
24 H	8.7015811	10.6493338	10.7825646	9.0095096
25 H	10.7329858	11.6385175	10.4773574	8.0025616
26 H	9.6788762	10.1065542	8.5890321	6.1013335
27 H	7.2627525	7.6358211	6.2528039	3.8104146
28 H	5.6507813	5.8940306	4.6038873	2.2097959 *
29 H	0.0000000	2.5237250 *	4.3892708	5.0567908
30 H	2.5237250 *	0.0000000	2.5414763 *	4.3739805
31 H	4.3892708	2.5414763 *	0.0000000	2.5151060 *
32 H	5.0567908	4.3739805	2.5151060 *	0.0000000
33 H	2.2958737 *	4.6255553	5.8119515	5.4604652
34 H	6.1926863	7.8702191	7.9483331	6.3655026
35 H	6.5788699	8.6026433	8.9853702	7.5135481

H H H

1	CO	2.6698467 *	2.5003092 *	2.6169676 *
2	C	8.1176046	4.7310665	4.7251789
3	C	7.7883737	4.2635061	3.8998830
4	C	6.4865254	3.0033217	2.4689854 *
5	C	5.4037232	2.1019119 *	2.0853469 *
6	C	5.8222028	2.9864473 *	3.4254380
7	C	7.2754480	4.2367660	4.5580055
8	C	8.0916049	5.3829836	5.8892365
9	C	7.7245524	5.6006459	6.3110412
10	C	6.3947391	4.7640463	5.5694886
11	C	5.3114801	3.4202175	4.1687082
12	N	3.9516745	3.1235776	3.9231332
13	C	4.0280957	4.0454633	5.0391688
14	C	3.3257751	4.7102194	5.6270633
15	C	2.0383764 *	4.6861992	5.3302409
16	C	2.4992078 *	5.8700417	6.4625163
17	C	3.9225202	6.9144543	7.6914631
18	C	4.7261423	6.9636219	7.9331359
19	C	4.4833692	5.9806958	7.0206027
20	O	0.9915454 *	3.8140566	4.1066943
21	N	4.1553058	1.0436848 *	1.0404601 *
22	H	9.1947739	5.8026632	5.8082465
23	H	8.6546305	5.1007157	4.5598055
24	H	6.5015091	3.1366543	2.1775079 *
25	H	9.1749003	6.3214004	6.7541332
26	H	8.5791933	6.6490786	7.4069165
27	H	6.3934065	5.4212863	6.2974699
28	H	5.1025610	4.7415413	5.8702893
29	H	2.2958737 *	6.1926863	6.5788699
30	H	4.6255553	7.8702191	8.6026433
31	H	5.8119515	7.9483331	8.9853702
32	H	5.4604652	6.3655026	7.5135481
33	H	0.0000000	4.3280453	4.3980512
34	H	4.3280453	0.0000000	1.6615723 *
35	H	4.3980512	1.6615723 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.82 , TOTAL = 4328.8 SECONDS (72.1 MIN)
WALL CLOCK TIME: STEP = 0.82 , TOTAL = 4002.1 SECONDS (66.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.95 , TOTAL = 4329.7 SECONDS (72.2 MIN)
WALL CLOCK TIME: STEP = 0.96 , TOTAL = 4003.0 SECONDS (66.7 MIN)
CPU UTILIZATION: STEP = 99.40%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.633947032	-284.633947032	0.011344201	0.000593219	196930488
11401641						
2	1	-284.633997631	-0.000050599	0.001233818	0.000056868	155234419
14923396						
3	2	-284.633997523	0.000000108	0.001300832	0.000109700	138349731
16252325						
4	3	-284.633998475	-0.000000952	0.000489956	0.000026734	132745449
16671400						
5	4	-284.633998439	0.000000036	0.000256963	0.000033281	127545017
17140229						
6	5	-284.633998539	-0.000000100	0.000159693	0.000016018	120800692
17635531						
7	6	-284.633998550	-0.000000011	0.000080666	0.000016289	116014596
17966241						
8	7	-284.633998539	0.000000011	0.000141407	0.000013995	106449116
18706847						
9	8	-284.633998546	-0.000000007	0.000178770	0.000011379	138991006
16268395						
10	9	-284.633998561	-0.000000015	0.000264430	0.000012266	156726970
14946313						

-----DISABLING FDIFF OPTION-----

11	10	-284.633998573	-0.000000012	0.000222180	0.000012121	196929725
11401632						
12	11	-284.633998584	-0.000000010	0.000261893	0.000010099	196929925
11401630						
13	12	-284.633998593	-0.000000010	0.000166840	0.000008765	196929957
11401623						
14	13	-284.633998599	-0.000000005	0.000102062	0.000007255	196929937
11401626						
15	14	-284.633998601	-0.000000002	0.000025858	0.000003901	196929886
11401630						

16 15 -284.633998602 -0.000000001 0.000027865 0.000003343 196929862
11401631
17 16 -284.633998602 0.000000000 0.000035398 0.000002934 196929883
11401630

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 56.0 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 18.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6339986020 AFTER 17 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6085269338
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000252179

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 59.46 , TOTAL = 4389.2 SECONDS (73.2 MIN)
WALL CLOCK TIME: STEP = 54.56 , TOTAL = 4057.6 SECONDS (67.6
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.74 , TOTAL = 4392.9 SECONDS (73.2 MIN)
WALL CLOCK TIME: STEP = 3.71 , TOTAL = 4061.3 SECONDS (67.7
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.76, TOTAL = 4395.7 SECONDS (73.3 MIN)

WALL CLOCK TIME: STEP = 2.62, TOTAL = 4063.9 SECONDS (67.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 42 ENERGY= -284.6339986

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0007110	-0.0000652	0.0007865
2 C	6.0	-0.0000339	-0.0004659	-0.0006557
3 C	6.0	-0.0010276	0.0012700	-0.0002023
4 C	6.0	0.0003382	0.0000216	0.0001495
5 C	6.0	-0.0005471	-0.0000738	0.0003622
6 C	6.0	-0.0002466	0.0001941	0.0001077
7 C	6.0	-0.0001277	0.0005154	-0.0002806
8 C	6.0	0.0001184	0.0000847	-0.0001170
9 C	6.0	-0.0000098	0.0003589	-0.0001910
10 C	6.0	-0.0003566	-0.0003374	-0.0001906
11 C	6.0	0.0002233	-0.0004876	0.0000722
12 N	7.0	-0.0000824	-0.0000593	0.0004822
13 C	6.0	-0.0002383	-0.0004057	0.0005430
14 C	6.0	-0.0000148	0.0002801	0.0004650
15 C	6.0	0.0001098	0.0002715	0.0006513
16 C	6.0	0.0000656	-0.0006914	0.0003502
17 C	6.0	-0.0007096	-0.0000362	-0.0000081
18 C	6.0	0.0001853	0.0004032	-0.0000137
19 C	6.0	0.0001697	-0.0000695	0.0001303
20 O	8.0	0.0000784	-0.0001733	-0.0006078
21 N	7.0	0.0002693	-0.0004861	0.0000645
22 H	1.0	0.0002414	0.0004713	0.0001529
23 H	1.0	-0.0004310	-0.0002086	0.0000081
24 H	1.0	-0.0011917	0.0000274	0.0005014
25 H	1.0	0.0001222	0.0000522	0.0000542
26 H	1.0	-0.0002913	-0.0000851	-0.0007170
27 H	1.0	0.0001557	-0.0005032	-0.0002376
28 H	1.0	0.0002727	0.0001049	0.0007532
29 H	1.0	0.0001229	0.0003305	-0.0004818
30 H	1.0	-0.0000611	0.0002895	-0.0005261
31 H	1.0	0.0006589	0.0000366	0.0002108
32 H	1.0	0.0007817	-0.0000492	-0.0001221
33 H	1.0	-0.0005061	0.0001032	-0.0013318

34 H 1.0 0.0008286 -0.0004278 0.0004015
35 H 1.0 0.0004227 -0.0001900 -0.0005636

MAXIMUM GRADIENT = 0.0013318 RMS GRADIENT = 0.0004275
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0000778636
PREDICTED ENERGY CHANGE WAS -0.0000833050 RATIO= 0.935
GDIIS STEP HAS LENGTH = 0.153684
RADIUS OF STEP TAKEN= 0.10000 CURRENT TRUST RADIUS= 0.10000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 4395.7 SECONDS (73.3 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4063.9 SECONDS (67.7
MIN)
CPU UTILIZATION: STEP = 91.37% , TOTAL = 100.00%

INSERCH= 43

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1352096523	-1.7648548487	1.0143786231
C	6.0	4.9852815402	0.6880929540	0.4461939534
C	6.0	5.2096194254	-0.6758702532	0.2265364073
C	6.0	4.0829539243	-1.5455155481	0.0708583251
C	6.0	2.7658036899	-1.0603989395	0.1596145425
C	6.0	2.4748254954	0.3321816502	0.4795530603
C	6.0	3.6468790754	1.2144410661	0.5802896382
C	6.0	3.4881225521	2.6290429732	0.8244405309
C	6.0	2.2173176625	3.1871073254	1.0172306194
C	6.0	1.0720782772	2.3354067823	0.9997136918
C	6.0	1.1687849734	0.9540380393	0.7112683747
N	7.0	-0.0426625680	0.1397551036	0.7370603757
C	6.0	-1.2439191747	0.6802712809	0.5311669283
C	6.0	-2.5561985607	0.0391866366	0.5767513465
C	6.0	-2.8627519046	-1.3473088094	0.7895927883
C	6.0	-4.1755334123	-1.8525356316	0.7869521280
C	6.0	-5.2585468300	-0.9455796479	0.5757748986
C	6.0	-5.0084912707	0.4394977645	0.3676928304
C	6.0	-3.6788966113	0.9185555038	0.3581996043
O	8.0	-1.7628880293	-2.2869211294	1.0046717480
N	7.0	1.6843172684	-2.0591124605	-0.1797322795
H	1.0	5.8347583979	1.3891751373	0.5298128681
H	1.0	6.2335660785	-1.0793414552	0.1467825992
H	1.0	4.2594555830	-2.6139527975	-0.1571522524

H	1.0	4.3907312182	3.2640165122	0.8768105925
H	1.0	2.0904701254	4.2651831895	1.2181847811
H	1.0	0.0975990246	2.7806316525	1.2583739025
H	1.0	-1.2857646309	1.7529311608	0.2670846242
H	1.0	-4.3766449515	-2.9302856437	0.9359517085
H	1.0	-6.2920413935	-1.3334463630	0.5639965818
H	1.0	-5.8442212619	1.1400300895	0.2028914639
H	1.0	-3.4789326349	1.9900451012	0.1724792144
H	1.0	-2.1013528655	-3.2138656603	1.1028698035
H	1.0	1.3608493550	-1.9003756189	-1.1583752877
H	1.0	2.1062197804	-3.0091201162	-0.1750317348

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4647035	5.2494016	4.0648524
2 C	5.4647035	0.0000000	1.3996330 *	2.4380482 *
3 C	5.2494016	1.3996330 *	0.0000000	1.4317450 *
4 C	4.0648524	2.4380482 *	1.4317450 *	0.0000000
5 C	2.8542783 *	2.8399707 *	2.4747881 *	1.4064496 *
6 C	3.1870680	2.5357790 *	2.9256254 *	2.5057644 *
7 C	4.6256307	1.4444186 *	2.4780185 *	2.8402539 *
8 C	5.5303200	2.4802908 *	3.7740551	4.2835323
9 C	5.3718815	3.7726356	4.9499154	5.1743539
10 C	4.2059581	4.2817271	5.1754072	4.9989702
11 C	2.9244713 *	3.8349234	4.3840517	3.8923353
12 N	1.9328950 *	5.0661129	5.3396953	4.5060708
13 C	2.8485315 *	6.2297852	6.6015210	5.7915100
14 C	3.2695201	7.5704720	7.8065284	6.8443812
15 C	3.0352342	8.1149499	8.1197932	6.9856062
16 C	4.3176286	9.5126989	9.4752151	8.2951591
17 C	5.4732252	10.3740878	10.4774623	9.3743533
18 C	5.6333855	9.9971724	10.2797742	9.3103579
19 C	4.7094234	8.6676894	9.0313480	8.1486523
20 O	1.9686092 *	7.3959718	7.1983915	5.9662013
21 N	1.9779340 *	4.3399639	3.8086964	2.4657727 *
22 H	6.5320414	1.1045901 *	2.1788042 *	3.4484587
23 H	6.1977901	2.1844189 *	1.1034566 *	2.2018663 *
24 H	4.3706815	3.4342912	2.1923030 *	1.1066616 *
25 H	6.5892288	2.6784889 *	4.0762902	4.8862956
26 H	6.3423922	4.6659916	5.9267586	6.2490455
27 H	4.5521858	5.3784565	6.2565843	6.0007330
28 H	3.8668378	6.3633309	6.9347483	6.3040776
29 H	4.6606021	10.0487907	9.8733036	8.6157291

30 H	6.4574386	11.4576835	11.5253845	10.3888732
31 H	6.6970488	10.8416592	11.2020287	10.2848624
32 H	5.2792133	8.5681340	9.0885072	8.3482120
33 H	2.6663974 *	8.1164581	7.7884335	6.4879959
34 H	2.4982830 *	4.7340596	4.2697102	3.0077889
35 H	2.6168252 *	4.7269760	3.9033833	2.4718572 *

C C C C

1 CO	2.8542783 *	3.1870680	4.6256307	5.5303200
2 C	2.8399707 *	2.5357790 *	1.4444186 *	2.4802908 *
3 C	2.4747881 *	2.9256254 *	2.4780185 *	3.7740551
4 C	1.4064496 *	2.5057644 *	2.8402539 *	4.2835323
5 C	0.0000000	1.4581871 *	2.4755117 *	3.8178161
6 C	1.4581871 *	0.0000000	1.4704554 *	2.5340265 *
7 C	2.4755117 *	1.4704554 *	0.0000000	1.4442686 *
8 C	3.8178161	2.5340265 *	1.4442686 *	0.0000000
9 C	4.3677971	2.9165061 *	2.4750708 *	1.4012669 *
10 C	3.8866398	2.5002355 *	2.8393802 *	2.4401256 *
11 C	2.6292104 *	1.4649707 *	2.4951785 *	2.8631759 *
12 N	3.1082626	2.5379291 *	3.8460687	4.3209528
13 C	4.3870105	3.7353571	4.9201278	5.1260062
14 C	5.4503944	5.0404858	6.3134307	6.5804653
15 C	5.6709636	5.6041543	6.9986903	7.4930764
16 C	7.0144988	7.0067651	8.4047125	8.8779263
17 C	8.0359551	7.8388124	9.1636412	9.4521948
18 C	7.9203945	7.4849221	8.6925928	8.7860784
19 C	6.7446170	6.1827871	7.3351116	7.3830422
20 O	4.7673396	5.0093577	6.4579577	7.1952970
21 N	1.5106945 *	2.6034300 *	3.8917136	5.1225851
22 H	3.9441023	3.5226283	2.1954261 *	2.6703516 *
23 H	3.4678379	4.0288043	3.4842957	4.6635604
24 H	2.1782715 *	3.5028569	3.9466023	5.3895718
25 H	4.6749683	3.5247928	2.2004545 *	1.1048242 *
26 H	5.4716059	4.0201750	3.4837260	2.1875607 *
27 H	4.8041757	3.5003821	3.9382915	3.4215387
28 H	4.9337189	4.0256316	4.9718249	4.8855109
29 H	7.4238634	7.6022786	9.0378201	9.6318813
30 H	9.0709777	8.9240911	10.2603185	10.5556032
31 H	8.8868606	8.3627567	9.4988921	9.4708038
32 H	6.9499717	6.1878948	7.1794891	7.0266087
33 H	5.4052162	5.8227471	7.2749681	8.0906946
34 H	2.1015601 *	2.9846380 *	4.2368586	5.3826093
35 H	2.0843592 *	3.4247115	4.5587949	5.8904570

C C C N

1	CO	5.3718815	4.2059581	2.9244713 *	1.9328950 *
2	C	3.7726356	4.2817271	3.8349234	5.0661129
3	C	4.9499154	5.1754072	4.3840517	5.3396953
4	C	5.1743539	4.9989702	3.8923353	4.5060708
5	C	4.3677971	3.8866398	2.6292104 *	3.1082626
6	C	2.9165061 *	2.5002355 *	1.4649707 *	2.5379291 *
7	C	2.4750708 *	2.8393802 *	2.4951785 *	3.8460687
8	C	1.4012669 *	2.4401256 *	2.8631759 *	4.3209528
9	C	0.0000000	1.4273310 *	2.4858866 *	3.8042557
10	C	1.4273310 *	0.0000000	1.4144725 *	2.4763926 *
11	C	2.4858866 *	1.4144725 *	0.0000000	1.4599065 *
12	N	3.8042557	2.4763926 *	1.4599065 *	0.0000000
13	C	4.3012376	2.8849357 *	2.4348565 *	1.3332544 *
14	C	5.7349703	4.3146167	3.8380399	2.5206500 *
15	C	6.8132118	5.3934621	4.6428032	3.1885769
16	C	8.1436831	6.7172582	6.0369134	4.5882821
17	C	8.5535101	7.1429273	6.7035438	5.3300481
18	C	7.7578072	6.4005662	6.2081831	4.9885602
19	C	6.3518495	4.9990769	4.8606515	3.7379491
20	O	6.7681004	5.4224509	4.3800238	2.9865614 *
21	N	5.4073683	4.5910488	3.1841375	2.9424457 *
22	H	4.0689082	4.8784509	4.6897312	6.0123273
23	H	5.9237249	6.2473157	5.4868282	6.4207219
24	H	6.2611342	5.9994894	4.7996831	5.1856286
25	H	2.1793025 *	3.4483153	3.9679141	5.4254511
26	H	1.1039567 *	2.1929178 *	3.4742121	4.6691426
27	H	2.1717688 *	1.1021525 *	2.1870546 *	2.6954907 *
28	H	3.8589073	2.5368182 *	2.6192257 *	2.0900997 *
29	H	8.9949678	7.5776096	6.7742340	5.3148952
30	H	9.6462437	8.2389679	7.8050115	6.4230063
31	H	8.3571576	7.0639260	7.0338678	5.9113425
32	H	5.8816520	4.6384579	4.7921690	3.9433839
33	H	7.7220920	6.3934131	5.3121158	3.9520621
34	H	5.5990429	4.7626242	3.4176210	3.1184380
35	H	6.3108689	5.5689715	4.1678453	3.9198243

C C C C

1	CO	2.8485315 *	3.2695201	3.0352342	4.3176286
2	C	6.2297852	7.5704720	8.1149499	9.5126989
3	C	6.6015210	7.8065284	8.1197932	9.4752151
4	C	5.7915100	6.8443812	6.9856062	8.2951591
5	C	4.3870105	5.4503944	5.6709636	7.0144988
6	C	3.7353571	5.0404858	5.6041543	7.0067651
7	C	4.9201278	6.3134307	6.9986903	8.4047125

8 C	5.1260062	6.5804653	7.4930764	8.8779263
9 C	4.3012376	5.7349703	6.8132118	8.1436831
10 C	2.8849357 *	4.3146167	5.3934621	6.7172582
11 C	2.4348565 *	3.8380399	4.6428032	6.0369134
12 N	1.3332544 *	2.5206500 *	3.1885769	4.5882821
13 C	0.0000000	1.4612134 *	2.6073903 *	3.8826407
14 C	1.4612134 *	0.0000000	1.4358433 *	2.4990084 *
15 C	2.6073903 *	1.4358433 *	0.0000000	1.4066472 *
16 C	3.8826407	2.4990084 *	1.4066472 *	0.0000000
17 C	4.3315836	2.8761870 *	2.4386344 *	1.4283148 *
18 C	3.7758044	2.4935304 *	2.8239821 *	2.4744725 *
19 C	2.4527153 *	1.4427423 *	2.4466985 *	2.8477049 *
20 O	3.0492239	2.4946412 *	1.4624742 *	2.4610872 *
21 N	4.0723666	4.7913569	4.7034130	5.9426427
22 H	7.1140862	8.4989900	9.1215413	10.5252435
23 H	7.6913441	8.8710733	9.1229388	10.4573897
24 H	6.4508007	7.3505717	7.2956530	8.5217445
25 H	6.2084212	7.6648155	8.5956353	9.9783801
26 H	4.9438587	6.3136371	7.4978774	8.7678530
27 H	2.5961538 *	3.8759220	5.1013063	6.3204540
28 H	1.1054817 *	2.1556475 *	3.5172989	4.6497760
29 H	4.7972849	3.5015447	2.1952469 *	1.1064320 *
30 H	5.4350413	3.9800510	3.4367299	2.1906092 *
31 H	4.6348595	3.4875093	3.9268604	3.4757870
32 H	2.6152341 *	2.1956145 *	3.4494114	3.9532589
33 H	4.0281930	3.3265650	2.0400749 *	2.5010495 *
34 H	4.0372157	4.7027471	4.6839375	5.8684003
35 H	5.0332650	5.6209872	5.3275507	6.4593749

C C C O

1 CO	5.4732252	5.6333855	4.7094234	1.9686092 *
2 C	10.3740878	9.9971724	8.6676894	7.3959718
3 C	10.4774623	10.2797742	9.0313480	7.1983915
4 C	9.3743533	9.3103579	8.1486523	5.9662013
5 C	8.0359551	7.9203945	6.7446170	4.7673396
6 C	7.8388124	7.4849221	6.1827871	5.0093577
7 C	9.1636412	8.6925928	7.3351116	6.4579577
8 C	9.4521948	8.7860784	7.3830422	7.1952970
9 C	8.5535101	7.7578072	6.3518495	6.7681004
10 C	7.1429273	6.4005662	4.9990769	5.4224509
11 C	6.7035438	6.2081831	4.8606515	4.3800238
12 N	5.3300481	4.9885602	3.7379491	2.9865614 *
13 C	4.3315836	3.7758044	2.4527153 *	3.0492239
14 C	2.8761870 *	2.4935304 *	1.4427423 *	2.4946412 *
15 C	2.4386344 *	2.8239821 *	2.4466985 *	1.4624742 *

16 C	1.4283148 *	2.4744725 *	2.8477049 *	2.4610872 *
17 C	0.0000000	1.4227668 *	2.4530866 *	3.7686576
18 C	1.4227668 *	0.0000000	1.4132970 *	4.2863787
19 C	2.4530866 *	1.4132970 *	0.0000000	3.7899994
20 O	3.7686576	4.2863787	3.7899994	0.0000000
21 N	7.0720653	7.1649434	6.1579169	3.6521136
22 H	11.3364286	10.8859650	9.5268340	8.4536031
23 H	11.5008950	11.3463442	10.1140104	8.1324966
24 H	9.6908731	9.7720961	8.7041162	6.1421012
25 H	10.5318512	9.8276391	8.4195628	8.2883223
26 H	9.0317656	8.1089123	6.7249598	7.6042112
27 H	6.5604032	5.6873877	4.3057590	5.4042454
28 H	4.8125096	3.9489141	2.5360531 *	4.1342579
29 H	2.2014850 *	3.4752825	3.9540142	2.6926503 *
30 H	1.1039431 *	2.1975821 *	3.4557764	4.6493590
31 H	2.1981412 *	1.1028824 *	2.1821555 *	5.3892604
32 H	3.4565252	2.1867453 *	1.1056978 *	4.6829258
33 H	3.9231141	4.7264155	4.4855415	0.9916791 *
34 H	6.9090751	6.9550263	5.9703778	3.8191524
35 H	7.6851608	7.9250633	7.0127415	4.1089253

N H H H

1 CO	1.9779340 *	6.5320414	6.1977901	4.3706815
2 C	4.3399639	1.1045901 *	2.1844189 *	3.4342912
3 C	3.8086964	2.1788042 *	1.1034566 *	2.1923030 *
4 C	2.4657727 *	3.4484587	2.2018663 *	1.1066616 *
5 C	1.5106945 *	3.9441023	3.4678379	2.1782715 *
6 C	2.6034300 *	3.5226283	4.0288043	3.5028569
7 C	3.8917136	2.1954261 *	3.4842957	3.9466023
8 C	5.1225851	2.6703516 *	4.6635604	5.3895718
9 C	5.4073683	4.0689082	5.9237249	6.2611342
10 C	4.5910488	4.8784509	6.2473157	5.9994894
11 C	3.1841375	4.6897312	5.4868282	4.7996831
12 N	2.9424457 *	6.0123273	6.4207219	5.1856286
13 C	4.0723666	7.1140862	7.6913441	6.4508007
14 C	4.7913569	8.4989900	8.8710733	7.3505717
15 C	4.7034130	9.1215413	9.1229388	7.2956530
16 C	5.9426427	10.5252435	10.4573897	8.5217445
17 C	7.0720653	11.3364286	11.5008950	9.6908731
18 C	7.1649434	10.8859650	11.3463442	9.7720961
19 C	6.1579169	9.5268340	10.1140104	8.7041162
20 O	3.6521136	8.4536031	8.1324966	6.1421012
21 N	0.0000000	5.4424538	4.6650003	2.6343301 *
22 H	5.4424538	0.0000000	2.5296905 *	4.3564358
23 H	4.6650003	2.5296905 *	0.0000000	2.5188332 *

24 H	2.6343301 *	4.3564358	2.5188332 *	0.0000000
25 H	6.0643764	2.3917885 *	4.7742790	5.9696596
26 H	6.4896724	4.7712653	6.8466846	7.3429260
27 H	5.2923480	5.9482729	7.3338339	6.9589012
28 H	4.8531133	7.1346473	8.0359551	7.0710056
29 H	6.2240627	11.0948388	10.7993222	8.7107506
30 H	8.0437567	12.4287212	12.5351298	10.6533488
31 H	8.1890052	11.6862105	12.2801346	10.7845401
32 H	6.5710638	9.3398915	10.1859916	9.0104443
33 H	4.1605074	9.1922925	8.6568568	6.5120991
34 H	1.0428667 *	5.8040491	5.1108612	3.1485803
35 H	1.0394895 *	5.8089420	4.5675593	2.1892696 *

H H H H

1 CO	6.5892288	6.3423922	4.5521858	3.8668378
2 C	2.6784889 *	4.6659916	5.3784565	6.3633309
3 C	4.0762902	5.9267586	6.2565843	6.9347483
4 C	4.8862956	6.2490455	6.0007330	6.3040776
5 C	4.6749683	5.4716059	4.8041757	4.9337189
6 C	3.5247928	4.0201750	3.5003821	4.0256316
7 C	2.2004545 *	3.4837260	3.9382915	4.9718249
8 C	1.1048242 *	2.1875607 *	3.4215387	4.8855109
9 C	2.1793025 *	1.1039567 *	2.1717688 *	3.8589073
10 C	3.4483153	2.1929178 *	1.1021525 *	2.5368182 *
11 C	3.9679141	3.4742121	2.1870546 *	2.6192257 *
12 N	5.4254511	4.6691426	2.6954907 *	2.0900997 *
13 C	6.2084212	4.9438587	2.5961538 *	1.1054817 *
14 C	7.6648155	6.3136371	3.8759220	2.1556475 *
15 C	8.5956353	7.4978774	5.1013063	3.5172989
16 C	9.9783801	8.7678530	6.3204540	4.6497760
17 C	10.5318512	9.0317656	6.5604032	4.8125096
18 C	9.8276391	8.1089123	5.6873877	3.9489141
19 C	8.4195628	6.7249598	4.3057590	2.5360531 *
20 O	8.2883223	7.6042112	5.4042454	4.1342579
21 N	6.0643764	6.4896724	5.2923480	4.8531133
22 H	2.3917885 *	4.7712653	5.9482729	7.1346473
23 H	4.7742790	6.8466846	7.3338339	8.0359551
24 H	5.9696596	7.3429260	6.9589012	7.0710056
25 H	0.0000000	2.5318120 *	4.3370768	5.9057387
26 H	2.5318120 *	0.0000000	2.4853659 *	4.3145061
27 H	4.3370768	2.4853659 *	0.0000000	1.9880940 *
28 H	5.9057387	4.3145061	1.9880940 *	0.0000000
29 H	10.7349784	9.6787398	7.2620515	5.6509684
30 H	11.6342661	10.1014412	7.6312058	5.8886917
31 H	10.4747190	8.5881738	6.2538664	4.5999234

32 H	8.0031678	6.1063901	3.8204415	2.2079762 *
33 H	9.1739422	8.5744300	6.3869843	5.1022340
34 H	6.3240107	6.6478944	5.4174078	4.7310836
35 H	6.7585211	7.4065369	6.2936821	5.8632890

H H H H

1 CO	4.6606021	6.4574386	6.6970488	5.2792133
2 C	10.0487907	11.4576835	10.8416592	8.5681340
3 C	9.8733036	11.5253845	11.2020287	9.0885072
4 C	8.6157291	10.3888732	10.2848624	8.3482120
5 C	7.4238634	9.0709777	8.8868606	6.9499717
6 C	7.6022786	8.9240911	8.3627567	6.1878948
7 C	9.0378201	10.2603185	9.4988921	7.1794891
8 C	9.6318813	10.5556032	9.4708038	7.0266087
9 C	8.9949678	9.6462437	8.3571576	5.8816520
10 C	7.5776096	8.2389679	7.0639260	4.6384579
11 C	6.7742340	7.8050115	7.0338678	4.7921690
12 N	5.3148952	6.4230063	5.9113425	3.9433839
13 C	4.7972849	5.4350413	4.6348595	2.6152341 *
14 C	3.5015447	3.9800510	3.4875093	2.1956145 *
15 C	2.1952469 *	3.4367299	3.9268604	3.4494114
16 C	1.1064320 *	2.1906092 *	3.4757870	3.9532589
17 C	2.2014850 *	1.1039431 *	2.1981412 *	3.4565252
18 C	3.4752825	2.1975821 *	1.1028824 *	2.1867453 *
19 C	3.9540142	3.4557764	2.1821555 *	1.1056978 *
20 O	2.6926503 *	4.6493590	5.3892604	4.6829258
21 N	6.2240627	8.0437567	8.1890052	6.5710638
22 H	11.0948388	12.4287212	11.6862105	9.3398915
23 H	10.7993222	12.5351298	12.2801346	10.1859916
24 H	8.7107506	10.6533488	10.7845401	9.0104443
25 H	10.7349784	11.6342661	10.4747190	8.0031678
26 H	9.6787398	10.1014412	8.5881738	6.1063901
27 H	7.2620515	7.6312058	6.2538664	3.8204415
28 H	5.6509684	5.8886917	4.5999234	2.2079762 *
29 H	0.0000000	2.5213072 *	4.3884653	5.0594893
30 H	2.5213072 *	0.0000000	2.5394932 *	4.3717802
31 H	4.3884653	2.5394932 *	0.0000000	2.5135713 *
32 H	5.0594893	4.3717802	2.5135713 *	0.0000000
33 H	2.2989635 *	4.6247412	5.8116635	5.4629699
34 H	6.1940101	7.8647766	7.9378937	6.3505934
35 H	6.5778442	8.5956289	8.9759560	7.5037553

H H H

1 CO	2.6663974 *	2.4982830 *	2.6168252 *
------	-------------	-------------	-------------

2 C	8.1164581	4.7340596	4.7269760
3 C	7.7884335	4.2697102	3.9033833
4 C	6.4879959	3.0077889	2.4718572 *
5 C	5.4052162	2.1015601 *	2.0843592 *
6 C	5.8227471	2.9846380 *	3.4247115
7 C	7.2749681	4.2368586	4.5587949
8 C	8.0906946	5.3826093	5.8904570
9 C	7.7220920	5.5990429	6.3108689
10 C	6.3934131	4.7626242	5.5689715
11 C	5.3121158	3.4176210	4.1678453
12 N	3.9520621	3.1184380	3.9198243
13 C	4.0281930	4.0372157	5.0332650
14 C	3.3265650	4.7027471	5.6209872
15 C	2.0400749 *	4.6839375	5.3275507
16 C	2.5010495 *	5.8684003	6.4593749
17 C	3.9231141	6.9090751	7.6851608
18 C	4.7264155	6.9550263	7.9250633
19 C	4.4855415	5.9703778	7.0127415
20 O	0.9916791 *	3.8191524	4.1089253
21 N	4.1605074	1.0428667 *	1.0394895 *
22 H	9.1922925	5.8040491	5.8089420
23 H	8.6568568	5.1108612	4.5675593
24 H	6.5120991	3.1485803	2.1892696 *
25 H	9.1739422	6.3240107	6.7585211
26 H	8.5744300	6.6478944	7.4065369
27 H	6.3869843	5.4174078	6.2936821
28 H	5.1022340	4.7310836	5.8632890
29 H	2.2989635 *	6.1940101	6.5778442
30 H	4.6247412	7.8647766	8.5956289
31 H	5.8116635	7.9378937	8.9759560
32 H	5.4629699	6.3505934	7.5037553
33 H	0.0000000	4.3388166	4.4021155
34 H	4.3388166	0.0000000	1.6588719 *
35 H	4.4021155	1.6588719 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.83 , TOTAL = 4396.5 SECONDS (73.3 MIN)

WALL CLOCK TIME: STEP = 0.84 , TOTAL = 4064.8 SECONDS (67.7 MIN)

CPU UTILIZATION: STEP = 99.20% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.15, TOTAL = 4397.7 SECONDS (73.3 MIN)
 WALL CLOCK TIME: STEP = 1.15, TOTAL = 4065.9 SECONDS (67.8 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
 INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.633927780	-284.633927780	0.027894738	0.001113027	196952522
11400409						
2	1	-284.634130403	-0.000202622	0.003762308	0.000152444	161736953
14402303						
3	2	-284.634128335	0.000002068	0.003358749	0.000338633	146936320
15580691						
4	3	-284.634134323	-0.000005988	0.000650147	0.000079519	141868420
15986261						
5	4	-284.634133897	0.000000426	0.000693216	0.000167104	136365629
16461753						
6	5	-284.634134625	-0.000000729	0.000284749	0.000031102	130852214
16885288						
7	6	-284.634134610	0.000000016	0.000147009	0.000044743	124208725
17347145						
8	7	-284.634134707	-0.000000098	0.000221614	0.000025316	140571009
16115053						
9	8	-284.634134721	-0.000000013	0.000199842	0.000022590	161429313
14467125						
10	9	-284.634134756	-0.000000035	0.000356802	0.000018725	156718711
14957744						

-----DISABLING FDIFF OPTION-----

11	10	-284.634134746	0.000000010	0.000317693	0.000016334	196946164
11400906						
12	11	-284.634134767	-0.000000021	0.000311517	0.000018483	196946186
11400911						
13	12	-284.634134793	-0.000000026	0.000589587	0.000016030	196945892
11400910						
14	13	-284.634134826	-0.000000033	0.000147259	0.000013587	196945916
11400906						
15	14	-284.634134833	-0.000000007	0.000081966	0.000010540	196945909
11400902						
16	15	-284.634134838	-0.000000005	0.000045238	0.000008083	196945965
11400902						

17 16	-284.634134840	-0.000000002	0.000052527	0.000006239	196945914
11400906					
18 17	-284.634134842	-0.000000002	0.000109976	0.000004444	196945941
11400906					
19 18	-284.634134844	-0.000000002	0.000053389	0.000003954	196945896
11400906					
20 19	-284.634134845	-0.000000001	0.000046980	0.000004334	196945851
11400907					
21 20	-284.634134846	-0.000000001	0.000085490	0.000003640	196945897
11400905					
22 21	-284.634134848	-0.000000002	0.000043841	0.000002869	196945815
11400903					
23 22	-284.634134848	-0.000000001	0.000019197	0.000003410	196945834
11400905					
24 23	-284.634134849	0.000000000	0.000035437	0.000002705	196945831
11400906					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 81.6 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 26.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6341348486 AFTER 24 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6106025600
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000287724

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 85.28 , TOTAL = 4483.0 SECONDS (74.7 MIN)
WALL CLOCK TIME: STEP = 78.23 , TOTAL = 4144.1 SECONDS (69.1 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.85 , TOTAL = 4486.8 SECONDS (74.8 MIN)
 WALL CLOCK TIME: STEP = 3.82 , TOTAL = 4148.0 SECONDS (69.1 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
 USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.73 , TOTAL = 4489.6 SECONDS (74.8 MIN)
 WALL CLOCK TIME: STEP = 2.67 , TOTAL = 4150.6 SECONDS (69.2 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 43 ENERGY= -284.6341348

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0003286	0.0000409	0.0005821
2 C	6.0	0.0005222	-0.0003537	-0.0003074
3 C	6.0	-0.0001052	0.0003571	-0.0001466
4 C	6.0	-0.0006209	-0.0000003	-0.0000025
5 C	6.0	-0.0009035	-0.0008217	0.0001430
6 C	6.0	-0.0002689	-0.0001346	-0.0000372
7 C	6.0	-0.0001857	-0.0000056	-0.0003694
8 C	6.0	0.0006138	0.0005656	-0.0004065
9 C	6.0	-0.0005245	-0.0000392	-0.0004435
10 C	6.0	0.0007069	0.0008193	0.0000919
11 C	6.0	0.0002270	0.0002182	0.0001007
12 N	7.0	0.0000406	-0.0005012	0.0004512
13 C	6.0	-0.0006717	-0.0002818	0.0007420
14 C	6.0	0.0002353	0.0002992	0.0006919
15 C	6.0	-0.0004975	0.0001818	0.0000040
16 C	6.0	-0.0004835	-0.0008266	0.0001546
17 C	6.0	-0.0000828	0.0006134	0.0001304
18 C	6.0	0.0002131	-0.0003701	0.0004234
19 C	6.0	0.0000646	0.0005148	0.0003413
20 O	8.0	-0.0004352	0.0003246	-0.0005448
21 N	7.0	0.0000128	-0.0006234	-0.0000562

22 H	1.0	-0.0002919	-0.0000652	-0.0001185
23 H	1.0	-0.0003201	0.0003769	0.0001312
24 H	1.0	-0.0004425	0.0007671	0.0005857
25 H	1.0	-0.0003593	0.0003652	0.0002775
26 H	1.0	-0.0005158	-0.0001298	-0.0005248
27 H	1.0	0.0002954	-0.0007910	-0.0002147
28 H	1.0	0.0000653	-0.0003248	0.0006961
29 H	1.0	0.0001103	0.0001193	-0.0004785
30 H	1.0	0.0008340	0.0003611	-0.0004913
31 H	1.0	0.0009972	-0.0001459	0.0001636
32 H	1.0	0.0006580	-0.0001399	-0.0005861
33 H	1.0	-0.0002658	-0.0001633	-0.0012124
34 H	1.0	0.0010009	-0.0007444	0.0010158
35 H	1.0	0.0000490	0.0005384	-0.0007858

MAXIMUM GRADIENT = 0.0012124 RMS GRADIENT = 0.0004718
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001362466
 PREDICTED ENERGY CHANGE WAS -0.0001407756 RATIO= 0.968
 GDIIS STEP HAS LENGTH = 0.129451
 RADIUS OF STEP TAKEN= 0.12945 CURRENT TRUST RADIUS= 0.20000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 4489.6 SECONDS (74.8 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4150.7 SECONDS (69.2 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 44

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1325504423	-1.7653773548	1.0068559843
C	6.0	4.9855764740	0.6859056422	0.4501918233
C	6.0	5.2099478192	-0.6778876363	0.2318260350
C	6.0	4.0833907637	-1.5464219912	0.0671827212
C	6.0	2.7653558156	-1.0595650800	0.1519696815
C	6.0	2.4754929658	0.3320312190	0.4748975818
C	6.0	3.6476082804	1.2145417298	0.5794908295
C	6.0	3.4882849679	2.6297987761	0.8256880364
C	6.0	2.2173394261	3.1870765383	1.0232007158
C	6.0	1.0730108830	2.3348691664	1.0057328191
C	6.0	1.1692174111	0.9544116246	0.7094142190
N	7.0	-0.0412123945	0.1402169448	0.7334121882

C	6.0	-1.2429590312	0.6787121374	0.5241344421
C	6.0	-2.5557200662	0.0369531820	0.5706932510
C	6.0	-2.8633273897	-1.3482077534	0.7908457525
C	6.0	-4.1757898262	-1.8535974157	0.7930470186
C	6.0	-5.2569877175	-0.9447117551	0.5831332728
C	6.0	-5.0064157203	0.4390433140	0.3650896578
C	6.0	-3.6770391854	0.9167777258	0.3456468565
O	8.0	-1.7638486962	-2.2853360908	1.0162337142
N	7.0	1.6802299815	-2.0545341821	-0.1909501140
H	1.0	5.8356270324	1.3856599000	0.5340361395
H	1.0	6.2364801008	-1.0788667780	0.1574007796
H	1.0	4.2665356665	-2.6122076902	-0.1645315408
H	1.0	4.3885269621	3.2673535038	0.8813292187
H	1.0	2.0899409227	4.2630654851	1.2324165819
H	1.0	0.0982447461	2.7760090738	1.2719287218
H	1.0	-1.2868371901	1.7501271921	0.2551855414
H	1.0	-4.3785031117	-2.9304470903	0.9465627998
H	1.0	-6.2900274125	-1.3312569205	0.5783011703
H	1.0	-5.8426162259	1.1381821993	0.1962724627
H	1.0	-3.4774226557	1.9859404304	0.1426308876
H	1.0	-2.1003798907	-3.2112167494	1.1333562965
H	1.0	1.3524272940	-1.8898466395	-1.1669360476
H	1.0	2.0992955587	-3.0060896576	-0.1928024981

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4653934	5.2500733	4.0669481
2 C	5.4653934	0.0000000	1.3992706 *	2.4380159 *
3 C	5.2500733	1.3992706 *	0.0000000	1.4319882 *
4 C	4.0669481	2.4380159 *	1.4319882 *	0.0000000
5 C	2.8566879 *	2.8398916 *	2.4754969 *	1.4076344 *
6 C	3.1892761	2.5350260 *	2.9251091 *	2.5060234 *
7 C	4.6279791	1.4444145 *	2.4785206 *	2.8417049 *
8 C	5.5327524	2.4822570 *	3.7759217	4.2860589
9 C	5.3733985	3.7745637	4.9517600	5.1770770
10 C	4.2067195	4.2820411	5.1758944	5.0007684
11 C	2.9258165 *	3.8345649	4.3840613	3.8934607
12 N	1.9329394 *	5.0642469	5.3381240	4.5056591
13 C	2.8458074 *	6.2289786	6.6004404	5.7905120
14 C	3.2657972	7.5701264	7.8058584	6.8438580
15 C	3.0324866	8.1153530	8.1203205	6.9871217
16 C	4.3145443	9.5130047	9.4757234	8.2967041
17 C	5.4681034	10.3724013	10.4762279	9.3739496

18 C	5.6285262	9.9954035	10.2781019	9.3088884
19 C	4.7057546	8.6663223	9.0296429	8.1467274
20 O	1.9664116 *	7.3961761	7.1995155	5.9696651
21 N	1.9782980 *	4.3412428	3.8121914	2.4698162 *
22 H	6.5328154	1.1042064 *	2.1773915 *	3.4475191
23 H	6.2008732	2.1828670 *	1.1045777 *	2.2051170 *
24 H	4.3793954	3.4311013	2.1883144 *	1.1059533 *
25 H	6.5922282	2.6844405 *	4.0818518	4.8916640
26 H	6.3422692	4.6682602	5.9286290	6.2515404
27 H	4.5492451	5.3786425	6.2562548	6.0013508
28 H	3.8650281	6.3650427	6.9357060	6.3041201
29 H	4.6594664	10.0503919	9.8753868	8.6193087
30 H	6.4514825	11.4553306	11.5237306	10.3882310
31 H	6.6925571	10.8406082	11.2008279	10.2834517
32 H	5.2774213	8.5677908	9.0870425	8.3456082
33 H	2.6631620 *	8.1157288	7.7891851	6.4920942
34 H	2.4957892 *	4.7380772	4.2785330	3.0164799
35 H	2.6166073 *	4.7302102	3.9085792	2.4768641 *

C C C C

1 CO	2.8566879 *	3.1892761	4.6279791	5.5327524
2 C	2.8398916 *	2.5350260 *	1.4444145 *	2.4822570 *
3 C	2.4754969 *	2.9251091 *	2.4785206 *	3.7759217
4 C	1.4076344 *	2.5060234 *	2.8417049 *	4.2860589
5 C	0.0000000	1.4576842 *	2.4764300 *	3.8194147
6 C	1.4576842 *	0.0000000	1.4709245 *	2.5354560 *
7 C	2.4764300 *	1.4709245 *	0.0000000	1.4453199 *
8 C	3.8194147	2.5354560 *	1.4453199 *	0.0000000
9 C	4.3695916	2.9186578 *	2.4765785 *	1.4017390 *
10 C	3.8878177	2.5020196 *	2.8399591 *	2.4398665 *
11 C	2.6295445 *	1.4658483 *	2.4953896 *	2.8633051 *
12 N	3.1071494	2.5372088 *	3.8451610	4.3201718
13 C	4.3848264	3.7349026	4.9201449	5.1266308
14 C	5.4489935	5.0407690	6.3141171	6.5816311
15 C	5.6721735	5.6058923	7.0003314	7.4945800
16 C	7.0157658	7.0084060	8.4062264	8.8791863
17 C	8.0347426	7.8379235	9.1626535	9.4507012
18 C	7.9178078	7.4834796	8.6913461	8.7847311
19 C	6.7415054	6.1816087	7.3344261	7.3828687
20 O	4.7710754	5.0115541	6.4593928	7.1958159
21 N	1.5116400 *	2.6022088 *	3.8924303	5.1230451
22 H	3.9435600	3.5219500	2.1951705 *	2.6726311 *
23 H	3.4711822	4.0294493	3.4842704	4.6640524
24 H	2.1827535 *	3.5050316	3.9472334	5.3911818
25 H	4.6785547	3.5271806	2.2032029 *	1.1045396 *

26 H	5.4730199	4.0218796	3.4851308	2.1882309 *
27 H	4.8041044	3.5013705	3.9389887	3.4224086
28 H	4.9320678	4.0267105	4.9740102	4.8888738
29 H	7.4274018	7.6054911	9.0406935	9.6341735
30 H	9.0694840	8.9225314	10.2585426	10.5530354
31 H	8.8842129	8.3617254	9.4982655	9.4703116
32 H	6.9460402	6.1873275	7.1799699	7.0286701
33 H	5.4100008	5.8246705	7.2755394	8.0898268
34 H	2.1036271 *	2.9822199 *	4.2373447	5.3814156
35 H	2.0860158 *	3.4249670	4.5615171	5.8932040

C C C N

1 CO	5.3733985	4.2067195	2.9258165 *	1.9329394 *
2 C	3.7745637	4.2820411	3.8345649	5.0642469
3 C	4.9517600	5.1758944	4.3840613	5.3381240
4 C	5.1770770	5.0007684	3.8934607	4.5056591
5 C	4.3695916	3.8878177	2.6295445 *	3.1071494
6 C	2.9186578 *	2.5020196 *	1.4658483 *	2.5372088 *
7 C	2.4765785 *	2.8399591 *	2.4953896 *	3.8451610
8 C	1.4017390 *	2.4398665 *	2.8633051 *	4.3201718
9 C	0.0000000	1.4269024 *	2.4863255 *	3.8037333
10 C	1.4269024 *	0.0000000	1.4151761 *	2.4763179 *
11 C	2.4863255 *	1.4151761 *	0.0000000	1.4589822 *
12 N	3.8037333	2.4763179 *	1.4589822 *	0.0000000
13 C	4.3028624	2.8876478 *	2.4349402 *	1.3334051 *
14 C	5.7367358	4.3171015	3.8387671	2.5218822 *
15 C	6.8143942	5.3949969	4.6443627	3.1910875
16 C	8.1445360	6.7185115	6.0382954	4.5905972
17 C	8.5516607	7.1416471	6.7021436	5.3295372
18 C	7.7567671	6.4003131	6.2066584	4.9878054
19 C	6.3527187	5.0009672	4.8600356	3.7380001
20 O	6.7673634	5.4216399	4.3809794	2.9884396 *
21 N	5.4071371	4.5899485	3.1820661	2.9384932 *
22 H	4.0714112	4.8791401	4.6895747	6.0106672
23 H	5.9246412	6.2477736	5.4878130	6.4208549
24 H	6.2643125	6.0034730	4.8039499	5.1902637
25 H	2.1772981 *	3.4463967	3.9677713	5.4243390
26 H	1.1035189 *	2.1916828 *	3.4739680	4.6678368
27 H	2.1728793 *	1.1025578 *	2.1866921 *	2.6938538 *
28 H	3.8644436	2.5444306 *	2.6213911 *	2.0909550 *
29 H	8.9963941	7.5793180	6.7768407	5.3185056
30 H	9.6430578	8.2363530	7.8026793	6.4216029
31 H	8.3573120	7.0649263	7.0329864	5.9110693
32 H	5.8862931	4.6446896	4.7933870	3.9450296
33 H	7.7196497	6.3910692	5.3124809	3.9537620

34 H	5.5964204	4.7588641	3.4123396	3.1104201
35 H	6.3125198	5.5691641	4.1670866	3.9164899

	C	C	C	C
--	---	---	---	---

1 CO	2.8458074 *	3.2657972	3.0324866	4.3145443
2 C	6.2289786	7.5701264	8.1153530	9.5130047
3 C	6.6004404	7.8058584	8.1203205	9.4757234
4 C	5.7905120	6.8438580	6.9871217	8.2967041
5 C	4.3848264	5.4489935	5.6721735	7.0157658
6 C	3.7349026	5.0407690	5.6058923	7.0084060
7 C	4.9201449	6.3141171	7.0003314	8.4062264
8 C	5.1266308	6.5816311	7.4945800	8.8791863
9 C	4.3028624	5.7367358	6.8143942	8.1445360
10 C	2.8876478 *	4.3171015	5.3949969	6.7185115
11 C	2.4349402 *	3.8387671	4.6443627	6.0382954
12 N	1.3334051 *	2.5218822 *	3.1910875	4.5905972
13 C	0.0000000	1.4619726 *	2.6086649 *	3.8841218
14 C	1.4619726 *	0.0000000	1.4358831 *	2.4996497 *
15 C	2.6086649 *	1.4358831 *	0.0000000	1.4064072 *
16 C	3.8841218	2.4996497 *	1.4064072 *	0.0000000
17 C	4.3302901	2.8741377 *	2.4363011 *	1.4279796 *
18 C	3.7744328	2.4919588 *	2.8228288 *	2.4757400 *
19 C	2.4521989 *	1.4429462 *	2.4475474 *	2.8502452 *
20 O	3.0494376	2.4937109 *	1.4621432 *	2.4604208 *
21 N	4.0653432	4.7851534	4.7017798	5.9415144
22 H	7.1138073	8.4991211	9.1220497	10.5256041
23 H	7.6919170	8.8723530	9.1258037	10.4603833
24 H	6.4543742	7.3553914	7.3037928	8.5302583
25 H	6.2082434	7.6651515	8.5965682	9.9789506
26 H	4.9454499	6.3150668	7.4977489	8.7673253
27 H	2.5993611 *	3.8778457	5.1001485	6.3190154
28 H	1.1055266 *	2.1551274 *	3.5173758	4.6499649
29 H	4.7995951	3.5027532	2.1962437 *	1.1064651 *
30 H	5.4328454	3.9770728	3.4333272	2.1883683 *
31 H	4.6341615	3.4866291	3.9257884	3.4763768
32 H	2.6167190 *	2.1980274 *	3.4516430	3.9563631
33 H	4.0296239	3.3278420	2.0421079 *	2.5032513 *
34 H	4.0240830	4.6910051	4.6796228	5.8654950
35 H	5.0261743	5.6135734	5.3238861	6.4557598

	C	C	C	O
--	---	---	---	---

1 CO	5.4681034	5.6285262	4.7057546	1.9664116 *
2 C	10.3724013	9.9954035	8.6663223	7.3961761
3 C	10.4762279	10.2781019	9.0296429	7.1995155

4 C	9.3739496	9.3088884	8.1467274	5.9696651
5 C	8.0347426	7.9178078	6.7415054	4.7710754
6 C	7.8379235	7.4834796	6.1816087	5.0115541
7 C	9.1626535	8.6913461	7.3344261	6.4593928
8 C	9.4507012	8.7847311	7.3828687	7.1958159
9 C	8.5516607	7.7567671	6.3527187	6.7673634
10 C	7.1416471	6.4003131	5.0009672	5.4216399
11 C	6.7021436	6.2066584	4.8600356	4.3809794
12 N	5.3295372	4.9878054	3.7380001	2.9884396 *
13 C	4.3302901	3.7744328	2.4521989 *	3.0494376
14 C	2.8741377 *	2.4919588 *	1.4429462 *	2.4937109 *
15 C	2.4363011 *	2.8228288 *	2.4475474 *	1.4621432 *
16 C	1.4279796 *	2.4757400 *	2.8502452 *	2.4604208 *
17 C	0.0000000	1.4230627 *	2.4531164 *	3.7665461
18 C	1.4230627 *	0.0000000	1.4127456 *	4.2849122
19 C	2.4531164 *	1.4127456 *	0.0000000	3.7899231
20 O	3.7665461	4.2849122	3.7899231	0.0000000
21 N	7.0679488	7.1580961	6.1495499	3.6568074
22 H	11.3348641	10.8846000	9.5260779	8.4534465
23 H	11.5021323	11.3468010	10.1141435	8.1362413
24 H	9.6972699	9.7764134	8.7071466	6.1535833
25 H	10.5293099	9.8250084	8.4181660	8.2886843
26 H	9.0288356	8.1076309	6.7262220	7.6013152
27 H	6.5571882	5.6869433	4.3090031	5.3990728
28 H	4.8095532	3.9454131	2.5329272 *	4.1342107
29 H	2.2015815 *	3.4764710	3.9565503	2.6939636 *
30 H	1.1030011 *	2.1970619 *	3.4547786	4.6463260
31 H	2.1979693 *	1.1029622 *	2.1819845 *	5.3878714
32 H	3.4568217	2.1863665 *	1.1064227 *	4.6843698
33 H	3.9247883	4.7286019	4.4885052	0.9920816 *
34 H	6.9022018	6.9430336	5.9548787	3.8254174
35 H	7.6789491	7.9165218	7.0032035	4.1115858

N H H H

1 CO	1.9782980 *	6.5328154	6.2008732	4.3793954
2 C	4.3412428	1.1042064 *	2.1828670 *	3.4311013
3 C	3.8121914	2.1773915 *	1.1045777 *	2.1883144 *
4 C	2.4698162 *	3.4475191	2.2051170 *	1.1059533 *
5 C	1.5116400 *	3.9435600	3.4711822	2.1827535 *
6 C	2.6022088 *	3.5219500	4.0294493	3.5050316
7 C	3.8924303	2.1951705 *	3.4842704	3.9472334
8 C	5.1230451	2.6726311 *	4.6640524	5.3911818
9 C	5.4071371	4.0714112	5.9246412	6.2643125
10 C	4.5899485	4.8791401	6.2477736	6.0034730
11 C	3.1820661	4.6895747	5.4878130	4.8039499

12 N	2.9384932 *	6.0106672	6.4208549	5.1902637
13 C	4.0653432	7.1138073	7.6919170	6.4543742
14 C	4.7851534	8.4991211	8.8723530	7.3553914
15 C	4.7017798	9.1220497	9.1258037	7.3037928
16 C	5.9415144	10.5256041	10.4603833	8.5302583
17 C	7.0679488	11.3348641	11.5021323	9.6972699
18 C	7.1580961	10.8846000	11.3468010	9.7764134
19 C	6.1495499	9.5260779	10.1141435	8.7071466
20 O	3.6568074	8.4534465	8.1362413	6.1535833
21 N	0.0000000	5.4431484	4.6725465	2.6458788 *
22 H	5.4431484	0.0000000	2.5251592 *	4.3512056
23 H	4.6725465	2.5251592 *	0.0000000	2.5170331 *
24 H	2.6458788 *	4.3512056	2.5170331 *	0.0000000
25 H	6.0668892	2.3990585 *	4.7779320	5.9731019
26 H	6.4889060	4.7746584	6.8473124	7.3456388
27 H	5.2893137	5.9493791	7.3334967	6.9621080
28 H	4.8454074	7.1372327	8.0382257	7.0743253
29 H	6.2265083	11.0962792	10.8041194	8.7219552
30 H	8.0398931	12.4263869	12.5361178	10.6599090
31 H	8.1814787	11.6857475	12.2809358	10.7884455
32 H	6.5603424	9.3405797	10.1859299	9.0114486
33 H	4.1694979	9.1907924	8.6604065	6.5254071
34 H	1.0426529 *	5.8070069	5.1249906	3.1652248
35 H	1.0397486 *	5.8117064	4.5774585	2.2029235 *

H H H H

1 CO	6.5922282	6.3422692	4.5492451	3.8650281
2 C	2.6844405 *	4.6682602	5.3786425	6.3650427
3 C	4.0818518	5.9286290	6.2562548	6.9357060
4 C	4.8916640	6.2515404	6.0013508	6.3041201
5 C	4.6785547	5.4730199	4.8041044	4.9320678
6 C	3.5271806	4.0218796	3.5013705	4.0267105
7 C	2.2032029 *	3.4851308	3.9389887	4.9740102
8 C	1.1045396 *	2.1882309 *	3.4224086	4.8888738
9 C	2.1772981 *	1.1035189 *	2.1728793 *	3.8644436
10 C	3.4463967	2.1916828 *	1.1025578 *	2.5444306 *
11 C	3.9677713	3.4739680	2.1866921 *	2.6213911 *
12 N	5.4243390	4.6678368	2.6938538 *	2.0909550 *
13 C	6.2082434	4.9454499	2.5993611 *	1.1055266 *
14 C	7.6651515	6.3150668	3.8778457	2.1551274 *
15 C	8.5965682	7.4977489	5.1001485	3.5173758
16 C	9.9789506	8.7673253	6.3190154	4.6499649
17 C	10.5293099	9.0288356	6.5571882	4.8095532
18 C	9.8250084	8.1076309	5.6869433	3.9454131
19 C	8.4181660	6.7262220	4.3090031	2.5329272 *

20	O	8.2886843	7.6013152	5.3990728	4.1342107
21	N	6.0668892	6.4889060	5.2893137	4.8454074
22	H	2.3990585 *	4.7746584	5.9493791	7.1372327
23	H	4.7779320	6.8473124	7.3334967	8.0382257
24	H	5.9731019	7.3456388	6.9621080	7.0743253
25	H	0.0000000	2.5294668 *	4.3359554	5.9079429
26	H	2.5294668 *	0.0000000	2.4859106 *	4.3211653
27	H	4.3359554	2.4859106 *	0.0000000	2.0011627 *
28	H	5.9079429	4.3211653	2.0011627 *	0.0000000
29	H	10.7367502	9.6782800	7.2602188	5.6519179
30	H	11.6305876	10.0969391	7.6263212	5.8848317
31	H	10.4727725	8.5885944	6.2556648	4.5970719
32	H	8.0038027	6.1129754	3.8320907	2.2061145 *
33	H	9.1728568	8.5693347	6.3796572	5.1037211
34	H	6.3253462	6.6452349	5.4121386	4.7156714
35	H	6.7639063	7.4075606	6.2914472	5.8556116

H H H H

1	CO	4.6594664	6.4514825	6.6925571	5.2774213
2	C	10.0503919	11.4553306	10.8406082	8.5677908
3	C	9.8753868	11.5237306	11.2008279	9.0870425
4	C	8.6193087	10.3882310	10.2834517	8.3456082
5	C	7.4274018	9.0694840	8.8842129	6.9460402
6	C	7.6054911	8.9225314	8.3617254	6.1873275
7	C	9.0406935	10.2585426	9.4982655	7.1799699
8	C	9.6341735	10.5530354	9.4703116	7.0286701
9	C	8.9963941	9.6430578	8.3573120	5.8862931
10	C	7.5793180	8.2363530	7.0649263	4.6446896
11	C	6.7768407	7.8026793	7.0329864	4.7933870
12	N	5.3185056	6.4216029	5.9110693	3.9450296
13	C	4.7995951	5.4328454	4.6341615	2.6167190 *
14	C	3.5027532	3.9770728	3.4866291	2.1980274 *
15	C	2.1962437 *	3.4333272	3.9257884	3.4516430
16	C	1.1064651 *	2.1883683 *	3.4763768	3.9563631
17	C	2.2015815 *	1.1030011 *	2.1979693 *	3.4568217
18	C	3.4764710	2.1970619 *	1.1029622 *	2.1863665 *
19	C	3.9565503	3.4547786	2.1819845 *	1.1064227 *
20	O	2.6939636 *	4.6463260	5.3878714	4.6843698
21	N	6.2265083	8.0398931	8.1814787	6.5603424
22	H	11.0962792	12.4263869	11.6857475	9.3405797
23	H	10.8041194	12.5361178	12.2809358	10.1859299
24	H	8.7219552	10.6599090	10.7884455	9.0114486
25	H	10.7367502	11.6305876	10.4727725	8.0038027
26	H	9.6782800	10.0969391	8.5885944	6.1129754
27	H	7.2602188	7.6263212	6.2556648	3.8320907

28 H	5.6519179	5.8848317	4.5970719	2.2061145 *
29 H	0.0000000	2.5193156 *	4.3886566	5.0625210
30 H	2.5193156 *	0.0000000	2.5385532 *	4.3708526
31 H	4.3886566	2.5385532 *	0.0000000	2.5131080 *
32 H	5.0625210	4.3708526	2.5131080 *	0.0000000
33 H	2.3029479 *	4.6255250	5.8137535	5.4670126
34 H	6.1962319	7.8590705	7.9243894	6.3296241
35 H	6.5776706	8.5895521	8.9666232	7.4921736

H H H

1 CO	2.6631620 *	2.4957892 *	2.6166073 *
2 C	8.1157288	4.7380772	4.7302102
3 C	7.7891851	4.2785330	3.9085792
4 C	6.4920942	3.0164799	2.4768641 *
5 C	5.4100008	2.1036271 *	2.0860158 *
6 C	5.8246705	2.9822199 *	3.4249670
7 C	7.2755394	4.2373447	4.5615171
8 C	8.0898268	5.3814156	5.8932040
9 C	7.7196497	5.5964204	6.3125198
10 C	6.3910692	4.7588641	5.5691641
11 C	5.3124809	3.4123396	4.1670866
12 N	3.9537620	3.1104201	3.9164899
13 C	4.0296239	4.0240830	5.0261743
14 C	3.3278420	4.6910051	5.6135734
15 C	2.0421079 *	4.6796228	5.3238861
16 C	2.5032513 *	5.8654950	6.4557598
17 C	3.9247883	6.9022018	7.6789491
18 C	4.7286019	6.9430336	7.9165218
19 C	4.4885052	5.9548787	7.0032035
20 O	0.9920816 *	3.8254174	4.1115858
21 N	4.1694979	1.0426529 *	1.0397486 *
22 H	9.1907924	5.8070069	5.8117064
23 H	8.6604065	5.1249906	4.5774585
24 H	6.5254071	3.1652248	2.2029235 *
25 H	9.1728568	6.3253462	6.7639063
26 H	8.5693347	6.6452349	7.4075606
27 H	6.3796572	5.4121386	6.2914472
28 H	5.1037211	4.7156714	5.8556116
29 H	2.3029479 *	6.1962319	6.5776706
30 H	4.6255250	7.8590705	8.5895521
31 H	5.8137535	7.9243894	8.9666232
32 H	5.4670126	6.3296241	7.4921736
33 H	0.0000000	4.3542211	4.4088602
34 H	4.3542211	0.0000000	1.6591404 *
35 H	4.4088602	1.6591404 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.81 , TOTAL = 4490.4 SECONDS (74.8 MIN)
WALL CLOCK TIME: STEP = 0.82 , TOTAL = 4151.5 SECONDS (69.2 MIN)

CPU UTILIZATION: STEP = 99.14%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.93 , TOTAL = 4491.3 SECONDS (74.9 MIN)
WALL CLOCK TIME: STEP = 0.93 , TOTAL = 4152.4 SECONDS (69.2 MIN)

CPU UTILIZATION: STEP = 99.92%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.633921955	-284.633921955	0.038201966	0.001459074	196952655
11400855						
2	1	-284.634243427	-0.000321472	0.003332925	0.000148576	162694219
14342612						
3	2	-284.634245019	-0.000001591	0.002935521	0.000189475	146866270
15623426						
4	3	-284.634248347	-0.000003328	0.001103325	0.000082467	141044794
16063775						
5	4	-284.634248457	-0.000000110	0.000466747	0.000100591	135539067
16531332						
6	5	-284.634248828	-0.000000371	0.000359979	0.000051620	127365425
17120039						
7	6	-284.634248859	-0.000000031	0.000195633	0.000033532	127329524
17161267						
8	7	-284.634248965	-0.000000106	0.000235947	0.000029105	119994781
17686981						
9	8	-284.634248993	-0.000000028	0.000217951	0.000025172	143717273
15912309						
10	9	-284.634249039	-0.000000047	0.000342066	0.000019057	140934530
16198481						
11	10	-284.634249087	-0.000000048	0.000360143	0.000021260	163695925
14358603						

-----DISABLING FDIFF OPTION-----

12 11	-284.634249111	-0.000000024	0.000545175	0.000020323	196934583
11402579					
13 12	-284.634249158	-0.000000046	0.000477086	0.000019361	196934456
11402596					
14 13	-284.634249189	-0.000000031	0.000199288	0.000012508	196934196
11402603					
15 14	-284.634249201	-0.000000012	0.000105518	0.000008429	196934481
11402590					
16 15	-284.634249205	-0.000000004	0.000046293	0.000006352	196934461
11402593					
17 16	-284.634249207	-0.000000003	0.000052825	0.000005713	196934500
11402590					
18 17	-284.634249209	-0.000000002	0.000087391	0.000004571	196934444
11402592					
19 18	-284.634249211	-0.000000002	0.000095283	0.000004225	196934354
11402594					
20 19	-284.634249213	-0.000000002	0.000059063	0.000004988	196934412
11402588					
21 20	-284.634249215	-0.000000002	0.000115878	0.000004793	196934422
11402588					
22 21	-284.634249218	-0.000000003	0.000112226	0.000003049	196934421
11402589					
23 22	-284.634249219	-0.000000001	0.000018421	0.000003179	196934450
11402588					
24 23	-284.634249219	0.000000000	0.000017219	0.000001447	196934419
11402591					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 80.5 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 26.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.8, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.9 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6342492193 AFTER 24 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6088670267
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000312031

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 84.58 , TOTAL = 4575.9 SECONDS (76.3 MIN)
WALL CLOCK TIME: STEP = 77.65 , TOTAL = 4230.1 SECONDS (70.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.87 , TOTAL = 4579.8 SECONDS (76.3 MIN)
WALL CLOCK TIME: STEP = 3.86 , TOTAL = 4233.9 SECONDS (70.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.82 , TOTAL = 4582.6 SECONDS (76.4 MIN)
WALL CLOCK TIME: STEP = 2.65 , TOTAL = 4236.6 SECONDS (70.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 44 ENERGY= -284.6342492

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0002482	0.0000035	0.0004447
2 C	6.0	0.0006916	-0.0010532	-0.0001123
3 C	6.0	-0.0005093	0.0004006	0.0001319
4 C	6.0	-0.0004108	-0.0006232	-0.0001830
5 C	6.0	-0.0013087	0.0000098	0.0003059
6 C	6.0	-0.0000430	-0.0011810	-0.0003726
7 C	6.0	-0.0000024	-0.0002447	-0.0004224
8 C	6.0	0.0010814	0.0009267	-0.0006505
9 C	6.0	-0.0008765	0.0005328	-0.0005251
10 C	6.0	0.0013767	0.0016201	0.0002662

11	C	6.0	-0.0004209	0.0001458	0.0000603
12	N	7.0	0.0006716	-0.0003936	0.0004772
13	C	6.0	-0.0004661	-0.0001956	0.0009513
14	C	6.0	-0.0001662	-0.0001329	0.0008549
15	C	6.0	-0.0006862	0.0001875	-0.0005434
16	C	6.0	-0.0004948	-0.0012842	0.0000254
17	C	6.0	-0.0001405	0.0004056	0.0003282
18	C	6.0	0.0007851	0.0000342	0.0007198
19	C	6.0	-0.0001648	0.0004616	0.0006365
20	O	8.0	-0.0007025	0.0008766	-0.0004868
21	N	7.0	-0.0005683	-0.0003866	-0.0003112
22	H	1.0	-0.0004670	-0.0002890	-0.0003616
23	H	1.0	0.0005613	0.0004805	0.0001730
24	H	1.0	0.0002659	0.0013704	0.0006100
25	H	1.0	-0.0007910	0.0005813	0.0004167
26	H	1.0	-0.0006154	-0.0004681	-0.0003859
27	H	1.0	0.0001325	-0.0008000	-0.0000510
28	H	1.0	-0.0001894	-0.0004228	0.0006044
29	H	1.0	0.0000281	0.0000389	-0.0005214
30	H	1.0	0.0015150	0.0004542	-0.0004313
31	H	1.0	0.0009598	-0.0001310	0.0000607
32	H	1.0	0.0005482	0.0002961	-0.0011329
33	H	1.0	-0.0001155	-0.0006389	-0.0010438
34	H	1.0	0.0007815	-0.0008738	0.0012232
35	H	1.0	-0.0000113	0.0002924	-0.0007551

MAXIMUM GRADIENT = 0.0016201 RMS GRADIENT = 0.0006303
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001143707
 PREDICTED ENERGY CHANGE WAS -0.0000846034 RATIO= 1.352
 GDIIS STEP HAS LENGTH = 0.131361
 RADIUS OF STEP TAKEN= 0.12945 CURRENT TRUST RADIUS= 0.12945

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 0.02 , TOTAL = 4582.6 SECONDS (76.4 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4236.6 SECONDS (70.6
 MIN)
 CPU UTILIZATION: STEP = 91.92%, TOTAL = 100.00%

INSERCH= 45

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1304282031	-1.7650653007	0.9987719285

C	6.0	4.9857586242	0.6843580283	0.4542138057
C	6.0	5.2107716960	-0.6802728996	0.2368448019
C	6.0	4.0836468457	-1.5469869569	0.0633424667
C	6.0	2.7656920352	-1.0594435231	0.1436959015
C	6.0	2.4762135560	0.3328785188	0.4702488783
C	6.0	3.6479735928	1.2147045343	0.5789432360
C	6.0	3.4880840810	2.6301962370	0.8277452863
C	6.0	2.2176113303	3.1865084931	1.0298581252
C	6.0	1.0734454509	2.3338791818	1.0113207559
C	6.0	1.1702363939	0.9556342377	0.7070824955
N	7.0	-0.0405096059	0.1411779974	0.7286227701
C	6.0	-1.2422647252	0.6781502316	0.5157860495
C	6.0	-2.5543550759	0.0353210518	0.5634366673
C	6.0	-2.8629943317	-1.3492979891	0.7918515175
C	6.0	-4.1753418955	-1.8538505971	0.7983146140
C	6.0	-5.2554070554	-0.9440702768	0.5900773848
C	6.0	-5.0055795945	0.4376612660	0.3624677210
C	6.0	-3.6755938249	0.9145214781	0.3325865081
O	8.0	-1.7636954206	-2.2838037993	1.0274343123
N	7.0	1.6768961876	-2.0503098498	-0.2016340224
H	1.0	5.8367507916	1.3820836204	0.5389067592
H	1.0	6.2384554312	-1.0790419031	0.1679747974
H	1.0	4.2728026923	-2.6115773142	-0.1728010569
H	1.0	4.3871567737	3.2696776602	0.8858501676
H	1.0	2.0903913364	4.2614393756	1.2474567703
H	1.0	0.0989584140	2.7723454741	1.2850735146
H	1.0	-1.2883570753	1.7483766513	0.2427586878
H	1.0	-4.3793531425	-2.9304535492	0.9556801119
H	1.0	-6.2889978989	-1.3299474935	0.5931609892
H	1.0	-5.8422518381	1.1359176630	0.1912843891
H	1.0	-3.4768514151	1.9810426391	0.1143598175
H	1.0	-2.0990824046	-3.2074482374	1.1662993495
H	1.0	1.3437361327	-1.8799975110	-1.1759732108
H	1.0	2.0916227353	-3.0032021386	-0.2081552900

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4653867	5.2504474	4.0682335
2 C	5.4653867	0.0000000	1.4000349 *	2.4383368 *
3 C	5.2504474	1.4000349 *	0.0000000	1.4323780 *
4 C	4.0682335	2.4383368 *	1.4323780 *	0.0000000
5 C	2.8589635 *	2.8400635 *	2.4760577 *	1.4075369 *
6 C	3.1911462	2.5340899 *	2.9255361 *	2.5066529 *

7 C	4.6290831	1.4444700 *	2.4799816 *	2.8429905 *
8 C	5.5336631	2.4837152 *	3.7783623	4.2881075
9 C	5.3735819	3.7755480	4.9537741	5.1790173
10 C	4.2060415	4.2822287	5.1771029	5.0021093
11 C	2.9271983 *	3.8335027	4.3844317	3.8942874
12 N	1.9328641 *	5.0629751	5.3378444	4.5056814
13 C	2.8437411 *	6.2283308	6.6003637	5.7897560
14 C	3.2617433	7.5687841	7.8048658	6.8422849
15 C	3.0292337	8.1149664	8.1204264	6.9875339
16 C	4.3113481	9.5124482	9.4758462	8.2973034
17 C	5.4633584	10.3707142	10.4754599	9.3733071
18 C	5.6245412	9.9948045	10.2781025	9.3081868
19 C	4.7021051	8.6652637	9.0288442	8.1447733
20 O	1.9640813 *	7.3955187	7.1999677	5.9719163
21 N	1.9783584 *	4.3424780	3.8154346	2.4730538 *
22 H	6.5328508	1.1037126 *	2.1763285 *	3.4465910
23 H	6.2023261	2.1819169 *	1.1044880 *	2.2075146 *
24 H	4.3873035	3.4299626	2.1857567 *	1.1067503 *
25 H	6.5940220	2.6885892 *	4.0867663	4.8958038
26 H	6.3420863	4.6698926	5.9311576	6.2540395
27 H	4.5465432	5.3787392	6.2569955	6.0022497
28 H	3.8637782	6.3672111	6.9380868	6.3047631
29 H	4.6581235	10.0510522	9.8767673	8.6216365
30 H	6.4469279	11.4541201	11.5236166	10.3884346
31 H	6.6888448	10.8406111	11.2013371	10.2828892
32 H	5.2752228	8.5681188	9.0869356	8.3433045
33 H	2.6606863 *	8.1146900	7.7900236	6.4961363
34 H	2.4929585 *	4.7431800	4.2882815	3.0255429
35 H	2.6145631 *	4.7342217	3.9144751	2.4824250 *

C C C C

1 CO	2.8589635 *	3.1911462	4.6290831	5.5336631
2 C	2.8400635 *	2.5340899 *	1.4444700 *	2.4837152 *
3 C	2.4760577 *	2.9255361 *	2.4799816 *	3.7783623
4 C	1.4075369 *	2.5066529 *	2.8429905 *	4.2881075
5 C	0.0000000	1.4591077 *	2.4778237 *	3.8214154
6 C	1.4591077 *	0.0000000	1.4705282 *	2.5356172 *
7 C	2.4778237 *	1.4705282 *	0.0000000	1.4460580 *
8 C	3.8214154	2.5356172 *	1.4460580 *	0.0000000
9 C	4.3719314	2.9194591 *	2.4773517 *	1.4015827 *
10 C	3.8898728	2.5029025 *	2.8403692 *	2.4396687 *
11 C	2.6312395 *	1.4661143 *	2.4945378 *	2.8620160 *
12 N	3.1077965	2.5372035 *	3.8444468	4.3192604
13 C	4.3842218	3.7347513	4.9199909	5.1267926
14 C	5.4477145	5.0402227	6.3134829	6.5813606

15 C	5.6732911	5.6071639	7.0008672	7.4949223
16 C	7.0169481	7.0094651	8.4064511	8.8789436
17 C	8.0343387	7.8372772	9.1613656	9.4488361
18 C	7.9171868	7.4833031	8.6910667	8.7844189
19 C	6.7396128	6.1807761	7.3338558	7.3828858
20 O	4.7744531	5.0134130	6.4596336	7.1950302
21 N	1.5121327 *	2.6019073 *	3.8929123	5.1231983
22 H	3.9431774	3.5211867	2.1955328 *	2.6753407 *
23 H	3.4729036	4.0298080	3.4843599	4.6645779
24 H	2.1864748 *	3.5087129	3.9491725	5.3937989
25 H	4.6820114	3.5283449	2.2053340 *	1.1048278 *
26 H	5.4759578	4.0232451	3.4864833	2.1887569 *
27 H	4.8059149	3.5023250	3.9395906	3.4227954
28 H	4.9324418	4.0283221	4.9764632	4.8922597
29 H	7.4304554	7.6081387	9.0422475	9.6350279
30 H	9.0698733	8.9223892	10.2576244	10.5512606
31 H	8.8836126	8.3617916	9.4984665	9.4706451
32 H	6.9436853	6.1872518	7.1809639	7.0314042
33 H	5.4153183	5.8268116	7.2752371	8.0875918
34 H	2.1063699 *	2.9815051 *	4.2386817	5.3809817
35 H	2.0871910 *	3.4260147	4.5642621	5.8956231

C C C N

1 CO	5.3735819	4.2060415	2.9271983 *	1.9328641 *
2 C	3.7755480	4.2822287	3.8335027	5.0629751
3 C	4.9537741	5.1771029	4.3844317	5.3378444
4 C	5.1790173	5.0021093	3.8942874	4.5056814
5 C	4.3719314	3.8898728	2.6312395 *	3.1077965
6 C	2.9194591 *	2.5029025 *	1.4661143 *	2.5372035 *
7 C	2.4773517 *	2.8403692 *	2.4945378 *	3.8444468
8 C	1.4015827 *	2.4396687 *	2.8620160 *	4.3192604
9 C	0.0000000	1.4270375 *	2.4855539 *	3.8031422
10 C	1.4270375 *	0.0000000	1.4147397 *	2.4756317 *
11 C	2.4855539 *	1.4147397 *	0.0000000	1.4593522 *
12 N	3.8031422	2.4756317 *	1.4593522 *	0.0000000
13 C	4.3042855	2.8895513 *	2.4359297 *	1.3333619 *
14 C	5.7375251	4.3179748	3.8392958	2.5214899 *
15 C	6.8148912	5.3953238	4.6461649	3.1924813
16 C	8.1442423	6.7180519	6.0395973	4.5914958
17 C	8.5499177	7.1398020	6.7016014	5.3284251
18 C	7.7573229	6.4008748	6.2070733	4.9873732
19 C	6.3543670	5.0028622	4.8604535	3.7374780
20 O	6.7657317	5.4196517	4.3822985	2.9898486 *
21 N	5.4067747	4.5887390	3.1809071	2.9355544 *
22 H	4.0737149	4.8803860	4.6889763	6.0098277

23 H	5.9249431	6.2479269	5.4879312	6.4209551
24 H	6.2680140	6.0079590	4.8088576	5.1956607
25 H	2.1759097 *	3.4455978	3.9667785	5.4236943
26 H	1.1040881 *	2.1921285 *	3.4737641	4.6675991
27 H	2.1737884 *	1.1030948 *	2.1868127 *	2.6929781 *
28 H	3.8703441	2.5517860 *	2.6246369 *	2.0919548 *
29 H	8.9968143	7.5795321	6.7794855	5.3209058
30 H	9.6411348	8.2343218	7.8023739	6.4207606
31 H	8.3587991	7.0664305	7.0337430	5.9108758
32 H	5.8922144	4.6512616	4.7956447	3.9459937
33 H	7.7159020	6.3871168	5.3132458	3.9550702
34 H	5.5945360	4.7554252	3.4083439	3.1030264
35 H	6.3135622	5.5685046	4.1664131	3.9128849

C C C C

1 CO	2.8437411 *	3.2617433	3.0292337	4.3113481
2 C	6.2283308	7.5687841	8.1149664	9.5124482
3 C	6.6003637	7.8048658	8.1204264	9.4758462
4 C	5.7897560	6.8422849	6.9875339	8.2973034
5 C	4.3842218	5.4477145	5.6732911	7.0169481
6 C	3.7347513	5.0402227	5.6071639	7.0094651
7 C	4.9199909	6.3134829	7.0008672	8.4064511
8 C	5.1267926	6.5813606	7.4949223	8.8789436
9 C	4.3042855	5.7375251	6.8148912	8.1442423
10 C	2.8895513 *	4.3179748	5.3953238	6.7180519
11 C	2.4359297 *	3.8392958	4.6461649	6.0395973
12 N	1.3333619 *	2.5214899 *	3.1924813	4.5914958
13 C	0.0000000	1.4618759 *	2.6102726 *	3.8850730
14 C	1.4618759 *	0.0000000	1.4368721 *	2.5003471 *
15 C	2.6102726 *	1.4368721 *	0.0000000	1.4060125 *
16 C	3.8850730	2.5003471 *	1.4060125 *	0.0000000
17 C	4.3292528	2.8732558 *	2.4348636 *	1.4274466 *
18 C	3.7741066	2.4921412 *	2.8228116 *	2.4759410 *
19 C	2.4516370 *	1.4434201 *	2.4486978 *	2.8514093 *
20 O	3.0507123	2.4937475 *	1.4619365 *	2.4603647 *
21 N	4.0596412	4.7789828	4.6998976	5.9403017
22 H	7.1139664	8.4985310	9.1219511	10.5252346
23 H	7.6921955	8.8719621	9.1268093	10.4615884
24 H	6.4585159	7.3592255	7.3105063	8.5374681
25 H	6.2083289	7.6648288	8.5970031	9.9787067
26 H	4.9479187	6.3167736	7.4982651	8.7668645
27 H	2.6031397 *	3.8797081	5.0994487	6.3172991
28 H	1.1054651 *	2.1540995 *	3.5180355	4.6496629
29 H	4.8017551	3.5043247	2.1968698 *	1.1070042 *
30 H	5.4321229	3.9764807	3.4318148	2.1872595 *

31 H	4.6340839	3.4871300	3.9259334	3.4764621
32 H	2.6176419 *	2.1996595 *	3.4535466	3.9575358
33 H	4.0317713	3.3296050	2.0436475 *	2.5056921 *
34 H	4.0116792	4.6785796	4.6744580	5.8616310
35 H	5.0190888	5.6047379	5.3182368	6.4504912

C C C O

1 CO	5.4633584	5.6245412	4.7021051	1.9640813 *
2 C	10.3707142	9.9948045	8.6652637	7.3955187
3 C	10.4754599	10.2781025	9.0288442	7.1999677
4 C	9.3733071	9.3081868	8.1447733	5.9719163
5 C	8.0343387	7.9171868	6.7396128	4.7744531
6 C	7.8372772	7.4833031	6.1807761	5.0134130
7 C	9.1613656	8.6910667	7.3338558	6.4596336
8 C	9.4488361	8.7844189	7.3828858	7.1950302
9 C	8.5499177	7.7573229	6.3543670	6.7657317
10 C	7.1398020	6.4008748	5.0028622	5.4196517
11 C	6.7016014	6.2070733	4.8604535	4.3822985
12 N	5.3284251	4.9873732	3.7374780	2.9898486 *
13 C	4.3292528	3.7741066	2.4516370 *	3.0507123
14 C	2.8732558 *	2.4921412 *	1.4434201 *	2.4937475 *
15 C	2.4348636 *	2.8228116 *	2.4486978 *	1.4619365 *
16 C	1.4274466 *	2.4759410 *	2.8514093 *	2.4603647 *
17 C	0.0000000	1.4224633 *	2.4528503 *	3.7653973
18 C	1.4224633 *	0.0000000	1.4132058 *	4.2846663
19 C	2.4528503 *	1.4132058 *	0.0000000	3.7904424
20 O	3.7653973	4.2846663	3.7904424	0.0000000
21 N	7.0645171	7.1528801	6.1420490	3.6609833
22 H	11.3335597	10.8848148	9.5260633	8.4524655
23 H	11.5024025	11.3475345	10.1138403	8.1378462
24 H	9.7030585	9.7812446	8.7100974	6.1633846
25 H	10.5272119	9.8243444	8.4178862	8.2881955
26 H	9.0271940	8.1090868	6.7294451	7.5988554
27 H	6.5546926	5.6884321	4.3134657	5.3944882
28 H	4.8070143	3.9433550	2.5302733 *	4.1352317
29 H	2.2015572 *	3.4768172	3.9582011	2.6953608 *
30 H	1.1032773 *	2.1965479 *	3.4547678	4.6450832
31 H	2.1976743 *	1.1031256 *	2.1825191 *	5.3877884
32 H	3.4562773	2.1864568 *	1.1066114 *	4.6858856
33 H	3.9264866	4.7308239	4.4912247	0.9924147 *
34 H	6.8951857	6.9319660	5.9395927	3.8306912
35 H	7.6717694	7.9079348	6.9929784	4.1118966

N H H H

1 CO	1.9783584 *	6.5328508	6.2023261	4.3873035
2 C	4.3424780	1.1037126 *	2.1819169 *	3.4299626
3 C	3.8154346	2.1763285 *	1.1044880 *	2.1857567 *
4 C	2.4730538 *	3.4465910	2.2075146 *	1.1067503 *
5 C	1.5121327 *	3.9431774	3.4729036	2.1864748 *
6 C	2.6019073 *	3.5211867	4.0298080	3.5087129
7 C	3.8929123	2.1955328 *	3.4843599	3.9491725
8 C	5.1231983	2.6753407 *	4.6645779	5.3937989
9 C	5.4067747	4.0737149	5.9249431	6.2680140
10 C	4.5887390	4.8803860	6.2479269	6.0079590
11 C	3.1809071	4.6889763	5.4879312	4.8088576
12 N	2.9355544 *	6.0098277	6.4209551	5.1956607
13 C	4.0596412	7.1139664	7.6921955	6.4585159
14 C	4.7789828	8.4985310	8.8719621	7.3592255
15 C	4.6998976	9.1219511	9.1268093	7.3105063
16 C	5.9403017	10.5252346	10.4615884	8.5374681
17 C	7.0645171	11.3335597	11.5024025	9.7030585
18 C	7.1528801	10.8848148	11.3475345	9.7812446
19 C	6.1420490	9.5260633	10.1138403	8.7100974
20 O	3.6609833	8.4524655	8.1378462	6.1633846
21 N	0.0000000	5.4437226	4.6784394	2.6560465 *
22 H	5.4437226	0.0000000	2.5211299 *	4.3476188
23 H	4.6784394	2.5211299 *	0.0000000	2.5156676 *
24 H	2.6560465 *	4.3476188	2.5156676 *	0.0000000
25 H	6.0688056	2.4051411 *	4.7805872	5.9768704
26 H	6.4891464	4.7778595	6.8478068	7.3497218
27 H	5.2875506	5.9507860	7.3331111	6.9665629
28 H	4.8394453	7.1406608	8.0406962	7.0787277
29 H	6.2283372	11.0968670	10.8067601	8.7312629
30 H	8.0377913	12.4254512	12.5371777	10.6668132
31 H	8.1758191	11.6867678	12.2821039	10.7930813
32 H	6.5507839	9.3424931	10.1859795	9.0128663
33 H	4.1795006	9.1888450	8.6626383	6.5382851
34 H	1.0437139 *	5.8111244	5.1386772	3.1813510
35 H	1.0392518 *	5.8150509	4.5869476	2.2163407 *

H H H H

1 CO	6.5940220	6.3420863	4.5465432	3.8637782
2 C	2.6885892 *	4.6698926	5.3787392	6.3672111
3 C	4.0867663	5.9311576	6.2569955	6.9380868
4 C	4.8958038	6.2540395	6.0022497	6.3047631
5 C	4.6820114	5.4759578	4.8059149	4.9324418
6 C	3.5283449	4.0232451	3.5023250	4.0283221
7 C	2.2053340 *	3.4864833	3.9395906	4.9764632
8 C	1.1048278 *	2.1887569 *	3.4227954	4.8922597

9 C	2.1759097 *	1.1040881 *	2.1737884 *	3.8703441
10 C	3.4455978	2.1921285 *	1.1030948 *	2.5517860 *
11 C	3.9667785	3.4737641	2.1868127 *	2.6246369 *
12 N	5.4236943	4.6675991	2.6929781 *	2.0919548 *
13 C	6.2083289	4.9479187	2.6031397 *	1.1054651 *
14 C	7.6648288	6.3167736	3.8797081	2.1540995 *
15 C	8.5970031	7.4982651	5.0994487	3.5180355
16 C	9.9787067	8.7668645	6.3172991	4.6496629
17 C	10.5272119	9.0271940	6.5546926	4.8070143
18 C	9.8243444	8.1090868	5.6884321	3.9433550
19 C	8.4178862	6.7294451	4.3134657	2.5302733 *
20 O	8.2881955	7.5988554	5.3944882	4.1352317
21 N	6.0688056	6.4891464	5.2875506	4.8394453
22 H	2.4051411 *	4.7778595	5.9507860	7.1406608
23 H	4.7805872	6.8478068	7.3331111	8.0406962
24 H	5.9768704	7.3497218	6.9665629	7.0787277
25 H	0.0000000	2.5277425 *	4.3353620	5.9109543
26 H	2.5277425 *	0.0000000	2.4868898 *	4.3290696
27 H	4.3353620	2.4868898 *	0.0000000	2.0148391 *
28 H	5.9109543	4.3290696	2.0148391 *	0.0000000
29 H	10.7376999	9.6781223	7.2584910	5.6527839
30 H	11.6285208	10.0948439	7.6232235	5.8826244
31 H	10.4726383	8.5913453	6.2587738	4.5951837
32 H	8.0061478	6.1219531	3.8448858	2.2045696 *
33 H	9.1707748	8.5640270	6.3720816	5.1059185
34 H	6.3271383	6.6443776	5.4083748	4.7016820
35 H	6.7687034	7.4090367	6.2894669	5.8485116

H H H H

1 CO	4.6581235	6.4469279	6.6888448	5.2752228
2 C	10.0510522	11.4541201	10.8406111	8.5681188
3 C	9.8767673	11.5236166	11.2013371	9.0869356
4 C	8.6216365	10.3884346	10.2828892	8.3433045
5 C	7.4304554	9.0698733	8.8836126	6.9436853
6 C	7.6081387	8.9223892	8.3617916	6.1872518
7 C	9.0422475	10.2576244	9.4984665	7.1809639
8 C	9.6350279	10.5512606	9.4706451	7.0314042
9 C	8.9968143	9.6411348	8.3587991	5.8922144
10 C	7.5795321	8.2343218	7.0664305	4.6512616
11 C	6.7794855	7.8023739	7.0337430	4.7956447
12 N	5.3209058	6.4207606	5.9108758	3.9459937
13 C	4.8017551	5.4321229	4.6340839	2.6176419 *
14 C	3.5043247	3.9764807	3.4871300	2.1996595 *
15 C	2.1968698 *	3.4318148	3.9259334	3.4535466
16 C	1.1070042 *	2.1872595 *	3.4764621	3.9575358

17 C	2.2015572 *	1.1032773 *	2.1976743 *	3.4562773
18 C	3.4768172	2.1965479 *	1.1031256 *	2.1864568 *
19 C	3.9582011	3.4547678	2.1825191 *	1.1066114 *
20 O	2.6953608 *	4.6450832	5.3877884	4.6858856
21 N	6.2283372	8.0377913	8.1758191	6.5507839
22 H	11.0968670	12.4254512	11.6867678	9.3424931
23 H	10.8067601	12.5371777	12.2821039	10.1859795
24 H	8.7312629	10.6668132	10.7930813	9.0128663
25 H	10.7376999	11.6285208	10.4726383	8.0061478
26 H	9.6781223	10.0948439	8.5913453	6.1219531
27 H	7.2584910	7.6232235	6.2587738	3.8448858
28 H	5.6527839	5.8826244	4.5951837	2.2045696 *
29 H	0.0000000	2.5178925 *	4.3885930	5.0641015
30 H	2.5178925 *	0.0000000	2.5380264 *	4.3703632
31 H	4.3885930	2.5380264 *	0.0000000	2.5130206 *
32 H	5.0641015	4.3703632	2.5130206 *	0.0000000
33 H	2.3066688 *	4.6269740	5.8160811	5.4703987
34 H	6.1968665	7.8543631	7.9122412	6.3095685
35 H	6.5752060	8.5835127	8.9575795	7.4802818

H H H

1 CO	2.6606863 *	2.4929585 *	2.6145631 *
2 C	8.1146900	4.7431800	4.7342217
3 C	7.7900236	4.2882815	3.9144751
4 C	6.4961363	3.0255429	2.4824250 *
5 C	5.4153183	2.1063699 *	2.0871910 *
6 C	5.8268116	2.9815051 *	3.4260147
7 C	7.2752371	4.2386817	4.5642621
8 C	8.0875918	5.3809817	5.8956231
9 C	7.7159020	5.5945360	6.3135622
10 C	6.3871168	4.7554252	5.5685046
11 C	5.3132458	3.4083439	4.1664131
12 N	3.9550702	3.1030264	3.9128849
13 C	4.0317713	4.0116792	5.0190888
14 C	3.3296050	4.6785796	5.6047379
15 C	2.0436475 *	4.6744580	5.3182368
16 C	2.5056921 *	5.8616310	6.4504912
17 C	3.9264866	6.8951857	7.6717694
18 C	4.7308239	6.9319660	7.9079348
19 C	4.4912247	5.9395927	6.9929784
20 O	0.9924147 *	3.8306912	4.1118966
21 N	4.1795006	1.0437139 *	1.0392518 *
22 H	9.1888450	5.8111244	5.8150509
23 H	8.6626383	5.1386772	4.5869476
24 H	6.5382851	3.1813510	2.2163407 *

25 H	9.1707748	6.3271383	6.7687034
26 H	8.5640270	6.6443776	7.4090367
27 H	6.3720816	5.4083748	6.2894669
28 H	5.1059185	4.7016820	5.8485116
29 H	2.3066688 *	6.1968665	6.5752060
30 H	4.6269740	7.8543631	8.5835127
31 H	5.8160811	7.9122412	8.9575795
32 H	5.4703987	6.3095685	7.4802818
33 H	0.0000000	4.3705109	4.4150710
34 H	4.3705109	0.0000000	1.6606007 *
35 H	4.4150710	1.6606007 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.79 , TOTAL = 4583.4 SECONDS (76.4 MIN)
WALL CLOCK TIME: STEP = 0.79 , TOTAL = 4237.4 SECONDS (70.6 MIN)
CPU UTILIZATION: STEP = 99.69%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.91 , TOTAL = 4584.3 SECONDS (76.4 MIN)
WALL CLOCK TIME: STEP = 0.90 , TOTAL = 4238.3 SECONDS (70.6 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.634007589	-284.634007589	0.038108183	0.001527467	196947136
11402425						
2	1	-284.634335172	-0.000327583	0.004263954	0.000160980	162583220
14347200						
3	2	-284.634337523	-0.000002351	0.001903119	0.000199630	145690242
15743767						
4	3	-284.634339626	-0.000002102	0.001276955	0.000105143	139891393
16169357						
5	4	-284.634340009	-0.000000384	0.000897132	0.000080945	136506181
16471857						

6 5	-284.634340207	-0.000000198	0.000512824	0.000049313	129543340
16953262					
7 6	-284.634340329	-0.000000121	0.000218653	0.000020934	127726311
17141364					
8 7	-284.634340368	-0.000000040	0.000263550	0.000032636	120943746
17627896					
9 8	-284.634340407	-0.000000039	0.000161238	0.000020940	142488931
16025610					
10 9	-284.634340416	-0.000000009	0.000110813	0.000012334	140696740
16140961					
11 10	-284.634340436	-0.000000020	0.000145845	0.000013840	137798604
16388573					
12 11	-284.634340446	-0.000000010	0.000165833	0.000013778	156520728
14925753					
-----DISABLING FDIFF OPTION-----					
13 12	-284.634340446	0.000000001	0.000285179	0.000013014	196927161
11404196					
14 13	-284.634340459	-0.000000014	0.000251502	0.000012185	196927267
11404199					
15 14	-284.634340471	-0.000000012	0.000131844	0.000011512	196927246
11404201					
16 15	-284.634340477	-0.000000005	0.000074619	0.000007047	196927275
11404200					
17 16	-284.634340479	-0.000000002	0.000041086	0.000004894	196927333
11404196					
18 17	-284.634340480	-0.000000001	0.000047944	0.000003385	196927442
11404194					
19 18	-284.634340481	-0.000000001	0.000063315	0.000002919	196927390
11404199					
20 19	-284.634340482	-0.000000001	0.000043632	0.000002407	196927345
11404199					
21 20	-284.634340482	0.000000000	0.000025488	0.000002461	196927381
11404199					
22 21	-284.634340483	0.000000000	0.000059630	0.000001637	196927384
11404197					
23 22	-284.634340483	-0.000000001	0.000037649	0.000002624	196927427
11404196					
24 23	-284.634340483	0.000000000	0.000020827	0.000002967	196927429
11404198					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 81.0 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 25.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4

TIME TO SOLVE SCF EQUATIONS= 2.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6343404834 AFTER 24 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6063777375
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000302890

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 84.84 , TOTAL = 4669.1 SECONDS (77.8 MIN)
WALL CLOCK TIME: STEP = 77.68 , TOTAL = 4316.0 SECONDS (71.9
MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.73 , TOTAL = 4672.9 SECONDS (77.9 MIN)
WALL CLOCK TIME: STEP = 3.71 , TOTAL = 4319.7 SECONDS (72.0
MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.99 , TOTAL = 4675.9 SECONDS (77.9 MIN)
WALL CLOCK TIME: STEP = 2.79 , TOTAL = 4322.5 SECONDS (72.0
MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 45 ENERGY= -284.6343405

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0007821	-0.0000430	0.0002422
2 C	6.0	0.0006008	-0.0004485	0.0002044
3 C	6.0	0.0002248	-0.0008948	0.0001765
4 C	6.0	-0.0011748	0.0001655	-0.0000065
5 C	6.0	-0.0005923	-0.0007408	0.0000075
6 C	6.0	-0.0001036	-0.0007094	-0.0003334
7 C	6.0	-0.0001552	-0.0005056	-0.0004425
8 C	6.0	0.0007344	0.0010284	-0.0007990
9 C	6.0	-0.0006099	0.0003028	-0.0007531
10 C	6.0	0.0016024	0.0012098	0.0001511
11 C	6.0	-0.0000748	0.0009944	0.0001167
12 N	7.0	0.0006145	-0.0005011	0.0005426
13 C	6.0	-0.0006045	-0.0001714	0.0010611
14 C	6.0	0.0005076	0.0001041	0.0009128
15 C	6.0	-0.0010442	-0.0006013	-0.0008089
16 C	6.0	-0.0006527	-0.0008210	-0.0002372
17 C	6.0	0.0008230	0.0007329	0.0004449
18 C	6.0	0.0004422	-0.0004167	0.0010643
19 C	6.0	0.0000062	0.0009357	0.0007282
20 O	8.0	-0.0006844	0.0012916	-0.0004740
21 N	7.0	-0.0004534	-0.0007860	0.0002923
22 H	1.0	-0.0006393	-0.0006366	-0.0005937
23 H	1.0	0.0006619	0.0008019	0.0002764
24 H	1.0	0.0010144	0.0010234	0.0004130
25 H	1.0	-0.0008177	0.0009134	0.0004980
26 H	1.0	-0.0006965	-0.0001239	-0.0001352
27 H	1.0	-0.0000560	-0.0006300	0.0001894
28 H	1.0	-0.0004747	-0.0005904	0.0005542
29 H	1.0	-0.0000882	-0.0003469	-0.0005570
30 H	1.0	0.0013747	0.0003380	-0.0003506
31 H	1.0	0.0008761	-0.0000602	-0.0000100
32 H	1.0	0.0004281	0.0003586	-0.0015115
33 H	1.0	-0.0000323	-0.0009784	-0.0008455
34 H	1.0	0.0001759	-0.0007500	0.0005625
35 H	1.0	-0.0003506	0.0005554	-0.0005798

MAXIMUM GRADIENT = 0.0016024 RMS GRADIENT = 0.0006600
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000912641
 PREDICTED ENERGY CHANGE WAS -0.0000314031 RATIO= 2.906
 GDIIS STEP HAS LENGTH = 0.142736
 RADIUS OF STEP TAKEN= 0.12945 CURRENT TRUST RADIUS= 0.12945

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 4675.9 SECONDS (77.9 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4322.5 SECONDS (72.0 MIN)
CPU UTILIZATION: STEP = 92.42%, TOTAL = 100.00%

INSERCH= 46

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1290866579	-1.7638930060	0.9899634380
C	6.0	4.9862314656	0.6825512445	0.4582187092
C	6.0	5.2113613598	-0.6814840386	0.2416448174
C	6.0	4.0856973899	-1.5488030574	0.0590529576
C	6.0	2.7664901672	-1.0582706773	0.1354138520
C	6.0	2.4772582166	0.3335513340	0.4657664836
C	6.0	3.6485805057	1.2152678408	0.5792794993
C	6.0	3.4880692119	2.6295964990	0.8310426008
C	6.0	2.2177489470	3.1860980373	1.0378398032
C	6.0	1.0730513329	2.3332763344	1.0167203925
C	6.0	1.1709179354	0.9560483043	0.7042020745
N	7.0	-0.0399180535	0.1432519159	0.7222066405
C	6.0	-1.2415427230	0.6785821505	0.5054458784
C	6.0	-2.5534209622	0.0336119014	0.5544638924
C	6.0	-2.8609342739	-1.3495867643	0.7925873571
C	6.0	-4.1739550933	-1.8539004990	0.8030031533
C	6.0	-5.2559666714	-0.9447539755	0.5959588116
C	6.0	-5.0060428984	0.4366405805	0.3588225517
C	6.0	-3.6751942843	0.9108773467	0.3191330592
O	8.0	-1.7624876277	-2.2826181242	1.0388706614
N	7.0	1.6737575446	-2.0447243604	-0.2133194819
H	1.0	5.8384637307	1.3788927426	0.5444820632
H	1.0	6.2403354264	-1.0804443849	0.1777098523
H	1.0	4.2782310485	-2.6115893814	-0.1819778501
H	1.0	4.3867109666	3.2701554884	0.8897493966
H	1.0	2.0925024088	4.2595686211	1.2630195960
H	1.0	0.0998781527	2.7702134399	1.2971522452
H	1.0	-1.2899922767	1.7480764912	0.2291251380
H	1.0	-4.3793874822	-2.9295105600	0.9641343140
H	1.0	-6.2888581987	-1.3295644879	0.6084088778
H	1.0	-5.8440326342	1.1331221297	0.1876268915
H	1.0	-3.4781930482	1.9755590451	0.0900910561
H	1.0	-2.0974925098	-3.2027939605	1.2014205700
H	1.0	1.3352027406	-1.8704791648	-1.1840008986
H	1.0	2.0838405284	-3.0014200052	-0.2203714035

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4644028	5.2498672	4.0703349
2 C	5.4644028	0.0000000	1.3993498 *	2.4391058 *
3 C	5.2498672	1.3993498 *	0.0000000	1.4327252 *
4 C	4.0703349	2.4391058 *	1.4327252 *	0.0000000
5 C	2.8607788 *	2.8393512 *	2.4760146 *	1.4095250 *
6 C	3.1918592	2.5331413 *	2.9250380 *	2.5091334 *
7 C	4.6293517	1.4449058 *	2.4807154 *	2.8463652 *
8 C	5.5327000	2.4848487 *	3.7789390	4.2909382
9 C	5.3728218	3.7773274	4.9551824	5.1832947
10 C	4.2045906	4.2836662	5.1783329	5.0063663
11 C	2.9266282 *	3.8330048	4.3841367	3.8969779
12 N	1.9332506 *	5.0618882	5.3373275	4.5081621
13 C	2.8423700 *	6.2279545	6.5999502	5.7913728
14 C	3.2583018	7.5681401	7.8039133	6.8430521
15 C	3.0250342	8.1129155	8.1186117	6.9880935
16 C	4.3080418	9.5111241	9.4749063	8.2986990
17 C	5.4612295	10.3715822	10.4766314	9.3765575
18 C	5.6222987	9.9957940	10.2790701	9.3108318
19 C	4.6986129	8.6655510	9.0284268	8.1454962
20 O	1.9620196 *	7.3942272	7.1995673	5.9749306
21 N	1.9780708 *	4.3429805	3.8183841	2.4774137 *
22 H	6.5324224	1.1039170 *	2.1748840 *	3.4466265
23 H	6.2027590	2.1816543 *	1.1054613 *	2.2081450 *
24 H	4.3940226	3.4296470	2.1852906 *	1.1066525 *
25 H	6.5938647	2.6909737 *	4.0884646	4.8992884
26 H	6.3412657	4.6708057	5.9316515	6.2577587
27 H	4.5445945	5.3794602	6.2574413	6.0061259
28 H	3.8634945	6.3701501	6.9404986	6.3084371
29 H	4.6567876	10.0507591	9.8771493	8.6245688
30 H	6.4439306	11.4542051	11.5243036	10.3914032
31 H	6.6868972	10.8430095	11.2034570	10.2863401
32 H	5.2731147	8.5705233	9.0879702	8.3447307
33 H	2.6594745 *	8.1134088	7.7908612	6.5017326
34 H	2.4884127 *	4.7481428	4.2977646	3.0354372
35 H	2.6110240 *	4.7387764	3.9213452	2.4890972 *
	C	C	C	C
1 CO	2.8607788 *	3.1918592	4.6293517	5.5327000
2 C	2.8393512 *	2.5331413 *	1.4449058 *	2.4848487 *

3 C	2.4760146 *	2.9250380 *	2.4807154 *	3.7789390
4 C	1.4095250 *	2.5091334 *	2.8463652 *	4.2909382
5 C	0.0000000	1.4594370 *	2.4787250 *	3.8216410
6 C	1.4594370 *	0.0000000	1.4704779 *	2.5351507 *
7 C	2.4787250 *	1.4704779 *	0.0000000	1.4455013 *
8 C	3.8216410	2.5351507 *	1.4455013 *	0.0000000
9 C	4.3738033	2.9208964 *	2.4782510 *	1.4022028 *
10 C	3.8919182	2.5048448 *	2.8415925 *	2.4402035 *
11 C	2.6318913 *	1.4665875 *	2.4943160 *	2.8611260 *
12 N	3.1086829	2.5373513 *	3.8437830	4.3174586
13 C	4.3838236	3.7349834	4.9200394	5.1265680
14 C	5.4469501	5.0403932	6.3136161	6.5814311
15 C	5.6731515	5.6067874	6.9998401	7.4930116
16 C	7.0177263	7.0098012	8.4060639	8.8774517
17 C	8.0364670	7.8392462	9.1628016	9.4493073
18 C	7.9181400	7.4847752	8.6923741	8.7853280
19 C	6.7384416	6.1812198	7.3347125	7.3843341
20 O	4.7777506	5.0148017	6.4595734	7.1931490
21 N	1.5128683 *	2.6005704 *	3.8930307	5.1216886
22 H	3.9426037	3.5208859	2.1962633 *	2.6778221 *
23 H	3.4741735	4.0302743	3.4855052	4.6654278
24 H	2.1906385 *	3.5123966	3.9523169	5.3963502
25 H	4.6828849	3.5283729	2.2054005 *	1.1051332 *
26 H	5.4776974	4.0245821	3.4866383	2.1888399 *
27 H	4.8080918	3.5043488	3.9403662	3.4229914
28 H	4.9334994	4.0310119	4.9795576	4.8958405
29 H	7.4331611	7.6098314	9.0429846	9.6342233
30 H	9.0717506	8.9236258	10.2581533	10.5504896
31 H	8.8851579	8.3642427	9.5010444	9.4732014
32 H	6.9427837	6.1890808	7.1838882	7.0360205
33 H	5.4215937	5.8288309	7.2748666	8.0840867
34 H	2.1092941 *	2.9805660 *	4.2406024	5.3801408
35 H	2.0900773 *	3.4274767	4.5681844	5.8979383

C C C N

1 CO	5.3728218	4.2045906	2.9266282 *	1.9332506 *
2 C	3.7773274	4.2836662	3.8330048	5.0618882
3 C	4.9551824	5.1783329	4.3841367	5.3373275
4 C	5.1832947	5.0063663	3.8969779	4.5081621
5 C	4.3738033	3.8919182	2.6318913 *	3.1086829
6 C	2.9208964 *	2.5048448 *	1.4665875 *	2.5373513 *
7 C	2.4782510 *	2.8415925 *	2.4943160 *	3.8437830
8 C	1.4022028 *	2.4402035 *	2.8611260 *	4.3174586
9 C	0.0000000	1.4276146 *	2.4860191 *	3.8020517
10 C	1.4276146 *	0.0000000	1.4156280 *	2.4741961 *

11 C	2.4860191 *	1.4156280 *	0.0000000	1.4584533 *
12 N	3.8020517	2.4741961 *	1.4584533 *	0.0000000
13 C	4.3055520	2.8908061 *	2.4364847 *	1.3332162 *
14 C	5.7389793	4.3189627	3.8397930	2.5214788 *
15 C	6.8136340	5.3935108	4.6453845	3.1924369
16 C	8.1431329	6.7163384	6.0393080	4.5918850
17 C	8.5507674	7.1399574	6.7029554	5.3298085
18 C	7.7591075	6.4019875	6.2083747	4.9880378
19 C	6.3576685	5.0055652	4.8615967	3.7372383
20 O	6.7638111	5.4173105	4.3824458	2.9920507 *
21 N	5.4058144	4.5870182	3.1779443	2.9324279 *
22 H	4.0766369	4.8829307	4.6893807	6.0094731
23 H	5.9265850	6.2496602	5.4884871	6.4214868
24 H	6.2726965	6.0134642	4.8133926	5.2012606
25 H	2.1756362 *	3.4458967	3.9662129	5.4222358
26 H	1.1039618 *	2.1932956 *	3.4748873	4.6673075
27 H	2.1738398 *	1.1030059 *	2.1885866 *	2.6927741 *
28 H	3.8763609	2.5586599 *	2.6285140 *	2.0931500 *
29 H	8.9960163	7.5781779	6.7801934	5.3227242
30 H	9.6404348	8.2329116	7.8026574	6.4211674
31 H	8.3624096	7.0692161	7.0361734	5.9121371
32 H	5.8997786	4.6583719	4.7990382	3.9469804
33 H	7.7114207	6.3823614	5.3127867	3.9571810
34 H	5.5932492	4.7522056	3.4031687	3.0951086
35 H	6.3155686	5.5687589	4.1653114	3.9099572

C C C C

1 CO	2.8423700 *	3.2583018	3.0250342	4.3080418
2 C	6.2279545	7.5681401	8.1129155	9.5111241
3 C	6.5999502	7.8039133	8.1186117	9.4749063
4 C	5.7913728	6.8430521	6.9880935	8.2986990
5 C	4.3838236	5.4469501	5.6731515	7.0177263
6 C	3.7349834	5.0403932	5.6067874	7.0098012
7 C	4.9200394	6.3136161	6.9998401	8.4060639
8 C	5.1265680	6.5814311	7.4930116	8.8774517
9 C	4.3055520	5.7389793	6.8136340	8.1431329
10 C	2.8908061 *	4.3189627	5.3935108	6.7163384
11 C	2.4364847 *	3.8397930	4.6453845	6.0393080
12 N	1.3332162 *	2.5214788 *	3.1924369	4.5918850
13 C	0.0000000	1.4626735 *	2.6111967 *	3.8860071
14 C	1.4626735 *	0.0000000	1.4368388 *	2.5001211 *
15 C	2.6111967 *	1.4368388 *	0.0000000	1.4065790 *
16 C	3.8860071	2.5001211 *	1.4065790 *	0.0000000
17 C	4.3311676	2.8744869 *	2.4369515 *	1.4283430 *
18 C	3.7751153	2.4932032 *	2.8249338 *	2.4771445 *

19	C	2.4518021 *	1.4433817 *	2.4488520 *	2.8507699 *
20	O	3.0536261	2.4950244 *	1.4621176 *	2.4606112 *
21	N	4.0536400	4.7726315	4.6966472	5.9384399
22	H	7.1146644	8.4990358	9.1206185	10.5245578
23	H	7.6928594	8.8720469	9.1259861	10.4616764
24	H	6.4626374	7.3628055	7.3150605	8.5430516
25	H	6.2081544	7.6650546	8.5953371	9.9773984
26	H	4.9510846	6.3202346	7.4980308	8.7666761
27	H	2.6078977 *	3.8833710	5.0984066	6.3160323
28	H	1.1056757 *	2.1544109 *	3.5186455	4.6498189
29	H	4.8036234	3.5045796	2.1980190 *	1.1068436 *
30	H	5.4331066	3.9767639	3.4329266	2.1876038 *
31	H	4.6357878	3.4887845	3.9279379	3.4770895
32	H	2.6186396 *	2.2004555 *	3.4541430	3.9569040
33	H	4.0351098	3.3317783	2.0455720 *	2.5079766 *
34	H	3.9989450	4.6657493	4.6675257	5.8565587
35	H	5.0127238	5.5960685	5.3108791	6.4439198

C C C O

1	CO	5.4612295	5.6222987	4.6986129	1.9620196 *
2	C	10.3715822	9.9957940	8.6655510	7.3942272
3	C	10.4766314	10.2790701	9.0284268	7.1995673
4	C	9.3765575	9.3108318	8.1454962	5.9749306
5	C	8.0364670	7.9181400	6.7384416	4.7777506
6	C	7.8392462	7.4847752	6.1812198	5.0148017
7	C	9.1628016	8.6923741	7.3347125	6.4595734
8	C	9.4493073	8.7853280	7.3843341	7.1931490
9	C	8.5507674	7.7591075	6.3576685	6.7638111
10	C	7.1399574	6.4019875	5.0055652	5.4173105
11	C	6.7029554	6.2083747	4.8615967	4.3824458
12	N	5.3298085	4.9880378	3.7372383	2.9920507 *
13	C	4.3311676	3.7751153	2.4518021 *	3.0536261
14	C	2.8744869 *	2.4932032 *	1.4433817 *	2.4950244 *
15	C	2.4369515 *	2.8249338 *	2.4488520 *	1.4621176 *
16	C	1.4283430 *	2.4771445 *	2.8507699 *	2.4606112 *
17	C	0.0000000	1.4237087 *	2.4533327 *	3.7670210
18	C	1.4237087 *	0.0000000	1.4133767 *	4.2868968
19	C	2.4533327 *	1.4133767 *	0.0000000	3.7914222
20	O	3.7670210	4.2868968	3.7914222	0.0000000
21	N	7.0629982	7.1487238	6.1343600	3.6650177
22	H	11.3352711	10.8869478	9.5278282	8.4513634
23	H	11.5047080	11.3496861	10.1144991	8.1383043
24	H	9.7100181	9.7868235	8.7129707	6.1716266
25	H	10.5277256	9.8251980	8.4193891	8.2866263
26	H	9.0293932	8.1130572	6.7357984	7.5968018

27 H	6.5557401	5.6917884	4.3202806	5.3913099
28 H	4.8077912	3.9428058	2.5294649 *	4.1382894
29 H	2.2007278 *	3.4770782	3.9573342	2.6967054 *
30 H	1.1023153 *	2.1971319 *	3.4546344	4.6456043
31 H	2.1977547 *	1.1030056 *	2.1841581 *	5.3898893
32 H	3.4560974	2.1851343 *	1.1067144 *	4.6878461
33 H	3.9295404	4.7344610	4.4933135	0.9926602 *
34 H	6.8897560	6.9220302	5.9244775	3.8349318
35 H	7.6660968	7.9007704	6.9830951	4.1105483

N H H H

1 CO	1.9780708 *	6.5324224	6.2027590	4.3940226
2 C	4.3429805	1.1039170 *	2.1816543 *	3.4296470
3 C	3.8183841	2.1748840 *	1.1054613 *	2.1852906 *
4 C	2.4774137 *	3.4466265	2.2081450 *	1.1066525 *
5 C	1.5128683 *	3.9426037	3.4741735	2.1906385 *
6 C	2.6005704 *	3.5208859	4.0302743	3.5123966
7 C	3.8930307	2.1962633 *	3.4855052	3.9523169
8 C	5.1216886	2.6778221 *	4.6654278	5.3963502
9 C	5.4058144	4.0766369	5.9265850	6.2726965
10 C	4.5870182	4.8829307	6.2496602	6.0134642
11 C	3.1779443	4.6893807	5.4884871	4.8133926
12 N	2.9324279 *	6.0094731	6.4214868	5.2012606
13 C	4.0536400	7.1146644	7.6928594	6.4626374
14 C	4.7726315	8.4990358	8.8720469	7.3628055
15 C	4.6966472	9.1206185	9.1259861	7.3150605
16 C	5.9384399	10.5245578	10.4616764	8.5430516
17 C	7.0629982	11.3352711	11.5047080	9.7100181
18 C	7.1487238	10.8869478	11.3496861	9.7868235
19 C	6.1343600	9.5278282	10.1144991	8.7129707
20 O	3.6650177	8.4513634	8.1383043	6.1716266
21 N	0.0000000	5.4442809	4.6836282	2.6656332 *
22 H	5.4442809	0.0000000	2.5188017 *	4.3458046
23 H	4.6836282	2.5188017 *	0.0000000	2.5146836 *
24 H	2.6656332 *	4.3458046	2.5146836 *	0.0000000
25 H	6.0683462	2.4090808 *	4.7823261	5.9795727
26 H	6.4883769	4.7798343	6.8482228	7.3537908
27 H	5.2860427	5.9526171	7.3338893	6.9721059
28 H	4.8337262	7.1449725	8.0441910	7.0838410
29 H	6.2297519	11.0969784	10.8081462	8.7389362
30 H	8.0367867	12.4262530	12.5390692	10.6738781
31 H	8.1716972	11.6905291	12.2854355	10.7990599
32 H	6.5419669	9.3467949	10.1880631	9.0154349
33 H	4.1910549	9.1871009	8.6643942	6.5508141
34 H	1.0426903 *	5.8159634	5.1515762	3.1960460

35 H 1.0409055 * 5.8197368 4.5962012 2.2290787 *

H H H H

1 CO	6.5938647	6.3412657	4.5445945	3.8634945
2 C	2.6909737 *	4.6708057	5.3794602	6.3701501
3 C	4.0884646	5.9316515	6.2574413	6.9404986
4 C	4.8992884	6.2577587	6.0061259	6.3084371
5 C	4.6828849	5.4776974	4.8080918	4.9334994
6 C	3.5283729	4.0245821	3.5043488	4.0310119
7 C	2.2054005 *	3.4866383	3.9403662	4.9795576
8 C	1.1051332 *	2.1888399 *	3.4229914	4.8958405
9 C	2.1756362 *	1.1039618 *	2.1738398 *	3.8763609
10 C	3.4458967	2.1932956 *	1.1030059 *	2.5586599 *
11 C	3.9662129	3.4748873	2.1885866 *	2.6285140 *
12 N	5.4222358	4.6673075	2.6927741 *	2.0931500 *
13 C	6.2081544	4.9510846	2.6078977 *	1.1056757 *
14 C	7.6650546	6.3202346	3.8833710	2.1544109 *
15 C	8.5953371	7.4980308	5.0984066	3.5186455
16 C	9.9773984	8.7666761	6.3160323	4.6498189
17 C	10.5277256	9.0293932	6.5557401	4.8077912
18 C	9.8251980	8.1130572	5.6917884	3.9428058
19 C	8.4193891	6.7357984	4.3202806	2.5294649 *
20 O	8.2866263	7.5968018	5.3913099	4.1382894
21 N	6.0683462	6.4883769	5.2860427	4.8337262
22 H	2.4090808 *	4.7798343	5.9526171	7.1449725
23 H	4.7823261	6.8482228	7.3338893	8.0441910
24 H	5.9795727	7.3537908	6.9721059	7.0838410
25 H	0.0000000	2.5261951 *	4.3350726	5.9142293
26 H	2.5261951 *	0.0000000	2.4879500 *	4.3379489
27 H	4.3350726	2.4879500 *	0.0000000	2.0290849 *
28 H	5.9142293	4.3379489	2.0290849 *	0.0000000
29 H	10.7371260	9.6776831	7.2568296	5.6537087
30 H	11.6277407	10.0952528	7.6222371	5.8825497
31 H	10.4751135	8.5976581	6.2642789	4.5955603
32 H	8.0107521	6.1339310	3.8588944	2.2043823 *
33 H	9.1673938	8.5584290	6.3650939	5.1096510
34 H	6.3275799	6.6437112	5.4053839	4.6885519
35 H	6.7726095	7.4109702	6.2889377	5.8431594

H H H H

1 CO	4.6567876	6.4439306	6.6868972	5.2731147
2 C	10.0507591	11.4542051	10.8430095	8.5705233
3 C	9.8771493	11.5243036	11.2034570	9.0879702
4 C	8.6245688	10.3914032	10.2863401	8.3447307

5 C	7.4331611	9.0717506	8.8851579	6.9427837
6 C	7.6098314	8.9236258	8.3642427	6.1890808
7 C	9.0429846	10.2581533	9.5010444	7.1838882
8 C	9.6342233	10.5504896	9.4732014	7.0360205
9 C	8.9960163	9.6404348	8.3624096	5.8997786
10 C	7.5781779	8.2329116	7.0692161	4.6583719
11 C	6.7801934	7.8026574	7.0361734	4.7990382
12 N	5.3227242	6.4211674	5.9121371	3.9469804
13 C	4.8036234	5.4331066	4.6357878	2.6186396 *
14 C	3.5045796	3.9767639	3.4887845	2.2004555 *
15 C	2.1980190 *	3.4329266	3.9279379	3.4541430
16 C	1.1068436 *	2.1876038 *	3.4770895	3.9569040
17 C	2.2007278 *	1.1023153 *	2.1977547 *	3.4560974
18 C	3.4770782	2.1971319 *	1.1030056 *	2.1851343 *
19 C	3.9573342	3.4546344	2.1841581 *	1.1067144 *
20 O	2.6967054 *	4.6456043	5.3898893	4.6878461
21 N	6.2297519	8.0367867	8.1716972	6.5419669
22 H	11.0969784	12.4262530	11.6905291	9.3467949
23 H	10.8081462	12.5390692	12.2854355	10.1880631
24 H	8.7389362	10.6738781	10.7990599	9.0154349
25 H	10.7371260	11.6277407	10.4751135	8.0107521
26 H	9.6776831	10.0952528	8.5976581	6.1339310
27 H	7.2568296	7.6222371	6.2642789	3.8588944
28 H	5.6537087	5.8825497	4.5955603	2.2043823 *
29 H	0.0000000	2.5164353 *	4.3878393	5.0631819
30 H	2.5164353 *	0.0000000	2.5376668 *	4.3694775
31 H	4.3878393	2.5376668 *	0.0000000	2.5132469 *
32 H	5.0631819	4.3694775	2.5132469 *	0.0000000
33 H	2.3104184 *	4.6290601	5.8193220	5.4732739
34 H	6.1961741	7.8505813	7.9021772	6.2915896
35 H	6.5712663	8.5781153	8.9505349	7.4701355

H H H

1 CO	2.6594745 *	2.4884127 *	2.6110240 *
2 C	8.1134088	4.7481428	4.7387764
3 C	7.7908612	4.2977646	3.9213452
4 C	6.5017326	3.0354372	2.4890972 *
5 C	5.4215937	2.1092941 *	2.0900773 *
6 C	5.8288309	2.9805660 *	3.4274767
7 C	7.2748666	4.2406024	4.5681844
8 C	8.0840867	5.3801408	5.8979383
9 C	7.7114207	5.5932492	6.3155686
10 C	6.3823614	4.7522056	5.5687589
11 C	5.3127867	3.4031687	4.1653114
12 N	3.9571810	3.0951086	3.9099572

13 C	4.0351098	3.9989450	5.0127238
14 C	3.3317783	4.6657493	5.5960685
15 C	2.0455720 *	4.6675257	5.3108791
16 C	2.5079766 *	5.8565587	6.4439198
17 C	3.9295404	6.8897560	7.6660968
18 C	4.7344610	6.9220302	7.9007704
19 C	4.4933135	5.9244775	6.9830951
20 O	0.9926602 *	3.8349318	4.1105483
21 N	4.1910549	1.0426903 *	1.0409055 *
22 H	9.1871009	5.8159634	5.8197368
23 H	8.6643942	5.1515762	4.5962012
24 H	6.5508141	3.1960460	2.2290787 *
25 H	9.1673938	6.3275799	6.7726095
26 H	8.5584290	6.6437112	7.4109702
27 H	6.3650939	5.4053839	6.2889377
28 H	5.1096510	4.6885519	5.8431594
29 H	2.3104184 *	6.1961741	6.5712663
30 H	4.6290601	7.8505813	8.5781153
31 H	5.8193220	7.9021772	8.9505349
32 H	5.4732739	6.2915896	7.4701355
33 H	0.0000000	4.3873335	4.4210395
34 H	4.3873335	0.0000000	1.6637510 *
35 H	4.4210395	1.6637510 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 4676.7 SECONDS (77.9 MIN)
WALL CLOCK TIME: STEP = 0.78 , TOTAL = 4323.3 SECONDS (72.1 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.82 , TOTAL = 4677.5 SECONDS (78.0 MIN)
WALL CLOCK TIME: STEP = 0.83 , TOTAL = 4324.1 SECONDS (72.1 MIN)

CPU UTILIZATION: STEP = 98.99%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.634100638	-284.634100638	0.034656249	0.001495227	196935024
11404992						
2	1	-284.634438840	-0.000338202	0.004491116	0.000223311	162477900
14364044						
3	2	-284.634436943	0.000001897	0.002018867	0.000500122	149114421
15432436						
4	3	-284.634445067	-0.000008124	0.000761035	0.000085050	142797627
15908566						
5	4	-284.634445174	-0.000000106	0.000250181	0.000134797	134592184
16585552						
6	5	-284.634445461	-0.000000287	0.000340953	0.000049680	123733387
17422098						
7	6	-284.634445477	-0.000000017	0.000222152	0.000029392	151331257
15281216						
8	7	-284.634445613	-0.000000136	0.000229131	0.000024151	144250504
15833610						
9	8	-284.634445632	-0.000000019	0.000181354	0.000016847	163564062
14300721						
10	9	-284.634445658	-0.000000025	0.000139954	0.000016743	158912376
14753397						
11	10	-284.634445665	-0.000000008	0.000062084	0.000016828	161171575
14485539						
12	11	-284.634445675	-0.000000010	0.000106644	0.000015064	152806145
15160873						

-----DISABLING FDIFF OPTION-----

13	12	-284.634445665	0.000000010	0.000124883	0.000010714	196913168
11407177						
14	13	-284.634445673	-0.000000008	0.000124668	0.000006274	196913282
11407179						
15	14	-284.634445677	-0.000000004	0.000069082	0.000005738	196913304
11407176						
16	15	-284.634445679	-0.000000002	0.000039558	0.000005680	196913264
11407181						
17	16	-284.634445681	-0.000000002	0.000087869	0.000004931	196913201
11407181						
18	17	-284.634445684	-0.000000002	0.000047710	0.000003566	196913240
11407175						
19	18	-284.634445684	-0.000000001	0.000018088	0.000002532	196913237
11407177						
20	19	-284.634445685	0.000000000	0.000012690	0.000001391	196913318
11407176						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 67.0 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 21.6 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 3.1 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6344456847 AFTER 20 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6027292658
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000272605

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 71.31 , TOTAL = 4748.8 SECONDS (79.1 MIN)
WALL CLOCK TIME: STEP = 65.31 , TOTAL = 4389.4 SECONDS (73.2
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.78 , TOTAL = 4752.6 SECONDS (79.2 MIN)
WALL CLOCK TIME: STEP = 3.75 , TOTAL = 4393.2 SECONDS (73.2
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84 , TOTAL = 4755.4 SECONDS (79.3 MIN)
WALL CLOCK TIME: STEP = 2.64 , TOTAL = 4395.8 SECONDS (73.3
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 46 ENERGY= -284.6344457

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0010936	-0.0001226	0.0000104
2 C	6.0	0.0006161	-0.0014950	0.0001651
3 C	6.0	-0.0003347	0.0000915	0.0005818
4 C	6.0	0.0002898	-0.0009703	-0.0001187
5 C	6.0	-0.0011956	0.0000155	0.0001335
6 C	6.0	0.0000038	-0.0008599	-0.0004335
7 C	6.0	-0.0003357	0.0002665	-0.0002775
8 C	6.0	0.0007871	0.0002039	-0.0009803
9 C	6.0	-0.0007264	0.0011262	-0.0006581
10 C	6.0	0.0006888	0.0013531	0.0002380
11 C	6.0	0.0000035	0.0003074	-0.0000504
12 N	7.0	0.0008781	0.0000149	0.0006259
13 C	6.0	-0.0002231	-0.0002185	0.0010790
14 C	6.0	0.0001040	-0.0000516	0.0008232
15 C	6.0	-0.0000955	-0.0003288	-0.0009550
16 C	6.0	-0.0002140	-0.0013968	-0.0002671
17 C	6.0	-0.0007867	-0.0001347	0.0005207
18 C	6.0	0.0004263	0.0010865	0.0009618
19 C	6.0	0.0004453	0.0006236	0.0007937
20 O	8.0	-0.0007080	0.0012188	-0.0004207
21 N	7.0	-0.0013971	0.0006558	-0.0009808
22 H	1.0	-0.0004793	-0.0006383	-0.0007486
23 H	1.0	0.0012582	0.0005614	0.0002924
24 H	1.0	0.0013897	0.0011254	0.0002983
25 H	1.0	-0.0007453	0.0011202	0.0004320
26 H	1.0	-0.0005980	-0.0002142	-0.0000184
27 H	1.0	0.0002056	-0.0004569	0.0003472
28 H	1.0	-0.0007194	-0.0005641	0.0005230
29 H	1.0	-0.0002686	-0.0002062	-0.0007092
30 H	1.0	0.0019668	0.0006200	-0.0002160
31 H	1.0	0.0007806	-0.0002794	0.0000378
32 H	1.0	0.0002056	0.0003918	-0.0016694
33 H	1.0	0.0000751	-0.0012593	-0.0006219
34 H	1.0	-0.0001525	-0.0008079	0.0013770
35 H	1.0	-0.0000510	-0.0007779	-0.0001155

MAXIMUM GRADIENT = 0.0019668 RMS GRADIENT = 0.0007207
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001052013
 PREDICTED ENERGY CHANGE WAS -0.0000859520 RATIO= 1.224
 GDIIS STEP HAS LENGTH = 0.170863

RADIUS OF STEP TAKEN= 0.17086 CURRENT TRUST RADIUS= 0.18307

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 4755.4 SECONDS (79.3 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4395.8 SECONDS (73.3 MIN)
CPU UTILIZATION: STEP = 92.04% , TOTAL = 100.00%

INSERCH= 47

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1292904044	-1.7636113943	0.9785622189
C	6.0	4.9866491760	0.6823688080	0.4630419235
C	6.0	5.2122788747	-0.6825882695	0.2468608734
C	6.0	4.0880031133	-1.5496291669	0.0539705146
C	6.0	2.7698068466	-1.0566520212	0.1251123521
C	6.0	2.4789923964	0.3346342608	0.4612531693
C	6.0	3.6495766750	1.2152327702	0.5806664669
C	6.0	3.4870208501	2.6287985723	0.8370260170
C	6.0	2.2175631214	3.1833817850	1.0494216667
C	6.0	1.0721196066	2.3303898805	1.0238188321
C	6.0	1.1714833532	0.9558159945	0.7013119932
N	7.0	-0.0399239563	0.1445050269	0.7133160437
C	6.0	-1.2403044062	0.6791162105	0.4905125248
C	6.0	-2.5513484124	0.0311358171	0.5419579595
C	6.0	-2.8582400648	-1.3502190602	0.7959060455
C	6.0	-4.1724627827	-1.8512662700	0.8115369061
C	6.0	-5.2559031232	-0.9449702333	0.6026101337
C	6.0	-5.0075847209	0.4335723373	0.3510842889
C	6.0	-3.6752558429	0.9049828801	0.3003368871
O	8.0	-1.7597202290	-2.2824106459	1.0535271217
N	7.0	1.6724425691	-2.0379476682	-0.2276806684
H	1.0	5.8409689689	1.3768181896	0.5527503460
H	1.0	6.2412990219	-1.0828343077	0.1893187387
H	1.0	4.2828184778	-2.6129491791	-0.1939259460
H	1.0	4.3867297740	3.2681454597	0.8931364265
H	1.0	2.0957142455	4.2563626082	1.2823240585
H	1.0	0.0999612031	2.7676151222	1.3123424709
H	1.0	-1.2901239020	1.7481193981	0.2101767368
H	1.0	-4.3796083188	-2.9268486304	0.9795447774
H	1.0	-6.2918301917	-1.3291481800	0.6279162361
H	1.0	-5.8472299591	1.1307071633	0.1801054095
H	1.0	-3.4795731947	1.9674417554	0.0624027663

H 1.0 -2.0961459700 -3.1959862876 1.2468935848
H 1.0 1.3245723904 -1.8537527946 -1.1967388746
H 1.0 2.0739610063 -2.9972249310 -0.2375130012

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4628303	5.2479300	4.0708801
2 C	5.4628303	0.0000000	1.4002681 *	2.4406391 *
3 C	5.2479300	1.4002681 *	0.0000000	1.4328163 *
4 C	4.0708801	2.4406391 *	1.4328163 *	0.0000000
5 C	2.8636507 *	2.8377420 *	2.4739475 *	1.4091590 *
6 C	3.1923883	2.5316526 *	2.9243052 *	2.5110244 *
7 C	4.6286336	1.4441407 *	2.4809653 *	2.8485238 *
8 C	5.5306104	2.4854251 *	3.7802239	4.2934385
9 C	5.3701625	3.7771345	4.9556181	5.1856399
10 C	4.2014071	4.2841552	5.1790559	5.0090625
11 C	2.9254605 *	3.8323669	4.3839392	3.8990247
12 N	1.9338814 *	5.0614595	5.3373494	4.5104999
13 C	2.8426925 *	6.2270150	6.5991997	5.7921271
14 C	3.2553902	7.5664879	7.8019480	6.8423635
15 C	3.0215219	8.1107644	8.1166777	6.9885998
16 C	4.3058868	9.5094736	9.4740722	8.3006137
17 C	5.4600204	10.3719617	10.4775110	9.3795097
18 C	5.6221732	9.9979571	10.2811618	9.3140261
19 C	4.6963770	8.6662927	9.0283728	8.1457968
20 O	1.9603912 *	7.3927052	7.1985355	5.9776208
21 N	1.9777768 *	4.3429466	3.8200301	2.4804667 *
22 H	6.5319894	1.1046130 *	2.1748505 *	3.4475737
23 H	6.2002429	2.1828909 *	1.1056177 *	2.2074646 *
24 H	4.3986246	3.4330897	2.1873461 *	1.1090785 *
25 H	6.5917877	2.6890752 *	4.0874809	4.8994275
26 H	6.3402824	4.6692783	5.9311377	6.2600006
27 H	4.5435980	5.3804538	6.2589893	6.0105388
28 H	3.8648941	6.3716282	6.9419686	6.3106098
29 H	4.6565319	10.0508709	9.8781491	8.6286653
30 H	6.4453472	11.4576385	11.5285632	10.3980270
31 H	6.6883039	10.8468427	11.2073740	10.2912083
32 H	5.2710532	8.5725635	9.0887280	8.3449428
33 H	2.6601253 *	8.1130789	7.7929653	6.5097816
34 H	2.4836987 *	4.7536924	4.3092770	3.0484938
35 H	2.6043013 *	4.7448856	3.9295292	2.4973710 *

C C C C

1	CO	2.8636507 *	3.1923883	4.6286336	5.5306104
2	C	2.8377420 *	2.5316526 *	1.4441407 *	2.4854251 *
3	C	2.4739475 *	2.9243052 *	2.4809653 *	3.7802239
4	C	1.4091590 *	2.5110244 *	2.8485238 *	4.2934385
5	C	0.0000000	1.4605620 *	2.4785046 *	3.8214870
6	C	1.4605620 *	0.0000000	1.4696873 *	2.5338738 *
7	C	2.4785046 *	1.4696873 *	0.0000000	1.4457914 *
8	C	3.8214870	2.5338738 *	1.4457914 *	0.0000000
9	C	4.3746094	2.9205564 *	2.4787103 *	1.4014983 *
10	C	3.8938244	2.5057557 *	2.8431047 *	2.4404277 *
11	C	2.6337562 *	1.4673360 *	2.4945539 *	2.8598956 *
12	N	3.1118080	2.5386265 *	3.8440173	4.3158265
13	C	4.3849060	3.7353303	4.9200087	5.1253231
14	C	5.4471769	5.0401342	6.3130861	6.5800319
15	C	5.6754786	5.6068506	6.9985391	7.4897669
16	C	7.0212319	7.0101866	8.4048212	8.8735179
17	C	8.0406777	7.8412995	9.1637617	9.4480418
18	C	7.9220989	7.4880413	8.6954094	8.7871202
19	C	6.7392543	6.1827149	7.3367575	7.3863241
20	O	4.7834144	5.0166121	6.4589163	7.1899333
21	N	1.5138073 *	2.5989031 *	3.8917435	5.1190639
22	H	3.9416606	3.5209950	2.1975189 *	2.6812943 *
23	H	3.4721846	4.0296547	3.4858701	4.6670967
24	H	2.1938666 *	3.5172854	3.9567620	5.4011180
25	H	4.6806168	3.5258294	2.2035160 *	1.1051647 *
26	H	5.4792029	4.0250482	3.4864427	2.1870046 *
27	H	4.8127550	3.5076400	3.9427162	3.4230642
28	H	4.9352828	4.0332638	4.9821554	4.8979228
29	H	7.4392088	7.6122468	9.0434371	9.6316863
30	H	9.0796658	8.9287892	10.2619529	10.5515400
31	H	8.8904942	8.3689160	9.5056262	9.4765004
32	H	6.9428976	6.1910941	7.1874330	7.0406581
33	H	5.4325538	5.8321868	7.2743413	8.0788528
34	H	2.1145598 *	2.9783655 *	4.2406942	5.3763975
35	H	2.0932085 *	3.4283539	4.5712998	5.8994502

C C C N

1	CO	5.3701625	4.2014071	2.9254605 *	1.9338814 *
2	C	3.7771345	4.2841552	3.8323669	5.0614595
3	C	4.9556181	5.1790559	4.3839392	5.3373494
4	C	5.1856399	5.0090625	3.8990247	4.5104999
5	C	4.3746094	3.8938244	2.6337562 *	3.1118080
6	C	2.9205564 *	2.5057557 *	1.4673360 *	2.5386265 *
7	C	2.4787103 *	2.8431047 *	2.4945539 *	3.8440173

8 C	1.4014983 *	2.4404277 *	2.8598956 *	4.3158265
9 C	0.0000000	1.4283877 *	2.4854602 *	3.8005245
10 C	1.4283877 *	0.0000000	1.4153929 *	2.4720731 *
11 C	2.4854602 *	1.4153929 *	0.0000000	1.4580388 *
12 N	3.8005245	2.4720731 *	1.4580388 *	0.0000000
13 C	4.3058766	2.8910941 *	2.4367436 *	1.3328030 *
14 C	5.7390497	4.3183654	3.8392582	2.5198153 *
15 C	6.8104027	5.3894855	4.6438579	3.1912265
16 C	8.1385933	6.7109579	6.0373521	4.5902753
17 C	8.5495982	7.1378759	6.7032848	5.3296952
18 C	7.7622090	6.4041622	6.2109806	4.9892309
19 C	6.3621965	5.0092699	4.8635631	3.7369127
20 O	6.7597105	5.4127745	4.3820226	2.9938875 *
21 N	5.4028167	4.5835588	3.1743674	2.9292958 *
22 H	4.0791451	4.8860136	4.6907792	6.0107636
23 H	5.9271264	6.2503524	5.4882842	6.4214249
24 H	6.2776306	6.0189775	4.8185000	5.2069899
25 H	2.1764407 *	3.4471878	3.9650314	5.4207682
26 H	1.1047074 *	2.1963474 *	3.4764041	4.6682002
27 H	2.1739888 *	1.1043114 *	2.1918335 *	2.6942730 *
28 H	3.8817752	2.5653941 *	2.6321985 *	2.0946905 *
29 H	8.9923562	7.5737609	6.7799054	5.3232463
30 H	9.6410771	8.2326614	7.8056068	6.4238056
31 H	8.3672021	7.0730820	7.0402116	5.9145339
32 H	5.9084752	4.6662576	4.8024909	3.9468941
33 H	7.7034679	6.3740492	5.3115462	3.9587417
34 H	5.5870739	4.7435913	3.3940698	3.0827252
35 H	6.3148018	5.5657995	4.1620176	3.9042352

C C C C

1 CO	2.8426925 *	3.2553902	3.0215219	4.3058868
2 C	6.2270150	7.5664879	8.1107644	9.5094736
3 C	6.5991997	7.8019480	8.1166777	9.4740722
4 C	5.7921271	6.8423635	6.9885998	8.3006137
5 C	4.3849060	5.4471769	5.6754786	7.0212319
6 C	3.7353303	5.0401342	5.6068506	7.0101866
7 C	4.9200087	6.3130861	6.9985391	8.4048212
8 C	5.1253231	6.5800319	7.4897669	8.8735179
9 C	4.3058766	5.7390497	6.8104027	8.1385933
10 C	2.8910941 *	4.3183654	5.3894855	6.7109579
11 C	2.4367436 *	3.8392582	4.6438579	6.0373521
12 N	1.3328030 *	2.5198153 *	3.1912265	4.5902753
13 C	0.0000000	1.4633392 *	2.6132705 *	3.8863151
14 C	1.4633392 *	0.0000000	1.4376416 *	2.4988242 *
15 C	2.6132705 *	1.4376416 *	0.0000000	1.4065824 *

16 C	3.8863151	2.4988242 *	1.4065824 *	0.0000000
17 C	4.3330423	2.8759482 *	2.4393397 *	1.4278886 *
18 C	3.7778477	2.4962942 *	2.8283318 *	2.4758701 *
19 C	2.4527884 *	1.4440074 *	2.4492936 *	2.8470071 *
20 O	3.0589900	2.4981744 *	1.4635900 *	2.4628787 *
21 N	4.0475094	4.7659060	4.6955070	5.9395069
22 H	7.1158340	8.4995275	9.1198736	10.5240826
23 H	7.6921764	8.8699455	9.1236536	10.4605964
24 H	6.4661454	7.3646825	7.3190827	8.5488536
25 H	6.2071485	7.6641038	8.5923415	9.9737060
26 H	4.9550659	6.3242292	7.4974678	8.7644061
27 H	2.6141048 *	3.8873196	5.0964909	6.3117730
28 H	1.1062721 *	2.1561073 *	3.5216144	4.6502783
29 H	4.8059717	3.5048093	2.1986463 *	1.1081576 *
30 H	5.4378229	3.9810759	3.4377617	2.1904433 *
31 H	4.6394019	3.4932549	3.9329716	3.4778896
32 H	2.6186610 *	2.2001943 *	3.4541215	3.9526989
33 H	4.0399253	3.3344356	2.0472015 *	2.5117522 *
34 H	3.9800547	4.6474330	4.6604828	5.8523990
35 H	5.0029852	5.5831918	5.3016215	6.4367334

C C C O

1 CO	5.4600204	5.6221732	4.6963770	1.9603912 *
2 C	10.3719617	9.9979571	8.6662927	7.3927052
3 C	10.4775110	10.2811618	9.0283728	7.1985355
4 C	9.3795097	9.3140261	8.1457968	5.9776208
5 C	8.0406777	7.9220989	6.7392543	4.7834144
6 C	7.8412995	7.4880413	6.1827149	5.0166121
7 C	9.1637617	8.6954094	7.3367575	6.4589163
8 C	9.4480418	8.7871202	7.3863241	7.1899333
9 C	8.5495982	7.7622090	6.3621965	6.7597105
10 C	7.1378759	6.4041622	5.0092699	5.4127745
11 C	6.7032848	6.2109806	4.8635631	4.3820226
12 N	5.3296952	4.9892309	3.7369127	2.9938875 *
13 C	4.3330423	3.7778477	2.4527884 *	3.0589900
14 C	2.8759482 *	2.4962942 *	1.4440074 *	2.4981744 *
15 C	2.4393397 *	2.8283318 *	2.4492936 *	1.4635900 *
16 C	1.4278886 *	2.4758701 *	2.8470071 *	2.4628787 *
17 C	0.0000000	1.4231328 *	2.4519669 *	3.7703273
18 C	1.4231328 *	0.0000000	1.4141794 *	4.2916912
19 C	2.4519669 *	1.4141794 *	0.0000000	3.7942127
20 O	3.7703273	4.2916912	3.7942127	0.0000000
21 N	7.0629991	7.1460580	6.1267872	3.6716477
22 H	11.3372729	10.8913497	9.5312578	8.4505153
23 H	11.5054541	11.3517859	10.1144354	8.1364703

24 H	9.7161635	9.7923399	8.7149922	6.1788080
25 H	10.5268760	9.8276025	8.4220877	8.2833113
26 H	9.0311767	8.1202087	6.7453792	7.5942267
27 H	6.5553255	5.6972624	4.3296441	5.3877788
28 H	4.8097963	3.9455549	2.5313756 *	4.1445064
29 H	2.1995032 *	3.4758806	3.9547906	2.6989975 *
30 H	1.1051597 *	2.1984326 *	3.4561700	4.6507929
31 H	2.1992304 *	1.1046424 *	2.1869793 *	5.3962927
32 H	3.4538841	2.1842417 *	1.1062202 *	4.6905722
33 H	3.9327140	4.7384223	4.4952759	0.9925691 *
34 H	6.8823107	6.9082434	5.9034008	3.8419143
35 H	7.6579674	7.8908242	6.9692182	4.1079016

N H H H

1 CO	1.9777768 *	6.5319894	6.2002429	4.3986246
2 C	4.3429466	1.1046130 *	2.1828909 *	3.4330897
3 C	3.8200301	2.1748505 *	1.1056177 *	2.1873461 *
4 C	2.4804667 *	3.4475737	2.2074646 *	1.1090785 *
5 C	1.5138073 *	3.9416606	3.4721846	2.1938666 *
6 C	2.5989031 *	3.5209950	4.0296547	3.5172854
7 C	3.8917435	2.1975189 *	3.4858701	3.9567620
8 C	5.1190639	2.6812943 *	4.6670967	5.4011180
9 C	5.4028167	4.0791451	5.9271264	6.2776306
10 C	4.5835588	4.8860136	6.2503524	6.0189775
11 C	3.1743674	4.6907792	5.4882842	4.8185000
12 N	2.9292958 *	6.0107636	6.4214249	5.2069899
13 C	4.0475094	7.1158340	7.6921764	6.4661454
14 C	4.7659060	8.4995275	8.8699455	7.3646825
15 C	4.6955070	9.1198736	9.1236536	7.3190827
16 C	5.9395069	10.5240826	10.4605964	8.5488536
17 C	7.0629991	11.3372729	11.5054541	9.7161635
18 C	7.1460580	10.8913497	11.3517859	9.7923399
19 C	6.1267872	9.5312578	10.1144354	8.7149922
20 O	3.6716477	8.4505153	8.1364703	6.1788080
21 N	0.0000000	5.4448426	4.6862116	2.6731683 *
22 H	5.4448426	0.0000000	2.5183799 *	4.3478273
23 H	4.6862116	2.5183799 *	0.0000000	2.5147115 *
24 H	2.6731683 *	4.3478273	2.5147115 *	0.0000000
25 H	6.0645041	2.4099363 *	4.7818209	5.9816199
26 H	6.4867261	4.7802706	6.8474490	7.3586808
27 H	5.2856223	5.9557087	7.3350646	6.9796570
28 H	4.8272998	7.1489654	8.0459347	7.0880113
29 H	6.2349706	11.0979233	10.8087242	8.7471827
30 H	8.0413981	12.4311190	12.5432199	10.6839489
31 H	8.1701982	11.6967273	12.2895233	10.8061438

32 H	6.5322706	9.3521005	10.1889964	9.0166740
33 H	4.2092377	9.1864122	8.6658447	6.5655983
34 H	1.0459518 *	5.8219532	5.1662048	3.2145346
35 H	1.0399647 *	5.8264156	4.6058423	2.2424583 *

H H H H

1 CO	6.5917877	6.3402824	4.5435980	3.8648941
2 C	2.6890752 *	4.6692783	5.3804538	6.3716282
3 C	4.0874809	5.9311377	6.2589893	6.9419686
4 C	4.8994275	6.2600006	6.0105388	6.3106098
5 C	4.6806168	5.4792029	4.8127550	4.9352828
6 C	3.5258294	4.0250482	3.5076400	4.0332638
7 C	2.2035160 *	3.4864427	3.9427162	4.9821554
8 C	1.1051647 *	2.1870046 *	3.4230642	4.8979228
9 C	2.1764407 *	1.1047074 *	2.1739888 *	3.8817752
10 C	3.4471878	2.1963474 *	1.1043114 *	2.5653941 *
11 C	3.9650314	3.4764041	2.1918335 *	2.6321985 *
12 N	5.4207682	4.6682002	2.6942730 *	2.0946905 *
13 C	6.2071485	4.9550659	2.6141048 *	1.1062721 *
14 C	7.6641038	6.3242292	3.8873196	2.1561073 *
15 C	8.5923415	7.4974678	5.0964909	3.5216144
16 C	9.9737060	8.7644061	6.3117730	4.6502783
17 C	10.5268760	9.0311767	6.5553255	4.8097963
18 C	9.8276025	8.1202087	5.6972624	3.9455549
19 C	8.4220877	6.7453792	4.3296441	2.5313756 *
20 O	8.2833113	7.5942267	5.3877788	4.1445064
21 N	6.0645041	6.4867261	5.2856223	4.8272998
22 H	2.4099363 *	4.7802706	5.9557087	7.1489654
23 H	4.7818209	6.8474490	7.3350646	8.0459347
24 H	5.9816199	7.3586808	6.9796570	7.0880113
25 H	0.0000000	2.5252311 *	4.3362022	5.9163824
26 H	2.5252311 *	0.0000000	2.4900402 *	4.3479517
27 H	4.3362022	2.4900402 *	0.0000000	2.0460883 *
28 H	5.9163824	4.3479517	2.0460883 *	0.0000000
29 H	10.7347148	9.6757429	7.2528763	5.6561619
30 H	11.6291484	10.0983703	7.6227886	5.8873719
31 H	10.4790738	8.6066817	6.2714042	4.5988387
32 H	8.0162754	6.1490810	3.8750088	2.2053634 *
33 H	9.1617586	8.5504650	6.3554474	5.1155288
34 H	6.3228339	6.6388194	5.3992780	4.6679258
35 H	6.7736352	7.4111342	6.2874564	5.8340197

H H H H

1 CO	4.6565319	6.4453472	6.6883039	5.2710532
------	-----------	-----------	-----------	-----------

2 C	10.0508709	11.4576385	10.8468427	8.5725635
3 C	9.8781491	11.5285632	11.2073740	9.0887280
4 C	8.6286653	10.3980270	10.2912083	8.3449428
5 C	7.4392088	9.0796658	8.8904942	6.9428976
6 C	7.6122468	8.9287892	8.3689160	6.1910941
7 C	9.0434371	10.2619529	9.5056262	7.1874330
8 C	9.6316863	10.5515400	9.4765004	7.0406581
9 C	8.9923562	9.6410771	8.3672021	5.9084752
10 C	7.5737609	8.2326614	7.0730820	4.6662576
11 C	6.7799054	7.8056068	7.0402116	4.8024909
12 N	5.3232463	6.4238056	5.9145339	3.9468941
13 C	4.8059717	5.4378229	4.6394019	2.6186610 *
14 C	3.5048093	3.9810759	3.4932549	2.2001943 *
15 C	2.1986463 *	3.4377617	3.9329716	3.4541215
16 C	1.1081576 *	2.1904433 *	3.4778896	3.9526989
17 C	2.1995032 *	1.1051597 *	2.1992304 *	3.4538841
18 C	3.4758806	2.1984326 *	1.1046424 *	2.1842417 *
19 C	3.9547906	3.4561700	2.1869793 *	1.1062202 *
20 O	2.6989975 *	4.6507929	5.3962927	4.6905722
21 N	6.2349706	8.0413981	8.1701982	6.5322706
22 H	11.0979233	12.4311190	11.6967273	9.3521005
23 H	10.8087242	12.5432199	12.2895233	10.1889964
24 H	8.7471827	10.6839489	10.8061438	9.0166740
25 H	10.7347148	11.6291484	10.4790738	8.0162754
26 H	9.6757429	10.0983703	8.6066817	6.1490810
27 H	7.2528763	7.6227886	6.2714042	3.8750088
28 H	5.6561619	5.8873719	4.5988387	2.2053634 *
29 H	0.0000000	2.5165218 *	4.3882543	5.0601671
30 H	2.5165218 *	0.0000000	2.5395063 *	4.3699085
31 H	4.3882543	2.5395063 *	0.0000000	2.5139167 *
32 H	5.0601671	4.3699085	2.5139167 *	0.0000000
33 H	2.3147593 *	4.6337872	5.8248557	5.4752058
34 H	6.1988243	7.8494691	7.8890716	6.2663211
35 H	6.5677043	8.5742586	8.9420073	7.4551732

H H H

1 CO	2.6601253 *	2.4836987 *	2.6043013 *
2 C	8.1130789	4.7536924	4.7448856
3 C	7.7929653	4.3092770	3.9295292
4 C	6.5097816	3.0484938	2.4973710 *
5 C	5.4325538	2.1145598 *	2.0932085 *
6 C	5.8321868	2.9783655 *	3.4283539
7 C	7.2743413	4.2406942	4.5712998
8 C	8.0788528	5.3763975	5.8994502
9 C	7.7034679	5.5870739	6.3148018

10 C	6.3740492	4.7435913	5.5657995
11 C	5.3115462	3.3940698	4.1620176
12 N	3.9587417	3.0827252	3.9042352
13 C	4.0399253	3.9800547	5.0029852
14 C	3.3344356	4.6474330	5.5831918
15 C	2.0472015 *	4.6604828	5.3016215
16 C	2.5117522 *	5.8523990	6.4367334
17 C	3.9327140	6.8823107	7.6579674
18 C	4.7384223	6.9082434	7.8908242
19 C	4.4952759	5.9034008	6.9692182
20 O	0.9925691 *	3.8419143	4.1079016
21 N	4.2092377	1.0459518 *	1.0399647 *
22 H	9.1864122	5.8219532	5.8264156
23 H	8.6658447	5.1662048	4.6058423
24 H	6.5655983	3.2145346	2.2424583 *
25 H	9.1617586	6.3228339	6.7736352
26 H	8.5504650	6.6388194	7.4111342
27 H	6.3554474	5.3992780	6.2874564
28 H	5.1155288	4.6679258	5.8340197
29 H	2.3147593 *	6.1988243	6.5677043
30 H	4.6337872	7.8494691	8.5742586
31 H	5.8248557	7.8890716	8.9420073
32 H	5.4752058	6.2663211	7.4551732
33 H	0.0000000	4.4129632	4.4308872
34 H	4.4129632	0.0000000	1.6700976 *
35 H	4.4308872	1.6700976 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.81 , TOTAL = 4756.3 SECONDS (79.3 MIN)
WALL CLOCK TIME: STEP = 0.81 , TOTAL = 4396.6 SECONDS (73.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.17 , TOTAL = 4757.4 SECONDS (79.3 MIN)
WALL CLOCK TIME: STEP = 1.17 , TOTAL = 4397.8 SECONDS (73.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
 INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.633993003	-284.633993003	0.040534000	0.002196272	196923330
11407856						
2	1	-284.634595485	-0.000602481	0.006764563	0.000197509	164818122
14170029						
3	2	-284.634597472	-0.000001987	0.003079961	0.000264956	150023486
15413301						
4	3	-284.634604262	-0.000006790	0.001385760	0.000182929	143738821
15874954						
5	4	-284.634604537	-0.000000275	0.000485462	0.000254090	138870720
16315564						
6	5	-284.634605240	-0.000000703	0.000678890	0.000076407	131581356
16883947						
7	6	-284.634605399	-0.000000159	0.000302299	0.000057451	155113448
15017866						
8	7	-284.634605627	-0.000000228	0.000346196	0.000044382	146234585
15668488						
9	8	-284.634605692	-0.000000065	0.000294103	0.000032437	167871275
13985798						
10	9	-284.634605737	-0.000000045	0.000314513	0.000015922	161456668
14523273						

-----DISABLING FDIFF OPTION-----

11	10	-284.634605768	-0.000000031	0.000150143	0.000016313	196897705
11410109						
12	11	-284.634605778	-0.000000010	0.000090444	0.000014177	196897830
11410098						
13	12	-284.634605786	-0.000000008	0.000091555	0.000010786	196897723
11410105						
14	13	-284.634605792	-0.000000006	0.000090082	0.000005869	196897645
11410115						
15	14	-284.634605797	-0.000000005	0.000062410	0.000007247	196897666
11410108						
16	15	-284.634605799	-0.000000002	0.000052380	0.000007991	196897644
11410105						
17	16	-284.634605801	-0.000000002	0.000164414	0.000007698	196897714
11410098						
18	17	-284.634605807	-0.000000006	0.000122532	0.000005814	196897726
11410095						
19	18	-284.634605809	-0.000000002	0.000051153	0.000003467	196897834
11410095						
20	19	-284.634605810	-0.000000001	0.000031502	0.000003447	196897799
11410098						

21 20 -284.634605811 -0.000000001 0.000022414 0.000002397 196897784
11410097

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 71.4 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 22.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.3
TIME TO SOLVE SCF EQUATIONS= 1.8 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6346058107 AFTER 21 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5972224939
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000194313

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 74.39 , TOTAL = 4831.8 SECONDS (80.5 MIN)
WALL CLOCK TIME: STEP = 68.83 , TOTAL = 4466.6 SECONDS (74.4
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.67 , TOTAL = 4835.5 SECONDS (80.6 MIN)
WALL CLOCK TIME: STEP = 3.67 , TOTAL = 4470.3 SECONDS (74.5
MIN)
CPU UTILIZATION: STEP = 99.98% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.75 , TOTAL = 4838.2 SECONDS (80.6 MIN)

WALL CLOCK TIME: STEP = 2.66 , TOTAL = 4472.9 SECONDS (74.5 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 47 ENERGY= -284.6346058

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0012054	-0.0002043	-0.0003042
2 C	6.0	-0.0005189	-0.0007158	0.0002271
3 C	6.0	-0.0004234	-0.0003714	0.0007342
4 C	6.0	0.0000239	0.0002150	0.0004022
5 C	6.0	0.0005929	-0.0001187	-0.0001232
6 C	6.0	0.0000231	-0.0001037	-0.0003030
7 C	6.0	0.0002470	-0.0001439	-0.0003035
8 C	6.0	-0.0001942	0.0006296	-0.0006657
9 C	6.0	-0.0004036	0.0006161	-0.0006858
10 C	6.0	0.0004907	0.0001973	-0.0002629
11 C	6.0	0.0001205	0.0003885	0.0000052
12 N	7.0	0.0005545	0.0003735	0.0007361
13 C	6.0	0.0003266	-0.0002303	0.0009524
14 C	6.0	0.0006139	-0.0000436	0.0006167
15 C	6.0	-0.0000827	-0.0009061	-0.0006111
16 C	6.0	-0.0002432	0.0006641	-0.0006732
17 C	6.0	0.0013015	0.0001914	0.0004318
18 C	6.0	0.0003156	0.0003129	0.0010558
19 C	6.0	0.0005778	0.0007197	0.0004842
20 O	8.0	-0.0000523	0.0003919	-0.0003202
21 N	7.0	-0.0002257	-0.0005853	0.0004825
22 H	1.0	0.0000068	-0.0004880	-0.0008178
23 H	1.0	0.0012893	0.0003605	0.0003745
24 H	1.0	0.0018443	-0.0004170	-0.0002347
25 H	1.0	-0.0005668	0.0009041	0.0001224
26 H	1.0	-0.0002969	0.0003006	0.0001478
27 H	1.0	-0.0002588	0.0002540	0.0008062
28 H	1.0	-0.0009044	-0.0002759	0.0004776
29 H	1.0	-0.0005603	-0.0010005	-0.0007770
30 H	1.0	0.0000307	0.0001744	0.0000212
31 H	1.0	-0.0001678	0.0003957	-0.0000082
32 H	1.0	0.0000148	0.0000511	-0.0014852
33 H	1.0	0.0001165	-0.0011439	-0.0004170
34 H	1.0	-0.0016835	0.0000176	-0.0007160
35 H	1.0	-0.0007024	-0.0004098	0.0006307

MAXIMUM GRADIENT = 0.0018443 RMS GRADIENT = 0.0005911
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0001601260
PREDICTED ENERGY CHANGE WAS -0.0001118339 RATIO= 1.432
GDIIS STEP HAS LENGTH = 0.133267
RADIUS OF STEP TAKEN= 0.13327 CURRENT TRUST RADIUS= 0.17086

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 4838.3 SECONDS (80.6 MIN)
WALL CLOCK TIME: STEP = 0.03 , TOTAL = 4473.0 SECONDS (74.5
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 48

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1330879983	-1.7647731507	0.9712576665
C	6.0	4.9881262668	0.6855526311	0.4657938742
C	6.0	5.2144424532	-0.6820959173	0.2484030604
C	6.0	4.0904649928	-1.5504809852	0.0501069185
C	6.0	2.7720352548	-1.0544934735	0.1192219247
C	6.0	2.4808045301	0.3352369219	0.4602582361
C	6.0	3.6491685511	1.2157020347	0.5834465669
C	6.0	3.4851428610	2.6254638076	0.8433818856
C	6.0	2.2173121188	3.1786688763	1.0597245986
C	6.0	1.0699794644	2.3259014769	1.0299645044
C	6.0	1.1713233989	0.9533633027	0.7005836933
N	7.0	-0.0406998797	0.1430693153	0.7060890716
C	6.0	-1.2392006727	0.6791221520	0.4774828461
C	6.0	-2.5506525956	0.0286676635	0.5318759255
C	6.0	-2.8553929772	-1.3497705235	0.8020771818
C	6.0	-4.1713924530	-1.8482927295	0.8225374744
C	6.0	-5.2600083634	-0.9458669203	0.6058907435
C	6.0	-5.0102451405	0.4314520555	0.3399777114
C	6.0	-3.6755934099	0.8984211055	0.2852752536
O	8.0	-1.7571120066	-2.2831164960	1.0640771224
N	7.0	1.6730040582	-2.0294454292	-0.2399223379
H	1.0	5.8424133469	1.3782561354	0.5604793429
H	1.0	6.2387574050	-1.0852496110	0.1955243320
H	1.0	4.2807015496	-2.6131507539	-0.2012435190
H	1.0	4.3881997087	3.2633884062	0.8933377877
H	1.0	2.0980587426	4.2525754858	1.2941424214

H	1.0	0.0995612922	2.7646015804	1.3212762038
H	1.0	-1.2862456122	1.7475856389	0.1949430145
H	1.0	-4.3797739912	-2.9211998984	0.9983923132
H	1.0	-6.2955343807	-1.3279244796	0.6407433881
H	1.0	-5.8490712536	1.1294592193	0.1700944696
H	1.0	-3.4796215335	1.9608220475	0.0489568995
H	1.0	-2.0968234639	-3.1900392489	1.2778121614
H	1.0	1.3211418250	-1.8366157696	-1.2050891653
H	1.0	2.0696389151	-2.9936894700	-0.2539865712

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4617750	5.2454620	4.0688171
2 C	5.4617750	0.0000000	1.4031893 *	2.4450844 *
3 C	5.2454620	1.4031893 *	0.0000000	1.4341336 *
4 C	4.0688171	2.4450844 *	1.4341336 *	0.0000000
5 C	2.8626045 *	2.8388258 *	2.4740090 *	1.4103324 *
6 C	3.1910712	2.5316821 *	2.9244871 *	2.5129988 *
7 C	4.6256299	1.4448904 *	2.4827351 *	2.8514842 *
8 C	5.5251067	2.4828990 *	3.7794746	4.2935085
9 C	5.3655788	3.7743600	4.9544463	5.1858353
10 C	4.1970026	4.2849629	5.1802954	5.0109674
11 C	2.9222359 *	3.8333840	4.3847470	3.9004800
12 N	1.9340061 *	5.0637064	5.3391849	4.5127540
13 C	2.8459821 *	6.2273412	6.5996138	5.7930231
14 C	3.2575988	7.5676318	7.8027074	6.8432635
15 C	3.0218980	8.1102664	8.1163162	6.9893266
16 C	4.3078585	9.5102272	9.4754178	8.3032300
17 C	5.4671372	10.3781222	10.4838682	9.3864693
18 C	5.6281254	10.0023911	10.2855535	9.3185304
19 C	4.6977899	8.6682143	9.0295145	8.1464157
20 O	1.9621803 *	7.3938609	7.1993863	5.9798869
21 N	1.9769547 *	4.3427278	3.8204186	2.4814595 *
22 H	6.5302196	1.1039067 *	2.1764167 *	3.4506962
23 H	6.1921493	2.1846886 *	1.1020663 *	2.2028951 *
24 H	4.3928580	3.4390162	2.1915809 *	1.1084377 *
25 H	6.5874468	2.6810339 *	4.0823357	4.8962254
26 H	6.3382844	4.6650084	5.9292833	6.2604130
27 H	4.5430026	5.3807399	6.2604145	6.0135781
28 H	3.8670191	6.3693812	6.9401121	6.3092977
29 H	4.6587533	10.0523569	9.8805394	8.6326742
30 H	6.4519193	11.4632323	11.5347558	10.4051605
31 H	6.6936293	10.8503153	11.2111195	10.2951861

32 H	5.2708983	8.5733784	9.0890892	8.3447864
33 H	2.6641817 *	8.1164092	7.7976966	6.5175110
34 H	2.4805481 *	4.7539414	4.3131596	3.0539386
35 H	2.6003246 *	4.7510499	3.9351810	2.5018117 *

C C C C

1 CO	2.8626045 *	3.1910712	4.6256299	5.5251067
2 C	2.8388258 *	2.5316821 *	1.4448904 *	2.4828990 *
3 C	2.4740090 *	2.9244871 *	2.4827351 *	3.7794746
4 C	1.4103324 *	2.5129988 *	2.8514842 *	4.2935085
5 C	0.0000000	1.4602985 *	2.4776309 *	3.8177239
6 C	1.4602985 *	0.0000000	1.4681514 *	2.5299443 *
7 C	2.4776309 *	1.4681514 *	0.0000000	1.4428787 *
8 C	3.8177239	2.5299443 *	1.4428787 *	0.0000000
9 C	4.3717189	2.9178577 *	2.4759427 *	1.4000839 *
10 C	3.8927517	2.5055415 *	2.8432618 *	2.4408123 *
11 C	2.6328214 *	1.4678479 *	2.4944457 *	2.8583338 *
12 N	3.1128843	2.5407372 *	3.8445690	4.3142437
13 C	4.3844940	3.7359058	4.9188718	5.1226507
14 C	5.4474331	5.0412969	6.3126454	6.5780858
15 C	5.6763922	5.6063441	6.9956250	7.4837550
16 C	7.0239560	7.0107612	8.4027616	8.8677768
17 C	8.0475071	7.8474595	9.1676779	9.4492579
18 C	7.9259482	7.4926330	8.6982625	8.7885562
19 C	6.7389439	6.1845801	7.3376911	7.3871715
20 O	4.7870075	5.0179984	6.4576007	7.1849915
21 N	1.5124105 *	2.5950948 *	3.8876914	5.1113183
22 H	3.9421061	3.5211287	2.1993804 *	2.6818436 *
23 H	3.4676982	4.0261738	3.4858044	4.6659947
24 H	2.1927573 *	3.5171300	3.9591269	5.4006702
25 H	4.6749703	3.5213329	2.1989132 *	1.1067769 *
26 H	5.4771949	4.0233566	3.4833361	2.1851041 *
27 H	4.8137863	3.5090574	3.9424858	3.4219738
28 H	4.9322434	4.0318467	4.9791714	4.8946186
29 H	7.4435146	7.6132455	9.0415738	9.6253012
30 H	9.0866698	8.9343609	10.2650102	10.5513975
31 H	8.8935772	8.3726826	9.5076210	9.4772833
32 H	6.9412014	6.1917990	7.1875261	7.0413637
33 H	5.4413851	5.8352930	7.2738658	8.0726175
34 H	2.1143810 *	2.9723970 *	4.2349985	5.3655650
35 H	2.0959786 *	3.4294247	4.5733123	5.8976904

C C C N

1 CO	5.3655788	4.1970026	2.9222359 *	1.9340061 *
------	-----------	-----------	-------------	-------------

2 C	3.7743600	4.2849629	3.8333840	5.0637064
3 C	4.9544463	5.1802954	4.3847470	5.3391849
4 C	5.1858353	5.0109674	3.9004800	4.5127540
5 C	4.3717189	3.8927517	2.6328214 *	3.1128843
6 C	2.9178577 *	2.5055415 *	1.4678479 *	2.5407372 *
7 C	2.4759427 *	2.8432618 *	2.4944457 *	3.8445690
8 C	1.4000839 *	2.4408123 *	2.8583338 *	4.3142437
9 C	0.0000000	1.4298497 *	2.4849667 *	3.7998080
10 C	1.4298497 *	0.0000000	1.4151408 *	2.4704777 *
11 C	2.4849667 *	1.4151408 *	0.0000000	1.4579462 *
12 N	3.7998080	2.4704777 *	1.4579462 *	0.0000000
13 C	4.3051388	2.8895382 *	2.4363104 *	1.3326731 *
14 C	5.7388692	4.3167525	3.8388318	2.5185910 *
15 C	6.8048132	5.3824758	4.6399538	3.1875197
16 C	8.1327822	6.7036485	6.0339673	4.5871237
17 C	8.5514959	7.1381407	6.7065692	5.3326356
18 C	7.7654890	6.4057905	6.2140339	4.9913507
19 C	6.3659750	5.0112597	4.8649874	3.7363206
20 O	6.7547883	5.4070932	4.3798017	2.9934267 *
21 N	5.3953506	4.5766033	3.1675516	2.9243015 *
22 H	4.0782460	4.8882076	4.6924668	6.0131448
23 H	5.9245139	6.2488805	5.4854275	6.4188027
24 H	6.2763677	6.0182096	4.8167985	5.2052389
25 H	2.1789022 *	3.4508165	3.9650553	5.4209413
26 H	1.1056439 *	2.1997295 *	3.4779234	4.6699182
27 H	2.1736443 *	1.1040977 *	2.1942008 *	2.6963976 *
28 H	3.8821081	2.5658345 *	2.6317498 *	2.0945470 *
29 H	8.9851937	7.5652417	6.7761060	5.3200330
30 H	9.6412387	8.2312047	7.8078051	6.4258110
31 H	8.3700205	7.0741864	7.0426110	5.9158629
32 H	5.9126860	4.6684610	4.8032155	3.9448992
33 H	7.6954383	6.3651922	5.3086497	3.9577928
34 H	5.5754446	4.7312892	3.3820139	3.0702391
35 H	6.3123412	5.5629037	4.1590144	3.9005808

C C C C

1 CO	2.8459821 *	3.2575988	3.0218980	4.3078585
2 C	6.2273412	7.5676318	8.1102664	9.5102272
3 C	6.5996138	7.8027074	8.1163162	9.4754178
4 C	5.7930231	6.8432635	6.9893266	8.3032300
5 C	4.3844940	5.4474331	5.6763922	7.0239560
6 C	3.7359058	5.0412969	5.6063441	7.0107612
7 C	4.9188718	6.3126454	6.9956250	8.4027616
8 C	5.1226507	6.5780858	7.4837550	8.8677768
9 C	4.3051388	5.7388692	6.8048132	8.1327822

10 C	2.8895382 *	4.3167525	5.3824758	6.7036485
11 C	2.4363104 *	3.8388318	4.6399538	6.0339673
12 N	1.3326731 *	2.5185910 *	3.1875197	4.5871237
13 C	0.0000000	1.4649081 *	2.6141623 *	3.8864685
14 C	1.4649081 *	0.0000000	1.4373473 *	2.4968504 *
15 C	2.6141623 *	1.4373473 *	0.0000000	1.4074081 *
16 C	3.8864685	2.4968504 *	1.4074081 *	0.0000000
17 C	4.3386602	2.8802438 *	2.4461812 *	1.4305218 *
18 C	3.7816695	2.4997311 *	2.8336686 *	2.4766457 *
19 C	2.4537818 *	1.4431822 *	2.4483012 *	2.8423413 *
20 O	3.0638510	2.5014577 *	1.4649231 *	2.4649875 *
21 N	4.0412801	4.7613840	4.6961794	5.9429460
22 H	7.1165254	8.5009272	9.1187902	10.5240486
23 H	7.6884566	8.8660968	9.1181933	10.4568925
24 H	6.4628980	7.3609828	7.3161894	8.5481594
25 H	6.2063679	7.6643163	8.5883176	9.9700007
26 H	4.9571970	6.3271609	7.4943374	8.7606519
27 H	2.6179181 *	3.8900027	5.0920900	6.3062334
28 H	1.1061900 *	2.1603073 *	3.5248334	4.6527721
29 H	4.8059199	3.5021481	2.1981054 *	1.1070129 *
30 H	5.4425546	3.9845118	3.4439917	2.1944956 *
31 H	4.6420036	3.4960254	3.9380315	3.4795538
32 H	2.6164623 *	2.1975929 *	3.4520826	3.9479525
33 H	4.0430748	3.3350346	2.0465435 *	2.5122490 *
34 H	3.9642578	4.6354204	4.6593109	5.8548560
35 H	4.9973005	5.5766761	5.2984601	6.4359390

C C C O

1 CO	5.4671372	5.6281254	4.6977899	1.9621803 *
2 C	10.3781222	10.0023911	8.6682143	7.3938609
3 C	10.4838682	10.2855535	9.0295145	7.1993863
4 C	9.3864693	9.3185304	8.1464157	5.9798869
5 C	8.0475071	7.9259482	6.7389439	4.7870075
6 C	7.8474595	7.4926330	6.1845801	5.0179984
7 C	9.1676779	8.6982625	7.3376911	6.4576007
8 C	9.4492579	8.7885562	7.3871715	7.1849915
9 C	8.5514959	7.7654890	6.3659750	6.7547883
10 C	7.1381407	6.4057905	5.0112597	5.4070932
11 C	6.7065692	6.2140339	4.8649874	4.3798017
12 N	5.3326356	4.9913507	3.7363206	2.9934267 *
13 C	4.3386602	3.7816695	2.4537818 *	3.0638510
14 C	2.8802438 *	2.4997311 *	1.4431822 *	2.5014577 *
15 C	2.4461812 *	2.8336686 *	2.4483012 *	1.4649231 *
16 C	1.4305218 *	2.4766457 *	2.8423413 *	2.4649875 *
17 C	0.0000000	1.4248154 *	2.4524607 *	3.7773607

18 C	1.4248154 *	0.0000000	1.4150434 *	4.2983808
19 C	2.4524607 *	1.4150434 *	0.0000000	3.7959564
20 O	3.7773607	4.2983808	3.7959564	0.0000000
21 N	7.0679702	7.1454965	6.1201086	3.6783773
22 H	11.3431644	10.8961119	9.5340669	8.4505648
23 H	11.5069302	11.3517095	10.1112490	8.1316171
24 H	9.7188707	9.7920487	8.7103655	6.1777950
25 H	10.5303549	9.8314209	8.4254121	8.2799592
26 H	9.0354106	8.1264629	6.7530159	7.5914782
27 H	6.5577694	5.7023377	4.3367869	5.3845004
28 H	4.8181278	3.9523936	2.5373654 *	4.1501408
29 H	2.1979105 *	3.4743746	3.9489126	2.6999668 *
30 H	1.1043083 *	2.1995077 *	3.4564524	4.6571323
31 H	2.2008844 *	1.1044019 *	2.1887556 *	5.4026853
32 H	3.4538085	2.1832257 *	1.1058694 *	4.6913242
33 H	3.9361817	4.7415987	4.4936791	0.9917638 *
34 H	6.8836487	6.9005669	5.8880367	3.8502111
35 H	7.6587659	7.8872775	6.9603895	4.1092856

N H H H

1 CO	1.9769547 *	6.5302196	6.1921493	4.3928580
2 C	4.3427278	1.1039067 *	2.1846886 *	3.4390162
3 C	3.8204186	2.1764167 *	1.1020663 *	2.1915809 *
4 C	2.4814595 *	3.4506962	2.2028951 *	1.1084377 *
5 C	1.5124105 *	3.9421061	3.4676982	2.1927573 *
6 C	2.5950948 *	3.5211287	4.0261738	3.5171300
7 C	3.8876914	2.1993804 *	3.4858044	3.9591269
8 C	5.1113183	2.6818436 *	4.6659947	5.4006702
9 C	5.3953506	4.0782460	5.9245139	6.2763677
10 C	4.5766033	4.8882076	6.2488805	6.0182096
11 C	3.1675516	4.6924668	5.4854275	4.8167985
12 N	2.9243015 *	6.0131448	6.4188027	5.2052389
13 C	4.0412801	7.1165254	7.6884566	6.4628980
14 C	4.7613840	8.5009272	8.8660968	7.3609828
15 C	4.6961794	9.1187902	9.1181933	7.3161894
16 C	5.9429460	10.5240486	10.4568925	8.5481594
17 C	7.0679702	11.3431644	11.5069302	9.7188707
18 C	7.1454965	10.8961119	11.3517095	9.7920487
19 C	6.1201086	9.5340669	10.1112490	8.7103655
20 O	3.6783773	8.4505648	8.1316171	6.1777950
21 N	0.0000000	5.4439918	4.6826513	2.6725071 *
22 H	5.4439918	0.0000000	2.5217338 *	4.3532166
23 H	4.6826513	2.5217338 *	0.0000000	2.5151321 *
24 H	2.6725071 *	4.3532166	2.5151321 *	0.0000000
25 H	6.0556301	2.4040083 *	4.7772544	5.9785765

26 H	6.4805720	4.7770456	6.8443206	7.3578737
27 H	5.2816616	5.9566027	7.3333758	6.9799871
28 H	4.8179072	7.1475730	8.0405613	7.0826468
29 H	6.2421768	11.0982072	10.8059483	8.7485917
30 H	8.0476896	12.4362225	12.5445439	10.6872595
31 H	8.1687459	11.7006458	12.2890676	10.8054300
32 H	6.5234375	9.3542168	10.1856234	9.0114617
33 H	4.2263572	9.1877837	8.6650675	6.5721558
34 H	1.0452451 *	5.8219009	5.1680956	3.2202029
35 H	1.0427289 *	5.8319028	4.6071414	2.2441902 *

H H H H

1 CO	6.5874468	6.3382844	4.5430026	3.8670191
2 C	2.6810339 *	4.6650084	5.3807399	6.3693812
3 C	4.0823357	5.9292833	6.2604145	6.9401121
4 C	4.8962254	6.2604130	6.0135781	6.3092977
5 C	4.6749703	5.4771949	4.8137863	4.9322434
6 C	3.5213329	4.0233566	3.5090574	4.0318467
7 C	2.1989132 *	3.4833361	3.9424858	4.9791714
8 C	1.1067769 *	2.1851041 *	3.4219738	4.8946186
9 C	2.1789022 *	1.1056439 *	2.1736443 *	3.8821081
10 C	3.4508165	2.1997295 *	1.1040977 *	2.5658345 *
11 C	3.9650553	3.4779234	2.1942008 *	2.6317498 *
12 N	5.4209413	4.6699182	2.6963976 *	2.0945470 *
13 C	6.2063679	4.9571970	2.6179181 *	1.1061900 *
14 C	7.6643163	6.3271609	3.8900027	2.1603073 *
15 C	8.5883176	7.4943374	5.0920900	3.5248334
16 C	9.9700007	8.7606519	6.3062334	4.6527721
17 C	10.5303549	9.0354106	6.5577694	4.8181278
18 C	9.8314209	8.1264629	5.7023377	3.9523936
19 C	8.4254121	6.7530159	4.3367869	2.5373654 *
20 O	8.2799592	7.5914782	5.3845004	4.1501408
21 N	6.0556301	6.4805720	5.2816616	4.8179072
22 H	2.4040083 *	4.7770456	5.9566027	7.1475730
23 H	4.7772544	6.8443206	7.3333758	8.0405613
24 H	5.9785765	7.3578737	6.9799871	7.0826468
25 H	0.0000000	2.5266343 *	4.3387025	5.9147902
26 H	2.5266343 *	0.0000000	2.4917453 *	4.3516353
27 H	4.3387025	2.4917453 *	0.0000000	2.0550933 *
28 H	5.9147902	4.3516353	2.0550933 *	0.0000000
29 H	10.7302158	9.6702036	7.2454839	5.6580038
30 H	11.6312567	10.1005602	7.6229353	5.8949533
31 H	10.4822923	8.6124453	6.2757580	4.6045712
32 H	8.0194931	6.1573645	3.8827062	2.2085470 *
33 H	9.1569686	8.5434078	6.3469475	5.1195490

34 H	6.3103314	6.6278208	5.3894324	4.6481243
35 H	6.7707533	7.4098493	6.2865391	5.8260783

H H H H

1 CO	4.6587533	6.4519193	6.6936293	5.2708983
2 C	10.0523569	11.4632323	10.8503153	8.5733784
3 C	9.8805394	11.5347558	11.2111195	9.0890892
4 C	8.6326742	10.4051605	10.2951861	8.3447864
5 C	7.4435146	9.0866698	8.8935772	6.9412014
6 C	7.6132455	8.9343609	8.3726826	6.1917990
7 C	9.0415738	10.2650102	9.5076210	7.1875261
8 C	9.6253012	10.5513975	9.4772833	7.0413637
9 C	8.9851937	9.6412387	8.3700205	5.9126860
10 C	7.5652417	8.2312047	7.0741864	4.6684610
11 C	6.7761060	7.8078051	7.0426110	4.8032155
12 N	5.3200330	6.4258110	5.9158629	3.9448992
13 C	4.8059199	5.4425546	4.6420036	2.6164623 *
14 C	3.5021481	3.9845118	3.4960254	2.1975929 *
15 C	2.1981054 *	3.4439917	3.9380315	3.4520826
16 C	1.1070129 *	2.1944956 *	3.4795538	3.9479525
17 C	2.1979105 *	1.1043083 *	2.2008844 *	3.4538085
18 C	3.4743746	2.1995077 *	1.1044019 *	2.1832257 *
19 C	3.9489126	3.4564524	2.1887556 *	1.1058694 *
20 O	2.6999668 *	4.6571323	5.4026853	4.6913242
21 N	6.2421768	8.0476896	8.1687459	6.5234375
22 H	11.0982072	12.4362225	11.7006458	9.3542168
23 H	10.8059483	12.5445439	12.2890676	10.1856234
24 H	8.7485917	10.6872595	10.8054300	9.0114617
25 H	10.7302158	11.6312567	10.4822923	8.0194931
26 H	9.6702036	10.1005602	8.6124453	6.1573645
27 H	7.2454839	7.6229353	6.2757580	3.8827062
28 H	5.6580038	5.8949533	4.6045712	2.2085470 *
29 H	0.0000000	2.5172559 *	4.3877957	5.0542893
30 H	2.5172559 *	0.0000000	2.5415693 *	4.3698318
31 H	4.3877957	2.5415693 *	0.0000000	2.5139870 *
32 H	5.0542893	4.3698318	2.5139870 *	0.0000000
33 H	2.3156453 *	4.6370790	5.8279043	5.4729871
34 H	6.2074225	7.8536374	7.8803989	6.2482393
35 H	6.5702842	8.5762136	8.9379064	7.4453509

H H H

1 CO	2.6641817 *	2.4805481 *	2.6003246 *
2 C	8.1164092	4.7539414	4.7510499
3 C	7.7976966	4.3131596	3.9351810

4 C	6.5175110	3.0539386	2.5018117 *
5 C	5.4413851	2.1143810 *	2.0959786 *
6 C	5.8352930	2.9723970 *	3.4294247
7 C	7.2738658	4.2349985	4.5733123
8 C	8.0726175	5.3655650	5.8976904
9 C	7.6954383	5.5754446	6.3123412
10 C	6.3651922	4.7312892	5.5629037
11 C	5.3086497	3.3820139	4.1590144
12 N	3.9577928	3.0702391	3.9005808
13 C	4.0430748	3.9642578	4.9973005
14 C	3.3350346	4.6354204	5.5766761
15 C	2.0465435 *	4.6593109	5.2984601
16 C	2.5122490 *	5.8548560	6.4359390
17 C	3.9361817	6.8836487	7.6587659
18 C	4.7415987	6.9005669	7.8872775
19 C	4.4936791	5.8880367	6.9603895
20 O	0.9917638 *	3.8502111	4.1092856
21 N	4.2263572	1.0452451 *	1.0427289 *
22 H	9.1877837	5.8219009	5.8319028
23 H	8.6650675	5.1680956	4.6071414
24 H	6.5721558	3.2202029	2.2441902 *
25 H	9.1569686	6.3103314	6.7707533
26 H	8.5434078	6.6278208	7.4098493
27 H	6.3469475	5.3894324	6.2865391
28 H	5.1195490	4.6481243	5.8260783
29 H	2.3156453 *	6.2074225	6.5702842
30 H	4.6370790	7.8536374	8.5762136
31 H	5.8279043	7.8803989	8.9379064
32 H	5.4729871	6.2482393	7.4453509
33 H	0.0000000	4.4361065	4.4434637
34 H	4.4361065	0.0000000	1.6744144 *
35 H	4.4434637	1.6744144 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.84 , TOTAL = 4839.1 SECONDS (80.7 MIN)
WALL CLOCK TIME: STEP = 0.85 , TOTAL = 4473.8 SECONDS (74.6 MIN)

CPU UTILIZATION: STEP = 99.34% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.85 , TOTAL = 4839.9 SECONDS (80.7 MIN)

WALL CLOCK TIME: STEP = 0.85 , TOTAL = 4474.7 SECONDS (74.6 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.634287854	-284.634287854	0.025237682	0.002211660	196904594
11409288						
2	1	-284.634741024	-0.000453170	0.015063589	0.000272609	164616508
14160234						
3	2	-284.634730452	0.000010572	0.003631767	0.000515313	153912654
15045698						
4	3	-284.634751694	-0.000021243	0.001905430	0.000183562	147534942
15560951						
5	4	-284.634750410	0.000001285	0.000806719	0.000379168	139863439
16200589						
6	5	-284.634752603	-0.000002193	0.000772267	0.000103573	134396214
16655061						
7	6	-284.634752591	0.000000011	0.000376180	0.000077478	128593126
17053939						
8	7	-284.634752913	-0.000000321	0.000421965	0.000058455	145419356
15783310						
9	8	-284.634752985	-0.000000072	0.000463655	0.000040601	166856717
14061351						

-----DISABLING FDIFF OPTION-----

10	9	-284.634753077	-0.000000092	0.000167526	0.000021898	196887191
11410941						
11	10	-284.634753096	-0.000000019	0.000127573	0.000019575	196886909
11410942						
12	11	-284.634753113	-0.000000017	0.000102266	0.000015656	196887005
11410942						
13	12	-284.634753121	-0.000000008	0.000101362	0.000011094	196887068
11410942						
14	13	-284.634753127	-0.000000006	0.000086014	0.000005844	196887020
11410941						
15	14	-284.634753129	-0.000000002	0.000041821	0.000006733	196887071
11410935						
16	15	-284.634753131	-0.000000002	0.000037878	0.000006329	196887040
11410937						
17	16	-284.634753132	-0.000000001	0.000066580	0.000005307	196887058
11410935						

18 17 -284.634753134 -0.000000002 0.000139374 0.000003669 196887058
11410940
19 18 -284.634753136 -0.000000002 0.000060898 0.000002110 196887079
11410935
20 19 -284.634753137 0.000000000 0.000023757 0.000001972 196887067
11410934
21 20 -284.634753137 0.000000000 0.000008501 0.000001361 196887085
11410934

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 71.3 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 22.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.7, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.0 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6347531371 AFTER 21 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5947104526
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000113493

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 74.57 , TOTAL = 4914.5 SECONDS (81.9 MIN)
WALL CLOCK TIME: STEP = 68.93 , TOTAL = 4543.6 SECONDS (75.7
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.72 , TOTAL = 4918.2 SECONDS (82.0 MIN)
WALL CLOCK TIME: STEP = 3.69 , TOTAL = 4547.3 SECONDS (75.8
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.

USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84 , TOTAL = 4921.1 SECONDS (82.0 MIN)
WALL CLOCK TIME: STEP = 2.66 , TOTAL = 4550.0 SECONDS (75.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 48 ENERGY= -284.6347531

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0003850	-0.0001062	-0.0005101
2 C	6.0	0.0001145	0.0027744	0.0003867
3 C	6.0	0.0027712	-0.0021708	0.0004363
4 C	6.0	0.0009223	-0.0019776	0.0001423
5 C	6.0	-0.0000831	0.0001547	-0.0001264
6 C	6.0	0.0008063	0.0005976	-0.0000910
7 C	6.0	-0.0010730	0.0014783	0.0000444
8 C	6.0	-0.0022658	-0.0013734	-0.0004685
9 C	6.0	0.0010484	-0.0002983	-0.0006601
10 C	6.0	-0.0010519	-0.0008480	-0.0004739
11 C	6.0	0.0002279	0.0000118	0.0000378
12 N	7.0	0.0001604	0.0003273	0.0007783
13 C	6.0	0.0010236	0.0007614	0.0003834
14 C	6.0	-0.0004551	-0.0004236	0.0002706
15 C	6.0	0.0010592	-0.0004437	0.0001769
16 C	6.0	0.0009589	-0.0002395	-0.0002781
17 C	6.0	-0.0018875	-0.0010384	0.0002903
18 C	6.0	-0.0003849	0.0021470	0.0001464
19 C	6.0	0.0014078	-0.0002526	0.0001626
20 O	8.0	0.0001054	-0.0011549	-0.0002453
21 N	7.0	-0.0006707	0.0020901	-0.0003625
22 H	1.0	-0.0002519	-0.0008817	-0.0007469
23 H	1.0	-0.0012096	0.0007510	0.0005786
24 H	1.0	0.0012826	-0.0001571	-0.0002331
25 H	1.0	0.0006602	0.0010949	-0.0002955
26 H	1.0	-0.0000454	0.0009747	0.0001407
27 H	1.0	0.0000726	0.0005396	0.0008722
28 H	1.0	-0.0006570	-0.0003057	0.0006476
29 H	1.0	-0.0006011	-0.0001446	-0.0010847

30 H	1.0	0.0004055	0.0007108	0.0001702
31 H	1.0	-0.0001597	0.0002488	0.0002945
32 H	1.0	-0.0000299	-0.0001279	-0.0008927
33 H	1.0	0.0001431	-0.0003807	-0.0004399
34 H	1.0	-0.0018360	0.0002082	-0.0001674
35 H	1.0	-0.0001222	-0.0025462	0.0011166

MAXIMUM GRADIENT = 0.0027744 RMS GRADIENT = 0.0009222
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001473264
 PREDICTED ENERGY CHANGE WAS -0.0001609630 RATIO= 0.915
 GDIIS STEP HAS LENGTH = 0.129410
 RADIUS OF STEP TAKEN= 0.12941 CURRENT TRUST RADIUS= 0.26653

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 4921.1 SECONDS (82.0 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4550.0 SECONDS (75.8 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 49

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1373457870	-1.7657984448	0.9648637249
C	6.0	4.9882679860	0.6845366613	0.4677216451
C	6.0	5.2109621859	-0.6780360035	0.2486597019
C	6.0	4.0914569689	-1.5472104345	0.0466495328
C	6.0	2.7746386365	-1.0524772236	0.1146369557
C	6.0	2.4804595827	0.3354995808	0.4603973897
C	6.0	3.6503192084	1.2136741393	0.5865812680
C	6.0	3.4857305542	2.6226374143	0.8503617940
C	6.0	2.2160298813	3.1744344878	1.0706721661
C	6.0	1.0681946381	2.3215100678	1.0363761714
C	6.0	1.1708777406	0.9499981912	0.7000203037
N	7.0	-0.0421072577	0.1415427837	0.6976541796
C	6.0	-1.2394241785	0.6776315652	0.4643528919
C	6.0	-2.5492172004	0.0273856833	0.5216027284
C	6.0	-2.8533867019	-1.3485465980	0.8075684507
C	6.0	-4.1711347018	-1.8440510114	0.8336701223
C	6.0	-5.2611386364	-0.9461100787	0.6080434225
C	6.0	-5.0118433565	0.4268410188	0.3282953171
C	6.0	-3.6772914226	0.8923126156	0.2712096707
O	8.0	-1.7544334229	-2.2827088420	1.0731021701

N	7.0	1.6738512586	-2.0232640429	-0.2507597301
H	1.0	5.8437868919	1.3817338685	0.5690409597
H	1.0	6.2376598781	-1.0889135109	0.1994387556
H	1.0	4.2754630349	-2.6136832003	-0.2075481521
H	1.0	4.3889410072	3.2565528973	0.8932929474
H	1.0	2.1002800984	4.2469893057	1.3042576412
H	1.0	0.0988429701	2.7612432739	1.3273442702
H	1.0	-1.2808943748	1.7479365546	0.1797770760
H	1.0	-4.3785856782	-2.9155507571	1.0192679609
H	1.0	-6.2993707245	-1.3278955503	0.6521171754
H	1.0	-5.8500073473	1.1279030709	0.1593803160
H	1.0	-3.4793687961	1.9548779580	0.0406668723
H	1.0	-2.0969053656	-3.1826835278	1.3070158302
H	1.0	1.3216616901	-1.8202442812	-1.2125234269
H	1.0	2.0663361660	-2.9869626312	-0.2703211023

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4573564	5.2381064	4.0652052
2 C	5.4573564	0.0000000	1.3979217 *	2.4417753 *
3 C	5.2381064	1.3979217 *	0.0000000	1.4316299 *
4 C	4.0652052	2.4417753 *	1.4316299 *	0.0000000
5 C	2.8612980 *	2.8358492 *	2.4685706 *	1.4083301 *
6 C	3.1874946	2.5319920 *	2.9202280 *	2.5121897 *
7 C	4.6218326	1.4436831 *	2.4755534 *	2.8475625 *
8 C	5.5211557	2.4819885 *	3.7726535	4.2895791
9 C	5.3607858	3.7747112	4.9484192	5.1826422
10 C	4.1925749	4.2860267	5.1749683	5.0086597
11 C	2.9178557 *	3.8336537	4.3790985	3.8977849
12 N	1.9343099 *	5.0648185	5.3355453	4.5124326
13 C	2.8489220 *	6.2276969	6.5948345	5.7916053
14 C	3.2603083	7.5662695	7.7969546	6.8413074
15 C	3.0237926	8.1080498	8.1114540	6.9892288
16 C	4.3111877	9.5090658	9.4723582	8.3052957
17 C	5.4720055	10.3792599	10.4816943	9.3886916
18 C	5.6326757	10.0044027	10.2826479	9.3191352
19 C	4.7008688	8.6702773	9.0259379	8.1458671
20 O	1.9641132 *	7.3915529	7.1952357	5.9807188
21 N	1.9760764 *	4.3397878	3.8170947	2.4819139 *
22 H	6.5289437	1.1082699 *	2.1784773 *	3.4528637
23 H	6.1852955	2.1858823 *	1.1069558 *	2.1999017 *
24 H	4.3837738	3.4412693	2.1977294 *	1.1116829 *
25 H	6.5806685	2.6749900 *	4.0709042	4.8868644

26 H	6.3341863	4.6616880	5.9200088	6.2545275
27 H	4.5416937	5.3812767	6.2550752	6.0119813
28 H	3.8696382	6.3652280	6.9306774	6.3037985
29 H	4.6603141	10.0500139	9.8772333	8.6348112
30 H	6.4591709	11.4671127	11.5357210	10.4107632
31 H	6.6985603	10.8517215	11.2077845	10.2957104
32 H	5.2705025	8.5730400	9.0828052	8.3415863
33 H	2.6676787 *	8.1153859	7.7973268	6.5237354
34 H	2.4792304 *	4.7477524	4.3088693	3.0548044
35 H	2.5957518 *	4.7499789	3.9356265	2.5048894 *

C C C C

1 CO	2.8612980 *	3.1874946	4.6218326	5.5211557
2 C	2.8358492 *	2.5319920 *	1.4436831 *	2.4819885 *
3 C	2.4685706 *	2.9202280 *	2.4755534 *	3.7726535
4 C	1.4083301 *	2.5121897 *	2.8475625 *	4.2895791
5 C	0.0000000	1.4603326 *	2.4748717 *	3.8148932
6 C	1.4603326 *	0.0000000	1.4682249 *	2.5285651 *
7 C	2.4748717 *	1.4682249 *	0.0000000	1.4428607 *
8 C	3.8148932	2.5285651 *	1.4428607 *	0.0000000
9 C	4.3695343	2.9158035 *	2.4771175 *	1.4018404 *
10 C	3.8917020	2.5040929 *	2.8455198 *	2.4433090 *
11 C	2.6314693 *	1.4662988 *	2.4960015 *	2.8598720 *
12 N	3.1144262	2.5411126 *	3.8465330	4.3156448
13 C	4.3850060	3.7355863	4.9205560	5.1243671
14 C	5.4474917	5.0394770	6.3123493	6.5775382
15 C	5.6782462	5.6041463	6.9937115	7.4804105
16 C	7.0276145	7.0095278	8.4015402	8.8644892
17 C	8.0516135	7.8483543	9.1694716	9.4499946
18 C	7.9286401	7.4940241	8.7016595	8.7922032
19 C	6.7404840	6.1857684	7.3414311	7.3917741
20 O	4.7900542	5.0164471	6.4554432	7.1813198
21 N	1.5125061 *	2.5923208 *	3.8839843	5.1068362
22 H	3.9435438	3.5239722	2.1999664 *	2.6794426 *
23 H	3.4642510	4.0266122	3.4851285	4.6660932
24 H	2.1894386 *	3.5165136	3.9585490	5.4001763
25 H	4.6669067	3.5159995	2.1938523 *	1.1043012 *
26 H	5.4730524	4.0195010	3.4811897	2.1826620 *
27 H	4.8140425	3.5082655	3.9441962	3.4231172
28 H	4.9288851	4.0275935	4.9767252	4.8923919
29 H	7.4470141	7.6110555	9.0388622	9.6201625
30 H	9.0940852	8.9380680	10.2693817	10.5543460
31 H	8.8960991	8.3734816	9.5103135	9.4798570
32 H	6.9399039	6.1901627	7.1888703	7.0437289
33 H	5.4489896	5.8349503	7.2716970	8.0669764

34 H	2.1123359 *	2.9645756 *	4.2265925	5.3551739
35 H	2.0957383 *	3.4269816	4.5704084	5.8939141

	C	C	C	N
--	---	---	---	---

1 CO	5.3607858	4.1925749	2.9178557 *	1.9343099 *
2 C	3.7747112	4.2860267	3.8336537	5.0648185
3 C	4.9484192	5.1749683	4.3790985	5.3355453
4 C	5.1826422	5.0086597	3.8977849	4.5124326
5 C	4.3695343	3.8917020	2.6314693 *	3.1144262
6 C	2.9158035 *	2.5040929 *	1.4662988 *	2.5411126 *
7 C	2.4771175 *	2.8455198 *	2.4960015 *	3.8465330
8 C	1.4018404 *	2.4433090 *	2.8598720 *	4.3156448
9 C	0.0000000	1.4304482 *	2.4855266 *	3.7995734
10 C	1.4304482 *	0.0000000	1.4158827 *	2.4697693 *
11 C	2.4855266 *	1.4158827 *	0.0000000	1.4577168 *
12 N	3.7995734	2.4697693 *	1.4577168 *	0.0000000
13 C	4.3060203	2.8904414 *	2.4370634 *	1.3324370 *
14 C	5.7369829	4.3143559	3.8369458	2.5158748 *
15 C	6.7989386	5.3759157	4.6356854	3.1836676
16 C	8.1263299	6.6965335	6.0300639	4.5836613
17 C	8.5499101	7.1359141	6.7063046	5.3319140
18 C	7.7680464	6.4076526	6.2159402	4.9916027
19 C	6.3701222	5.0147506	4.8674378	3.7363183
20 O	6.7487034	5.4006860	4.3757320	2.9916581 *
21 N	5.3903812	4.5717175	3.1618433	2.9206833 *
22 H	4.0775029	4.8895667	4.6946386	6.0165077
23 H	5.9252588	6.2493859	5.4845259	6.4185447
24 H	6.2751429	6.0158167	4.8126869	5.2011609
25 H	2.1816850 *	3.4528444	3.9640232	5.4199402
26 H	1.1037817 *	2.2010069 *	3.4783677	4.6703835
27 H	2.1723462 *	1.1034810 *	2.1962246 *	2.6980006 *
28 H	3.8803440	2.5653397 *	2.6303127 *	2.0936311 *
29 H	8.9766094	7.5560912	6.7705932	5.3154775
30 H	9.6414839	8.2308466	7.8099748	6.4276488
31 H	8.3713619	7.0749797	7.0439172	5.9156022
32 H	5.9148791	4.6697098	4.8030535	3.9413936
33 H	7.6857152	6.3550965	5.3033865	3.9552494
34 H	5.5641435	4.7197377	3.3696888	3.0589627
35 H	6.3074151	5.5573039	4.1524774	3.8948756

	C	C	C	C
--	---	---	---	---

1 CO	2.8489220 *	3.2603083	3.0237926	4.3111877
2 C	6.2276969	7.5662695	8.1080498	9.5090658
3 C	6.5948345	7.7969546	8.1114540	9.4723582

4 C	5.7916053	6.8413074	6.9892288	8.3052957
5 C	4.3850060	5.4474917	5.6782462	7.0276145
6 C	3.7355863	5.0394770	5.6041463	7.0095278
7 C	4.9205560	6.3123493	6.9937115	8.4015402
8 C	5.1243671	6.5775382	7.4804105	8.8644892
9 C	4.3060203	5.7369829	6.7989386	8.1263299
10 C	2.8904414 *	4.3143559	5.3759157	6.6965335
11 C	2.4370634 *	3.8369458	4.6356854	6.0300639
12 N	1.3324370 *	2.5158748 *	3.1836676	4.5836613
13 C	0.0000000	1.4634394 *	2.6130576 *	3.8846113
14 C	1.4634394 *	0.0000000	1.4378752 *	2.4960524 *
15 C	2.6130576 *	1.4378752 *	0.0000000	1.4080716 *
16 C	3.8846113	2.4960524 *	1.4080716 *	0.0000000
17 C	4.3395128	2.8826522 *	2.4492927 *	1.4301447 *
18 C	3.7831936	2.5022909 *	2.8356021 *	2.4736906 *
19 C	2.4549112 *	1.4433803 *	2.4470288 *	2.8368872 *
20 O	3.0658483	2.5044699 *	1.4665830 *	2.4678317 *
21 N	4.0365080	4.7577322	4.6979981	5.9474336
22 H	7.1188903	8.5017073	9.1187804	10.5249404
23 H	7.6874994	8.8633584	9.1150622	10.4554047
24 H	6.4574132	7.3541258	7.3110554	8.5452608
25 H	6.2059100	7.6618349	8.5828667	9.9646681
26 H	4.9597761	6.3273556	7.4896954	8.7551624
27 H	2.6224322 *	3.8904266	5.0868654	6.2996158
28 H	1.1082671 *	2.1646669 *	3.5291730	4.6565481
29 H	4.8034597	3.5007334	2.1969412 *	1.1070656 *
30 H	5.4461412	3.9896708	3.4495503	2.1974454 *
31 H	4.6425456	3.4982223	3.9411529	3.4793377
32 H	2.6130863 *	2.1935605 *	3.4485657	3.9419862
33 H	4.0431903	3.3355665	2.0459154 *	2.5136469 *
34 H	3.9510073	4.6265142	4.6620059	5.8615942
35 H	4.9896942	5.5692703	5.2962181	6.4366984

C C C O

1 CO	5.4720055	5.6326757	4.7008688	1.9641132 *
2 C	10.3792599	10.0044027	8.6702773	7.3915529
3 C	10.4816943	10.2826479	9.0259379	7.1952357
4 C	9.3886916	9.3191352	8.1458671	5.9807188
5 C	8.0516135	7.9286401	6.7404840	4.7900542
6 C	7.8483543	7.4940241	6.1857684	5.0164471
7 C	9.1694716	8.7016595	7.3414311	6.4554432
8 C	9.4499946	8.7922032	7.3917741	7.1813198
9 C	8.5499101	7.7680464	6.3701222	6.7487034
10 C	7.1359141	6.4076526	5.0147506	5.4006860
11 C	6.7063046	6.2159402	4.8674378	4.3757320

12 N	5.3319140	4.9916027	3.7363183	2.9916581 *
13 C	4.3395128	3.7831936	2.4549112 *	3.0658483
14 C	2.8826522 *	2.5022909 *	1.4433803 *	2.5044699 *
15 C	2.4492927 *	2.8356021 *	2.4470288 *	1.4665830 *
16 C	1.4301447 *	2.4736906 *	2.8368872 *	2.4678317 *
17 C	0.0000000	1.4231661 *	2.4498626 *	3.7815020
18 C	1.4231661 *	0.0000000	1.4145499 *	4.3019899
19 C	2.4498626 *	1.4145499 *	0.0000000	3.7975223
20 O	3.7815020	4.3019899	3.7975223	0.0000000
21 N	7.0704942	7.1440067	6.1161890	3.6841631
22 H	11.3463540	10.9002058	9.5383001	8.4507497
23 H	11.5069422	11.3518914	10.1112149	8.1278528
24 H	9.7155937	9.7870310	8.7044540	6.1732698
25 H	10.5293770	9.8336788	8.4285660	8.2738625
26 H	9.0356782	8.1319331	6.7602793	7.5861194
27 H	6.5567725	5.7067195	4.3436751	5.3796585
28 H	4.8253128	3.9607236	2.5462072 *	4.1555230
29 H	2.1969756 *	3.4713169	3.9435046	2.6999189 *
30 H	1.1070811 *	2.2003835 *	3.4568359	4.6631912
31 H	2.2021797 *	1.1056849 *	2.1883106 *	5.4074844
32 H	3.4514275	2.1831412 *	1.1051554 *	4.6902523
33 H	3.9374097	4.7416690	4.4917823	0.9909375 *
34 H	6.8856252	6.8946937	5.8778364	3.8600931
35 H	7.6569243	7.8811815	6.9520709	4.1108442

N H H H

1 CO	1.9760764 *	6.5289437	6.1852955	4.3837738
2 C	4.3397878	1.1082699 *	2.1858823 *	3.4412693
3 C	3.8170947	2.1784773 *	1.1069558 *	2.1977294 *
4 C	2.4819139 *	3.4528637	2.1999017 *	1.1116829 *
5 C	1.5125061 *	3.9435438	3.4642510	2.1894386 *
6 C	2.5923208 *	3.5239722	4.0266122	3.5165136
7 C	3.8839843	2.1999664 *	3.4851285	3.9585490
8 C	5.1068362	2.6794426 *	4.6660932	5.4001763
9 C	5.3903812	4.0775029	5.9252588	6.2751429
10 C	4.5717175	4.8895667	6.2493859	6.0158167
11 C	3.1618433	4.6946386	5.4845259	4.8126869
12 N	2.9206833 *	6.0165077	6.4185447	5.2011609
13 C	4.0365080	7.1188903	7.6874994	6.4574132
14 C	4.7577322	8.5017073	8.8633584	7.3541258
15 C	4.6979981	9.1187804	9.1150622	7.3110554
16 C	5.9474336	10.5249404	10.4554047	8.5452608
17 C	7.0704942	11.3463540	11.5069422	9.7155937
18 C	7.1440067	10.9002058	11.3518914	9.7870310
19 C	6.1161890	9.5383001	10.1112149	8.7044540

20	O	3.6841631	8.4507497	8.1278528	6.1732698
21	N	0.0000000	5.4455897	4.6801751	2.6681165 *
22	H	5.4455897	0.0000000	2.5289998 *	4.3618904
23	H	4.6801751	2.5289998 *	0.0000000	2.5180900 *
24	H	2.6681165 *	4.3618904	2.5180900 *	0.0000000
25	H	6.0462415	2.3951330 *	4.7730780	5.9736421
26	H	6.4742565	4.7711713	6.8418123	7.3543052
27	H	5.2785011	5.9567148	7.3335497	6.9778137
28	H	4.8101806	7.1446983	8.0359668	7.0743802
29	H	6.2482909	11.0980296	10.8033973	8.7457853
30	H	8.0542531	12.4420766	12.5474765	10.6873469
31	H	8.1674058	11.7037206	12.2893279	10.8008914
32	H	6.5166111	9.3556884	10.1838363	9.0039313
33	H	4.2414059	9.1887489	8.6646164	6.5745528
34	H	1.0441475 *	5.8203309	5.1667708	3.2193886
35	H	1.0407411 *	5.8360236	4.6068651	2.2413209 *

H H H H

1	CO	6.5806685	6.3341863	4.5416937	3.8696382
2	C	2.6749900 *	4.6616880	5.3812767	6.3652280
3	C	4.0709042	5.9200088	6.2550752	6.9306774
4	C	4.8868644	6.2545275	6.0119813	6.3037985
5	C	4.6669067	5.4730524	4.8140425	4.9288851
6	C	3.5159995	4.0195010	3.5082655	4.0275935
7	C	2.1938523 *	3.4811897	3.9441962	4.9767252
8	C	1.1043012 *	2.1826620 *	3.4231172	4.8923919
9	C	2.1816850 *	1.1037817 *	2.1723462 *	3.8803440
10	C	3.4528444	2.2010069 *	1.1034810 *	2.5653397 *
11	C	3.9640232	3.4783677	2.1962246 *	2.6303127 *
12	N	5.4199402	4.6703835	2.6980006 *	2.0936311 *
13	C	6.2059100	4.9597761	2.6224322 *	1.1082671 *
14	C	7.6618349	6.3273556	3.8904266	2.1646669 *
15	C	8.5828667	7.4896954	5.0868654	3.5291730
16	C	9.9646681	8.7551624	6.2996158	4.6565481
17	C	10.5293770	9.0356782	6.5567725	4.8253128
18	C	9.8336788	8.1319331	5.7067195	3.9607236
19	C	8.4285660	6.7602793	4.3436751	2.5462072 *
20	O	8.2738625	7.5861194	5.3796585	4.1555230
21	N	6.0462415	6.4742565	5.2785011	4.8101806
22	H	2.3951330 *	4.7711713	5.9567148	7.1446983
23	H	4.7730780	6.8418123	7.3335497	8.0359668
24	H	5.9736421	7.3543052	6.9778137	7.0743802
25	H	0.0000000	2.5274147 *	4.3403541	5.9103351
26	H	2.5274147 *	0.0000000	2.4927344 *	4.3522479
27	H	4.3403541	2.4927344 *	0.0000000	2.0609163 *

28 H	5.9103351	4.3522479	2.0609163 *	0.0000000
29 H	10.7228848	9.6622410	7.2365923	5.6611439
30 H	11.6325122	10.1024137	7.6232622	5.9049939
31 H	10.4835987	8.6166417	6.2785954	4.6110358
32 H	8.0207000	6.1630283	3.8870764	2.2125700 *
33 H	9.1488325	8.5332533	6.3365598	5.1232368
34 H	6.2941667	6.6145111	5.3792417	4.6307357
35 H	6.7623943	7.4034121	6.2821521	5.8159961

H H H H

1 CO	4.6603141	6.4591709	6.6985603	5.2705025
2 C	10.0500139	11.4671127	10.8517215	8.5730400
3 C	9.8772333	11.5357210	11.2077845	9.0828052
4 C	8.6348112	10.4107632	10.2957104	8.3415863
5 C	7.4470141	9.0940852	8.8960991	6.9399039
6 C	7.6110555	8.9380680	8.3734816	6.1901627
7 C	9.0388622	10.2693817	9.5103135	7.1888703
8 C	9.6201625	10.5543460	9.4798570	7.0437289
9 C	8.9766094	9.6414839	8.3713619	5.9148791
10 C	7.5560912	8.2308466	7.0749797	4.6697098
11 C	6.7705932	7.8099748	7.0439172	4.8030535
12 N	5.3154775	6.4276488	5.9156022	3.9413936
13 C	4.8034597	5.4461412	4.6425456	2.6130863 *
14 C	3.5007334	3.9896708	3.4982223	2.1935605 *
15 C	2.1969412 *	3.4495503	3.9411529	3.4485657
16 C	1.1070656 *	2.1974454 *	3.4793377	3.9419862
17 C	2.1969756 *	1.1070811 *	2.2021797 *	3.4514275
18 C	3.4713169	2.2003835 *	1.1056849 *	2.1831412 *
19 C	3.9435046	3.4568359	2.1883106 *	1.1051554 *
20 O	2.6999189 *	4.6631912	5.4074844	4.6902523
21 N	6.2482909	8.0542531	8.1674058	6.5166111
22 H	11.0980296	12.4420766	11.7037206	9.3556884
23 H	10.8033973	12.5474765	12.2893279	10.1838363
24 H	8.7457853	10.6873469	10.8008914	9.0039313
25 H	10.7228848	11.6325122	10.4835987	8.0207000
26 H	9.6622410	10.1024137	8.6166417	6.1630283
27 H	7.2365923	7.6232622	6.2785954	3.8870764
28 H	5.6611439	5.9049939	4.6110358	2.2125700 *
29 H	0.0000000	2.5189013 *	4.3879388	5.0484975
30 H	2.5189013 *	0.0000000	2.5447326 *	4.3706846
31 H	4.3879388	2.5447326 *	0.0000000	2.5135448 *
32 H	5.0484975	4.3706846	2.5135448 *	0.0000000
33 H	2.3152157 *	4.6400265	5.8295796	5.4689471
34 H	6.2187948	7.8612612	7.8744225	6.2347356
35 H	6.5730630	8.5783709	8.9322594	7.4346046

	H	H	H
1 CO	2.6676787 *	2.4792304 *	2.5957518 *
2 C	8.1153859	4.7477524	4.7499789
3 C	7.7973268	4.3088693	3.9356265
4 C	6.5237354	3.0548044	2.5048894 *
5 C	5.4489896	2.1123359 *	2.0957383 *
6 C	5.8349503	2.9645756 *	3.4269816
7 C	7.2716970	4.2265925	4.5704084
8 C	8.0669764	5.3551739	5.8939141
9 C	7.6857152	5.5641435	6.3074151
10 C	6.3550965	4.7197377	5.5573039
11 C	5.3033865	3.3696888	4.1524774
12 N	3.9552494	3.0589627	3.8948756
13 C	4.0431903	3.9510073	4.9896942
14 C	3.3355665	4.6265142	5.5692703
15 C	2.0459154 *	4.6620059	5.2962181
16 C	2.5136469 *	5.8615942	6.4366984
17 C	3.9374097	6.8856252	7.6569243
18 C	4.7416690	6.8946937	7.8811815
19 C	4.4917823	5.8778364	6.9520709
20 O	0.9909375 *	3.8600931	4.1108442
21 N	4.2414059	1.0441475 *	1.0407411 *
22 H	9.1887489	5.8203309	5.8360236
23 H	8.6646164	5.1667708	4.6068651
24 H	6.5745528	3.2193886	2.2413209 *
25 H	9.1488325	6.2941667	6.7623943
26 H	8.5332533	6.6145111	7.4034121
27 H	6.3365598	5.3792417	6.2821521
28 H	5.1232368	4.6307357	5.8159961
29 H	2.3152157 *	6.2187948	6.5730630
30 H	4.6400265	7.8612612	8.5783709
31 H	5.8295796	7.8744225	8.9322594
32 H	5.4689471	6.2347356	7.4346046
33 H	0.0000000	4.4599237	4.4563302
34 H	4.4599237	0.0000000	1.6743706 *
35 H	4.4563302	1.6743706 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.79 , TOTAL = 4921.9 SECONDS (82.0 MIN)

WALL CLOCK TIME: STEP = 0.79 , TOTAL = 4550.8 SECONDS (75.8 MIN)

CPU UTILIZATION: STEP = 99.47%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.92 , TOTAL = 4922.8 SECONDS (82.0 MIN)

WALL CLOCK TIME: STEP = 0.92 , TOTAL = 4551.7 SECONDS (75.9 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.634391826 -284.634391826 0.028796365 0.002204739 196942180
11406171

2 1 -284.634846804 -0.000454979 0.007133618 0.000338583 165073762
14112288

3 2 -284.634839349 0.000007455 0.003382393 0.000647470 151935361
15205382

4 3 -284.634857671 -0.000018322 0.000934131 0.000129933 146074687
15638914

5 4 -284.634857217 0.000000453 0.000479286 0.000227230 136693710
16417022

6 5 -284.634858278 -0.000001061 0.000486227 0.000088394 129184216
17032694

7 6 -284.634858220 0.000000058 0.000282474 0.000069773 152432750
15194544

8 7 -284.634858529 -0.000000309 0.000417733 0.000053312 167185060
13999541

-----DISABLING FDIFF OPTION-----

9 8 -284.634858608 -0.000000079 0.000441080 0.000031825 196945230
11405695

10 9 -284.634858671 -0.000000063 0.000238541 0.000021639 196945276
11405688

11 10 -284.634858687 -0.000000016 0.000122174 0.000018508 196945386
11405682

12 11 -284.634858706 -0.000000019 0.000093433 0.000014821 196945187
11405698

13 12 -284.634858714 -0.000000008 0.000105163 0.000010586 196945332
11405690

14 13 -284.634858723 -0.000000009 0.000139616 0.000007993 196945315
11405692

15	14	-284.634858728	-0.000000005	0.000052667	0.000011928	196945348
11405693						
16	15	-284.634858732	-0.000000004	0.000084971	0.000011806	196945313
11405694						
17	16	-284.634858736	-0.000000004	0.000177206	0.000009749	196945343
11405684						
18	17	-284.634858744	-0.000000007	0.000185386	0.000004907	196945266
11405685						
19	18	-284.634858747	-0.000000004	0.000059943	0.000004311	196945319
11405691						
20	19	-284.634858748	-0.000000001	0.000038714	0.000003311	196945280
11405695						
21	20	-284.634858749	-0.000000001	0.000014341	0.000002401	196945292
11405696						
22	21	-284.634858749	0.000000000	0.000017752	0.000001605	196945262
11405699						

 DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 74.5 SECONDS (3.4 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 23.9 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.0
 TIME TO SOLVE SCF EQUATIONS= 2.9 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6348587492 AFTER 22 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.5965697484
 INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000047096

 SPIN SZ = 1.500
 S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
 PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 78.40 , TOTAL = 5001.2 SECONDS (83.4 MIN)
 WALL CLOCK TIME: STEP = 71.67 , TOTAL = 4623.4 SECONDS (77.1 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
 END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.76 , TOTAL = 5005.0 SECONDS (83.4 MIN)
 WALL CLOCK TIME: STEP = 3.74 , TOTAL = 4627.1 SECONDS (77.1 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
 USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.83 , TOTAL = 5007.8 SECONDS (83.5 MIN)
 WALL CLOCK TIME: STEP = 2.66 , TOTAL = 4629.8 SECONDS (77.2 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 49 ENERGY= -284.6348587

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0004921	-0.0000518	-0.0005632
2 C	6.0	-0.0016851	-0.0028904	-0.0008272
3 C	6.0	-0.0041065	0.0035581	0.0010009
4 C	6.0	0.0024546	0.0015501	0.0010487
5 C	6.0	0.0022255	-0.0003608	-0.0002058
6 C	6.0	-0.0004972	0.0014053	0.0002735
7 C	6.0	0.0008680	0.0001530	-0.0002478
8 C	6.0	0.0001764	-0.0002067	-0.0000719
9 C	6.0	-0.0006097	0.0014831	0.0002584
10 C	6.0	-0.0023697	-0.0011548	-0.0003486
11 C	6.0	0.0010711	-0.0015019	-0.0001460
12 N	7.0	-0.0004950	0.0010306	0.0005078
13 C	6.0	0.0000407	-0.0011689	0.0003525
14 C	6.0	0.0008800	0.0005511	-0.0001896
15 C	6.0	0.0011905	-0.0004811	0.0009795
16 C	6.0	0.0000806	0.0010333	-0.0002924
17 C	6.0	0.0000617	0.0001797	-0.0001428
18 C	6.0	0.0001412	0.0003419	-0.0001593
19 C	6.0	0.0001205	-0.0009675	-0.0003251
20 O	8.0	0.0005246	-0.0026436	-0.0002031
21 N	7.0	-0.0006629	0.0009997	-0.0013175

22 H	1.0	0.0018218	0.0012993	-0.0002624
23 H	1.0	0.0015898	-0.0009996	0.0005381
24 H	1.0	0.0006887	-0.0024550	-0.0007672
25 H	1.0	-0.0003324	-0.0003549	-0.0008697
26 H	1.0	0.0005079	-0.0001917	-0.0003548
27 H	1.0	0.0006009	0.0006581	0.0007673
28 H	1.0	-0.0001344	0.0010016	0.0004706
29 H	1.0	-0.0005174	-0.0001509	-0.0011929
30 H	1.0	-0.0014596	0.0002738	0.0004139
31 H	1.0	-0.0007393	0.0009916	0.0004254
32 H	1.0	0.0002311	-0.0005568	-0.0000759
33 H	1.0	0.0001810	0.0004450	-0.0004782
34 H	1.0	-0.0015600	0.0004098	0.0005443
35 H	1.0	-0.0007793	-0.0012287	0.0014604

MAXIMUM GRADIENT = 0.0041065 RMS GRADIENT = 0.0011018
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001056121
 PREDICTED ENERGY CHANGE WAS -0.0001462940 RATIO= 0.722
 GDIIS STEP HAS LENGTH = 0.083258
 RADIUS OF STEP TAKEN= 0.08326 CURRENT TRUST RADIUS= 0.12941

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 5007.8 SECONDS (83.5 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4629.8 SECONDS (77.2
 MIN)
 CPU UTILIZATION: STEP = 91.97%, TOTAL = 100.00%

INSERCH= 50

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1384728712	-1.7687369408	0.9628368441
C	6.0	4.9893767845	0.6858319422	0.4694586870
C	6.0	5.2121017986	-0.6784850908	0.2487363115
C	6.0	4.0897969100	-1.5464599049	0.0445841739
C	6.0	2.7728181002	-1.0509477296	0.1128528425
C	6.0	2.4803836370	0.3343238590	0.4606131551
C	6.0	3.6501220133	1.2131842437	0.5881650948
C	6.0	3.4848326881	2.6214479013	0.8527597998
C	6.0	2.2159148493	3.1713259592	1.0751599224
C	6.0	1.0687258807	2.3188662312	1.0412005556
C	6.0	1.1700076646	0.9484728819	0.7011475922
N	7.0	-0.0417909116	0.1383669802	0.6953826673

C	6.0	-1.2384370295	0.6752677883	0.4594226772
C	6.0	-2.5495377126	0.0256881231	0.5181842611
C	6.0	-2.8546544456	-1.3478045607	0.8110887509
C	6.0	-4.1722449465	-1.8430215327	0.8425678804
C	6.0	-5.2610279760	-0.9454325091	0.6107133457
C	6.0	-5.0104816761	0.4261103821	0.3214235786
C	6.0	-3.6758894849	0.8909972846	0.2634205201
O	8.0	-1.7552767536	-2.2811072304	1.0795963675
N	7.0	1.6743756963	-2.0210913528	-0.2561984544
H	1.0	5.8424748304	1.3825903421	0.5727800779
H	1.0	6.2365415921	-1.0887479175	0.2017223659
H	1.0	4.2732708902	-2.6108832462	-0.2088039692
H	1.0	4.3882364823	3.2560735222	0.8940763968
H	1.0	2.0982404276	4.2441296085	1.3090243679
H	1.0	0.0973924429	2.7563807999	1.3321475744
H	1.0	-1.2768389373	1.7444696814	0.1721817674
H	1.0	-4.3799983233	-2.9128770584	1.0365998092
H	1.0	-6.2991893316	-1.3257947112	0.6579949766
H	1.0	-5.8465993432	1.1272796416	0.1484380902
H	1.0	-3.4762091133	1.9528075302	0.0309539955
H	1.0	-2.0978161394	-3.1807360537	1.3194982220
H	1.0	1.3225483904	-1.8086243980	-1.2190831456
H	1.0	2.0663551747	-2.9817594657	-0.2877601025

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4589009	5.2383489	4.0627031
2 C	5.4589009	0.0000000	1.3998878 *	2.4439495 *
3 C	5.2383489	1.3998878 *	0.0000000	1.4333969 *
4 C	4.0627031	2.4439495 *	1.4333969 *	0.0000000
5 C	2.8596274 *	2.8384333 *	2.4712947 *	1.4087676 *
6 C	3.1874189	2.5335119 *	2.9211227 *	2.5101073 *
7 C	4.6221113	1.4442282 *	2.4765713 *	2.8468281 *
8 C	5.5212285	2.4813669 *	3.7733090	4.2884245
9 C	5.3602801	3.7731480	4.9478437	5.1798672
10 C	4.1928524	4.2854630	5.1749086	5.0060824
11 C	2.9181800 *	3.8353931	4.3806613	3.8962719
12 N	1.9341851 *	5.0659064	5.3357407	4.5091239
13 C	2.8499940 *	6.2278309	6.5944285	5.7877666
14 C	3.2623731	7.5679189	7.7981735	6.8393502
15 C	3.0263877	8.1105619	8.1139870	6.9894490
16 C	4.3130350	9.5115521	9.4749536	8.3057849
17 C	5.4732468	10.3803552	10.4827828	9.3872074

18 C	5.6338707	10.0043260	10.2823454	9.3157256
19 C	4.7024174	8.6701433	9.0255127	8.1421724
20 O	1.9653101 *	7.3936018	7.1974364	5.9812911
21 N	1.9770502 *	4.3408806	3.8174673	2.4799203 *
22 H	6.5282958	1.1063109 *	2.1795427 *	3.4540131
23 H	6.1828895	2.1854602 *	1.1045374 *	2.2006148 *
24 H	4.3793273	3.4411014	2.1965676 *	1.1094437 *
25 H	6.5813326	2.6735392 *	4.0713596	4.8862082
26 H	6.3336481	4.6610109	5.9205134	6.2526821
27 H	4.5403489	5.3817205	6.2555843	6.0092887
28 H	3.8692200	6.3619609	6.9269706	6.2966085
29 H	4.6616606	10.0527382	9.8803654	8.6364705
30 H	6.4600790	11.4679515	11.5367381	10.4094189
31 H	6.6986004	10.8497147	11.2056110	10.2903663
32 H	5.2710743	8.5710943	9.0806319	8.3360366
33 H	2.6686958 *	8.1179566	7.8001725	6.5255513
34 H	2.4828211 *	4.7454311	4.3081707	3.0533997
35 H	2.5984893 *	4.7506486	3.9355588	2.5029690 *

C C C C

1 CO	2.8596274 *	3.1874189	4.6221113	5.5212285
2 C	2.8384333 *	2.5335119 *	1.4442282 *	2.4813669 *
3 C	2.4712947 *	2.9211227 *	2.4765713 *	3.7733090
4 C	1.4087676 *	2.5101073 *	2.8468281 *	4.2884245
5 C	0.0000000	1.4578863 *	2.4742428 *	3.8132554
6 C	1.4578863 *	0.0000000	1.4686568 *	2.5285635 *
7 C	2.4742428 *	1.4686568 *	0.0000000	1.4424068 *
8 C	3.8132554	2.5285635 *	1.4424068 *	0.0000000
9 C	4.3662079	2.9148229 *	2.4755672 *	1.4007070 *
10 C	3.8886252	2.5036509 *	2.8445351 *	2.4422608 *
11 C	2.6292156 *	1.4670109 *	2.4967588 *	2.8601130 *
12 N	3.1106003	2.5406456 *	3.8466802	4.3159625
13 C	4.3806505	3.7344171	4.9197498	5.1236323
14 C	5.4452649	5.0397102	6.3127510	6.5775022
15 C	5.6783893	5.6049104	6.9943174	7.4796924
16 C	7.0280698	7.0102917	8.4020557	8.8635450
17 C	8.0499492	7.8479144	9.1689001	9.4483491
18 C	7.9249579	7.4927206	8.7003846	8.7904602
19 C	6.7364420	6.1845347	7.3402798	7.3903804
20 O	4.7907753	5.0164169	6.4552237	7.1795020
21 N	1.5112754 *	2.5906463 *	3.8829193	5.1049695
22 H	3.9441644	3.5235070	2.1989420 *	2.6779905 *
23 H	3.4650696	4.0250317	3.4839340	4.6649014
24 H	2.1882003 *	3.5123794	3.9556247	5.3968363
25 H	4.6658674	3.5163069	2.1935796 *	1.1048055 *

26 H	5.4702583	4.0190068	3.4806040	2.1826386 *
27 H	4.8104400	3.5077883	3.9442177	3.4238532
28 H	4.9211381	4.0234842	4.9729519	4.8893552
29 H	7.4486826	7.6118930	9.0392648	9.6186338
30 H	9.0925266	8.9373293	10.2684023	10.5520493
31 H	8.8904611	8.3704766	9.5072844	9.4765095
32 H	6.9339451	6.1874949	7.1862453	7.0412036
33 H	5.4511530	5.8355157	7.2718757	8.0653054
34 H	2.1098364 *	2.9587479 *	4.2207905	5.3472934
35 H	2.0946634 *	3.4246008	4.5687104	5.8914172

C C C N

1 CO	5.3602801	4.1928524	2.9181800 *	1.9341851 *
2 C	3.7731480	4.2854630	3.8353931	5.0659064
3 C	4.9478437	5.1749086	4.3806613	5.3357407
4 C	5.1798672	5.0060824	3.8962719	4.5091239
5 C	4.3662079	3.8886252	2.6292156 *	3.1106003
6 C	2.9148229 *	2.5036509 *	1.4670109 *	2.5406456 *
7 C	2.4755672 *	2.8445351 *	2.4967588 *	3.8466802
8 C	1.4007070 *	2.4422608 *	2.8601130 *	4.3159625
9 C	0.0000000	1.4296445 *	2.4849312 *	3.8000403
10 C	1.4296445 *	0.0000000	1.4155818 *	2.4713184 *
11 C	2.4849312 *	1.4155818 *	0.0000000	1.4576559 *
12 N	3.8000403	2.4713184 *	1.4576559 *	0.0000000
13 C	4.3060406	2.8918648 *	2.4359142 *	1.3326296 *
14 C	5.7371419	4.3155583	3.8366685	2.5165234 *
15 C	6.7972750	5.3749734	4.6349630	3.1834407
16 C	8.1244302	6.6954119	6.0292706	4.5834719
17 C	8.5479872	7.1348966	6.7047204	5.3312499
18 C	7.7669256	6.4076024	6.2141372	4.9910449
19 C	6.3696293	5.0154887	4.8659663	3.7362703
20 O	6.7453251	5.3977978	4.3738656	2.9895668 *
21 N	5.3876690	4.5700424	3.1605712	2.9178750 *
22 H	4.0747881	4.8871985	4.6943461	6.0156219
23 H	5.9225469	6.2468294	5.4835627	6.4161492
24 H	6.2701850	6.0111604	4.8090821	5.1957375
25 H	2.1815028 *	3.4524127	3.9647495	5.4207671
26 H	1.1042860 *	2.1996065 *	3.4774248	4.6705007
27 H	2.1740192 *	1.1043359 *	2.1948110 *	2.6979322 *
28 H	3.8795125	2.5664761 *	2.6268753 *	2.0925221 *
29 H	8.9735770	7.5537907	6.7694252	5.3147496
30 H	9.6387302	8.2290081	7.8078844	6.4265233
31 H	8.3690545	7.0737986	7.0406132	5.9137888
32 H	5.9140027	4.6702282	4.8005393	3.9406711
33 H	7.6822307	6.3521700	5.3020181	3.9538848

34 H	5.5553182	4.7126943	3.3633525	3.0524378
35 H	6.3039971	5.5550008	4.1506751	3.8917912

	C	C	C	C
--	---	---	---	---

1 CO	2.8499940 *	3.2623731	3.0263877	4.3130350
2 C	6.2278309	7.5679189	8.1105619	9.5115521
3 C	6.5944285	7.7981735	8.1139870	9.4749536
4 C	5.7877666	6.8393502	6.9894490	8.3057849
5 C	4.3806505	5.4452649	5.6783893	7.0280698
6 C	3.7344171	5.0397102	5.6049104	7.0102917
7 C	4.9197498	6.3127510	6.9943174	8.4020557
8 C	5.1236323	6.5775022	7.4796924	8.8635450
9 C	4.3060406	5.7371419	6.7972750	8.1244302
10 C	2.8918648 *	4.3155583	5.3749734	6.6954119
11 C	2.4359142 *	3.8366685	4.6349630	6.0292706
12 N	1.3326296 *	2.5165234 *	3.1834407	4.5834719
13 C	0.0000000	1.4643742 *	2.6131685 *	3.8853327
14 C	1.4643742 *	0.0000000	1.4371400 *	2.4960928 *
15 C	2.6131685 *	1.4371400 *	0.0000000	1.4079331 *
16 C	3.8853327	2.4960928 *	1.4079331 *	0.0000000
17 C	4.3394465	2.8816343 *	2.4479966 *	1.4299899 *
18 C	3.7827826	2.5010594 *	2.8344554 *	2.4745084 *
19 C	2.4548178 *	1.4430290 *	2.4467532 *	2.8384220 *
20 O	3.0646194	2.5034654 *	1.4668952 *	2.4677595 *
21 N	4.0332300	4.7571440	4.7015456	5.9516358
22 H	7.1170547	8.5011787	9.1187666	10.5248263
23 H	7.6846253	8.8621276	9.1152775	10.4557376
24 H	6.4516850	7.3505604	7.3104629	8.5452754
25 H	6.2055569	7.6622057	8.5826598	9.9641992
26 H	4.9590336	6.3263353	7.4865770	8.7515700
27 H	2.6224265 *	3.8891462	5.0823637	6.2947592
28 H	1.1077792 *	2.1664925 *	3.5298532	4.6586357
29 H	4.8038864	3.5006437	2.1970392 *	1.1069782 *
30 H	5.4456309	3.9882252	3.4480056	2.1966982 *
31 H	4.6407096	3.4958306	3.9391474	3.4796505
32 H	2.6121480 *	2.1931490 *	3.4480401	3.9435392
33 H	4.0431458	3.3357626	2.0471742 *	2.5140003 *
34 H	3.9428097	4.6234026	4.6672236	5.8689302
35 H	4.9853568	5.5678321	5.3003408	6.4416222

	C	C	C	O
--	---	---	---	---

1 CO	5.4732468	5.6338707	4.7024174	1.9653101 *
2 C	10.3803552	10.0043260	8.6701433	7.3936018
3 C	10.4827828	10.2823454	9.0255127	7.1974364

4 C	9.3872074	9.3157256	8.1421724	5.9812911
5 C	8.0499492	7.9249579	6.7364420	4.7907753
6 C	7.8479144	7.4927206	6.1845347	5.0164169
7 C	9.1689001	8.7003846	7.3402798	6.4552237
8 C	9.4483491	8.7904602	7.3903804	7.1795020
9 C	8.5479872	7.7669256	6.3696293	6.7453251
10 C	7.1348966	6.4076024	5.0154887	5.3977978
11 C	6.7047204	6.2141372	4.8659663	4.3738656
12 N	5.3312499	4.9910449	3.7362703	2.9895668 *
13 C	4.3394465	3.7827826	2.4548178 *	3.0646194
14 C	2.8816343 *	2.5010594 *	1.4430290 *	2.5034654 *
15 C	2.4479966 *	2.8344554 *	2.4467532 *	1.4668952 *
16 C	1.4299899 *	2.4745084 *	2.8384220 *	2.4677595 *
17 C	0.0000000	1.4239354 *	2.4506633 *	3.7807631
18 C	1.4239354 *	0.0000000	1.4144329 *	4.3011873
19 C	2.4506633 *	1.4144329 *	0.0000000	3.7969914
20 O	3.7807631	4.3011873	3.7969914	0.0000000
21 N	7.0716619	7.1421118	6.1135588	3.6897794
22 H	11.3449947	10.8979218	9.5360698	8.4501699
23 H	11.5057342	11.3492139	10.1083870	8.1278253
24 H	9.7132996	9.7822560	8.6991559	6.1735010
25 H	10.5281172	9.8322188	8.4274219	8.2726987
26 H	9.0320554	8.1293638	6.7585028	7.5816191
27 H	6.5525994	5.7045685	4.3427514	5.3733091
28 H	4.8271779	3.9623771	2.5479763 *	4.1542236
29 H	2.1973690 *	3.4724377	3.9450013	2.7000269 *
30 H	1.1066571 *	2.2007315 *	3.4571025	4.6623504
31 H	2.2028908 *	1.1048326 *	2.1865570 *	5.4058373
32 H	3.4527517	2.1838427 *	1.1051488 *	4.6890610
33 H	3.9376220	4.7422689	4.4927306	0.9920777 *
34 H	6.8874330	6.8901720	5.8711290	3.8704231
35 H	7.6579649	7.8782169	6.9480514	4.1189134

N H H H

1 CO	1.9770502 *	6.5282958	6.1828895	4.3793273
2 C	4.3408806	1.1063109 *	2.1854602 *	3.4411014
3 C	3.8174673	2.1795427 *	1.1045374 *	2.1965676 *
4 C	2.4799203 *	3.4540131	2.2006148 *	1.1094437 *
5 C	1.5112754 *	3.9441644	3.4650696	2.1882003 *
6 C	2.5906463 *	3.5235070	4.0250317	3.5123794
7 C	3.8829193	2.1989420 *	3.4839340	3.9556247
8 C	5.1049695	2.6779905 *	4.6649014	5.3968363
9 C	5.3876690	4.0747881	5.9225469	6.2701850
10 C	4.5700424	4.8871985	6.2468294	6.0111604
11 C	3.1605712	4.6943461	5.4835627	4.8090821

12 N	2.9178750 *	6.0156219	6.4161492	5.1957375
13 C	4.0332300	7.1170547	7.6846253	6.4516850
14 C	4.7571440	8.5011787	8.8621276	7.3505604
15 C	4.7015456	9.1187666	9.1152775	7.3104629
16 C	5.9516358	10.5248263	10.4557376	8.5452754
17 C	7.0716619	11.3449947	11.5057342	9.7132996
18 C	7.1421118	10.8979218	11.3492139	9.7822560
19 C	6.1135588	9.5360698	10.1083870	8.6991559
20 O	3.6897794	8.4501699	8.1278253	6.1735010
21 N	0.0000000	5.4447502	4.6789222	2.6654000 *
22 H	5.4447502	0.0000000	2.5299180 *	4.3613193
23 H	4.6789222	2.5299180 *	0.0000000	2.5179078 *
24 H	2.6654000 *	4.3613193	2.5179078 *	0.0000000
25 H	6.0445547	2.3933198 *	4.7721127	5.9708244
26 H	6.4716750	4.7696702	6.8404120	7.3502219
27 H	5.2757899	5.9556621	7.3315775	6.9728054
28 H	4.8033975	7.1397524	8.0298743	7.0652649
29 H	6.2547625	11.0979785	10.8044152	8.7476453
30 H	8.0558629	12.4403625	12.5462714	10.6854905
31 H	8.1633961	11.6995600	12.2847838	10.7941307
32 H	6.5117473	9.3518230	10.1792803	8.9966215
33 H	4.2493561	9.1885666	8.6652961	6.5765637
34 H	1.0469344 *	5.8158714	5.1656790	3.2204109
35 H	1.0380401 *	5.8349943	4.6058159	2.2392544 *

H H H H

1 CO	6.5813326	6.3336481	4.5403489	3.8692200
2 C	2.6735392 *	4.6610109	5.3817205	6.3619609
3 C	4.0713596	5.9205134	6.2555843	6.9269706
4 C	4.8862082	6.2526821	6.0092887	6.2966085
5 C	4.6658674	5.4702583	4.8104400	4.9211381
6 C	3.5163069	4.0190068	3.5077883	4.0234842
7 C	2.1935796 *	3.4806040	3.9442177	4.9729519
8 C	1.1048055 *	2.1826386 *	3.4238532	4.8893552
9 C	2.1815028 *	1.1042860 *	2.1740192 *	3.8795125
10 C	3.4524127	2.1996065 *	1.1043359 *	2.5664761 *
11 C	3.9647495	3.4774248	2.1948110 *	2.6268753 *
12 N	5.4207671	4.6705007	2.6979322 *	2.0925221 *
13 C	6.2055569	4.9590336	2.6224265 *	1.1077792 *
14 C	7.6622057	6.3263353	3.8891462	2.1664925 *
15 C	8.5826598	7.4865770	5.0823637	3.5298532
16 C	9.9641992	8.7515700	6.2947592	4.6586357
17 C	10.5281172	9.0320554	6.5525994	4.8271779
18 C	9.8322188	8.1293638	5.7045685	3.9623771
19 C	8.4274219	6.7585028	4.3427514	2.5479763 *

20 O	8.2726987	7.5816191	5.3733091	4.1542236
21 N	6.0445547	6.4716750	5.2757899	4.8033975
22 H	2.3933198 *	4.7696702	5.9556621	7.1397524
23 H	4.7721127	6.8404120	7.3315775	8.0298743
24 H	5.9708244	7.3502219	6.9728054	7.0652649
25 H	0.0000000	2.5283431 *	4.3419974	5.9075509
26 H	2.5283431 *	0.0000000	2.4934562 *	4.3510771
27 H	4.3419974	2.4934562 *	0.0000000	2.0634914 *
28 H	5.9075509	4.3510771	2.0634914 *	0.0000000
29 H	10.7218565	9.6573566	7.2301356	5.6628346
30 H	11.6305770	10.0977583	7.6180639	5.9064830
31 H	10.4804391	8.6129085	6.2758407	4.6113119
32 H	8.0182908	6.1610152	3.8870892	2.2137252 *
33 H	9.1478074	8.5285187	6.3299650	5.1232792
34 H	6.2860999	6.6052144	5.3711319	4.6170239
35 H	6.7600614	7.4002845	6.2791057	5.8073863

H H H H

1 CO	4.6616606	6.4600790	6.6986004	5.2710743
2 C	10.0527382	11.4679515	10.8497147	8.5710943
3 C	9.8803654	11.5367381	11.2056110	9.0806319
4 C	8.6364705	10.4094189	10.2903663	8.3360366
5 C	7.4486826	9.0925266	8.8904611	6.9339451
6 C	7.6118930	8.9373293	8.3704766	6.1874949
7 C	9.0392648	10.2684023	9.5072844	7.1862453
8 C	9.6186338	10.5520493	9.4765095	7.0412036
9 C	8.9735770	9.6387302	8.3690545	5.9140027
10 C	7.5537907	8.2290081	7.0737986	4.6702282
11 C	6.7694252	7.8078844	7.0406132	4.8005393
12 N	5.3147496	6.4265233	5.9137888	3.9406711
13 C	4.8038864	5.4456309	4.6407096	2.6121480 *
14 C	3.5006437	3.9882252	3.4958306	2.1931490 *
15 C	2.1970392 *	3.4480056	3.9391474	3.4480401
16 C	1.1069782 *	2.1966982 *	3.4796505	3.9435392
17 C	2.1973690 *	1.1066571 *	2.2028908 *	3.4527517
18 C	3.4724377	2.2007315 *	1.1048326 *	2.1838427 *
19 C	3.9450013	3.4571025	2.1865570 *	1.1051488 *
20 O	2.7000269 *	4.6623504	5.4058373	4.6890610
21 N	6.2547625	8.0558629	8.1633961	6.5117473
22 H	11.0979785	12.4403625	11.6995600	9.3518230
23 H	10.8044152	12.5462714	12.2847838	10.1792803
24 H	8.7476453	10.6854905	10.7941307	8.9966215
25 H	10.7218565	11.6305770	10.4804391	8.0182908
26 H	9.6573566	10.0977583	8.6129085	6.1610152
27 H	7.2301356	7.6180639	6.2758407	3.8870892

28 H	5.6628346	5.9064830	4.6113119	2.2137252 *
29 H	0.0000000	2.5190209 *	4.3889197	5.0500540
30 H	2.5190209 *	0.0000000	2.5459889 *	4.3716851
31 H	4.3889197	2.5459889 *	0.0000000	2.5127771 *
32 H	5.0500540	4.3716851	2.5127771 *	0.0000000
33 H	2.3151966 *	4.6400356	5.8295589	5.4693311
34 H	6.2310929	7.8643139	7.8667863	6.2240691
35 H	6.5813484	8.5801519	8.9268875	7.4277553

H H H

1 CO	2.6686958 *	2.4828211 *	2.5984893 *
2 C	8.1179566	4.7454311	4.7506486
3 C	7.8001725	4.3081707	3.9355588
4 C	6.5255513	3.0533997	2.5029690 *
5 C	5.4511530	2.1098364 *	2.0946634 *
6 C	5.8355157	2.9587479 *	3.4246008
7 C	7.2718757	4.2207905	4.5687104
8 C	8.0653054	5.3472934	5.8914172
9 C	7.6822307	5.5553182	6.3039971
10 C	6.3521700	4.7126943	5.5550008
11 C	5.3020181	3.3633525	4.1506751
12 N	3.9538848	3.0524378	3.8917912
13 C	4.0431458	3.9428097	4.9853568
14 C	3.3357626	4.6234026	5.5678321
15 C	2.0471742 *	4.6672236	5.3003408
16 C	2.5140003 *	5.8689302	6.4416222
17 C	3.9376220	6.8874330	7.6579649
18 C	4.7422689	6.8901720	7.8782169
19 C	4.4927306	5.8711290	6.9480514
20 O	0.9920777 *	3.8704231	4.1189134
21 N	4.2493561	1.0469344 *	1.0380401 *
22 H	9.1885666	5.8158714	5.8349943
23 H	8.6652961	5.1656790	4.6058159
24 H	6.5765637	3.2204109	2.2392544 *
25 H	9.1478074	6.2860999	6.7600614
26 H	8.5285187	6.6052144	7.4002845
27 H	6.3299650	5.3711319	6.2791057
28 H	5.1232792	4.6170239	5.8073863
29 H	2.3151966 *	6.2310929	6.5813484
30 H	4.6400356	7.8643139	8.5801519
31 H	5.8295589	7.8667863	8.9268875
32 H	5.4693311	6.2240691	7.4277553
33 H	0.0000000	4.4750396	4.4680190
34 H	4.4750396	0.0000000	1.6723806 *
35 H	4.4680190	1.6723806 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.82 , TOTAL = 5008.6 SECONDS (83.5 MIN)
WALL CLOCK TIME: STEP = 0.82 , TOTAL = 4630.6 SECONDS (77.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.82 , TOTAL = 5009.5 SECONDS (83.5 MIN)
WALL CLOCK TIME: STEP = 0.82 , TOTAL = 4631.4 SECONDS (77.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.634836931	-284.634836931	0.024150928	0.001401703	196961030
11402926						
2	1	-284.634993370	-0.000156438	0.008656259	0.000175628	159406045
14541535						
3	2	-284.634988136	0.000005233	0.002979589	0.000334657	148415318
15476487						
4	3	-284.634997687	-0.000009550	0.001563505	0.000087469	142684561
15935823						
5	4	-284.634997111	0.000000576	0.000751936	0.000214428	134750644
16598983						
6	5	-284.634997883	-0.000000773	0.000383022	0.000021201	129512321
17029742						
7	6	-284.634997870	0.000000014	0.000256673	0.000031008	121181007
17573294						
8	7	-284.634997928	-0.000000058	0.000073580	0.000011951	139671073
16176555						
9	8	-284.634997937	-0.000000009	0.000104923	0.000010906	132966928
16735017						
10	9	-284.634997953	-0.000000017	0.000226444	0.000011962	152929801
15281171						

-----DISABLING FDIFF OPTION-----

11 10	-284.634997940	0.000000014	0.000139040	0.000014869	196956153
11403254					
12 11	-284.634997949	-0.000000010	0.000090756	0.000014009	196956214
11403262					
13 12	-284.634997958	-0.000000008	0.000265543	0.000011253	196956246
11403259					
14 13	-284.634997970	-0.000000012	0.000090047	0.000005486	196956145
11403264					
15 14	-284.634997972	-0.000000003	0.000027175	0.000003976	196956268
11403254					
16 15	-284.634997973	-0.000000001	0.000015675	0.000003508	196956264
11403254					
17 16	-284.634997973	-0.000000001	0.000030111	0.000002909	196956240
11403257					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 56.4 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 18.5 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.2 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6349979734 AFTER 17 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5975125956
INTEGRATED TOTAL ELECTRON NUMBER IS 113.0000017712

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 59.56 , TOTAL = 5069.0 SECONDS (84.5 MIN)
WALL CLOCK TIME: STEP = 54.87 , TOTAL = 4686.3 SECONDS (78.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.65 , TOTAL = 5072.7 SECONDS (84.5 MIN)
WALL CLOCK TIME: STEP = 3.63 , TOTAL = 4689.9 SECONDS (78.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.85 , TOTAL = 5075.5 SECONDS (84.6 MIN)
WALL CLOCK TIME: STEP = 2.69 , TOTAL = 4692.6 SECONDS (78.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 50 ENERGY= -284.6349980

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0006622	0.0001035	-0.0003662
2 C	6.0	-0.0001703	-0.0003294	-0.0004653
3 C	6.0	-0.0010123	0.0019095	0.0007211
4 C	6.0	0.0012993	-0.0006583	0.0003200
5 C	6.0	0.0005493	0.0009598	-0.0000803
6 C	6.0	0.0001150	-0.0001823	-0.0000811
7 C	6.0	0.0003887	0.0007278	-0.0000893
8 C	6.0	-0.0008360	-0.0002997	-0.0000442
9 C	6.0	0.0000339	0.0000898	0.0000074
10 C	6.0	-0.0007501	-0.0007526	-0.0002580
11 C	6.0	0.0001096	-0.0008990	0.0000553
12 N	7.0	-0.0003695	0.0003947	0.0003238
13 C	6.0	0.0002833	-0.0002838	0.0001302
14 C	6.0	0.0000077	-0.0002426	-0.0000343
15 C	6.0	0.0007358	0.0001420	0.0007775
16 C	6.0	0.0001097	0.0007338	-0.0001414
17 C	6.0	-0.0000763	-0.0004243	-0.0000042
18 C	6.0	-0.0001503	0.0009547	-0.0004873
19 C	6.0	0.0002411	-0.0008101	-0.0004130
20 O	8.0	0.0005885	-0.0017270	-0.0004276
21 N	7.0	0.0014275	-0.0014252	0.0011221
22 H	1.0	0.0007586	0.0005615	-0.0003305
23 H	1.0	0.0001301	-0.0002746	0.0007230

24 H	1.0	0.0004935	-0.0010405	-0.0003409
25 H	1.0	-0.0000127	-0.0001893	-0.0009187
26 H	1.0	0.0003291	0.0001292	-0.0003434
27 H	1.0	-0.0000278	0.0006153	0.0007953
28 H	1.0	0.0001067	0.0006960	0.0005357
29 H	1.0	-0.0004814	-0.0001299	-0.0011338
30 H	1.0	-0.0011568	0.0003173	0.0004315
31 H	1.0	-0.0001577	0.0007832	0.0005001
32 H	1.0	0.0003344	-0.0005181	0.0000862
33 H	1.0	-0.0000980	-0.0004897	-0.0002281
34 H	1.0	-0.0017524	0.0009104	-0.0014109
35 H	1.0	-0.0016527	0.0006479	0.0010691

MAXIMUM GRADIENT = 0.0019095 RMS GRADIENT = 0.0006725
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001392242
 PREDICTED ENERGY CHANGE WAS -0.0000948539 RATIO= 1.468
 GDIIS STEP HAS LENGTH = 0.158860
 RADIUS OF STEP TAKEN= 0.08326 CURRENT TRUST RADIUS= 0.08326

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 5075.6 SECONDS (84.6 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4692.6 SECONDS (78.2
 MIN)
 CPU UTILIZATION: STEP = 91.71%, TOTAL = 100.00%

INSERCH= 51

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1388758470	-1.7706619496	0.9603858545
C	6.0	4.9897229006	0.6861646980	0.4715693629
C	6.0	5.2130003172	-0.6797380227	0.2486276772
C	6.0	4.0878205106	-1.5445200133	0.0420495937
C	6.0	2.7712731609	-1.0501358535	0.1103159462
C	6.0	2.4802141902	0.3341541767	0.4602977261
C	6.0	3.6500399013	1.2119031680	0.5894890130
C	6.0	3.4850477680	2.6204399978	0.8554869652
C	6.0	2.2162786878	3.1685151267	1.0801475356
C	6.0	1.0694225460	2.3167392676	1.0459439603
C	6.0	1.1694046522	0.9475955034	0.7014348291
N	7.0	-0.0415225223	0.1360746785	0.6921243958
C	6.0	-1.2378060449	0.6733103952	0.4536025704
C	6.0	-2.5500779341	0.0245619167	0.5139860962

C	6.0	-2.8561662946	-1.3471764356	0.8138285845
C	6.0	-4.1730892804	-1.8420715874	0.8503562777
C	6.0	-5.2604609650	-0.9447326642	0.6134656167
C	6.0	-5.0092428548	0.4239167334	0.3157412090
C	6.0	-3.6752064809	0.8898244255	0.2554666359
O	8.0	-1.7562694637	-2.2783748322	1.0874673411
N	7.0	1.6730241063	-2.0170274715	-0.2630331587
H	1.0	5.8416332684	1.3826722476	0.5773179094
H	1.0	6.2357560693	-1.0890090313	0.2041137142
H	1.0	4.2712443942	-2.6080188975	-0.2108377709
H	1.0	4.3878546870	3.2556088001	0.8962512855
H	1.0	2.0969973192	4.2412200001	1.3153529260
H	1.0	0.0968701345	2.7517061837	1.3366232896
H	1.0	-1.2736383946	1.7410909999	0.1633695718
H	1.0	-4.3806672905	-2.9105761418	1.0527288324
H	1.0	-6.2987038771	-1.3247410034	0.6643992423
H	1.0	-5.8443193489	1.1254652812	0.1390194370
H	1.0	-3.4745959717	1.9509175936	0.0199675931
H	1.0	-2.0983737062	-3.1771765041	1.3345522093
H	1.0	1.3242139826	-1.7990727114	-1.2240997075
H	1.0	2.0674429865	-2.9777430740	-0.3046255644

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4594556	5.2386500	4.0606213
2 C	5.4594556	0.0000000	1.4018723 *	2.4441500 *
3 C	5.2386500	1.4018723 *	0.0000000	1.4340683 *
4 C	4.0606213	2.4441500 *	1.4340683 *	0.0000000
5 C	2.8585472 *	2.8402047 *	2.4735311 *	1.4079677 *
6 C	3.1878212	2.5341019 *	2.9224821 *	2.5077373 *
7 C	4.6218538	1.4439725 *	2.4773652 *	2.8441537 *
8 C	5.5217431	2.4804961 *	3.7742911	4.2862463
9 C	5.3596097	3.7715281	4.9478094	5.1761971
10 C	4.1928613	4.2845577	5.1753093	5.0027846
11 C	2.9185559 *	3.8361459	4.3822271	3.8939157
12 N	1.9339473 *	5.0660314	5.3359395	4.5053823
13 C	2.8504531 *	6.2275681	6.5943656	5.7836360
14 C	3.2638281	7.5688912	7.7994767	6.8371367
15 C	3.0283818	8.1123113	8.1164263	6.9895307
16 C	4.3139598	9.5127591	9.4769074	8.3056925
17 C	5.4731482	10.3800882	10.4831636	9.3849149
18 C	5.6333710	10.0036180	10.2818682	9.3116171
19 C	4.7034373	8.6700161	9.0257295	8.1385605

20 O	1.9660869 *	7.3943382	7.1993064	5.9820422
21 N	1.9776402 *	4.3413569	3.8185824	2.4794315 *
22 H	6.5277638	1.1054668 *	2.1809981 *	3.4541028
23 H	6.1813062	2.1852627 *	1.1025033 *	2.2016771 *
24 H	4.3760029	3.4399908	2.1946024 *	1.1084341 *
25 H	6.5818943	2.6729465 *	4.0727431	4.8847638
26 H	6.3326903	4.6602843	5.9214192	6.2497573
27 H	4.5381860	5.3809654	6.2556640	6.0050950
28 H	3.8681831	6.3590527	6.9241724	6.2892925
29 H	4.6619955	10.0537805	9.8823922	8.6372951
30 H	6.4597900	11.4677593	11.5372539	10.4074738
31 H	6.6978221	10.8480434	11.2042443	10.2852140
32 H	5.2717852	8.5701947	9.0800310	8.3311893
33 H	2.6690015 *	8.1185749	7.8020908	6.5272605
34 H	2.4855202 *	4.7421150	4.3063320	3.0504839
35 H	2.6032038 *	4.7504125	3.9346470	2.5012472 *

C C C C

1 CO	2.8585472 *	3.1878212	4.6218538	5.5217431
2 C	2.8402047 *	2.5341019 *	1.4439725 *	2.4804961 *
3 C	2.4735311 *	2.9224821 *	2.4773652 *	3.7742911
4 C	1.4079677 *	2.5077373 *	2.8441537 *	4.2862463
5 C	0.0000000	1.4572102 *	2.4735922 *	3.8128573
6 C	1.4572102 *	0.0000000	1.4682050 *	2.5284319 *
7 C	2.4735922 *	1.4682050 *	0.0000000	1.4428975 *
8 C	3.8128573	2.5284319 *	1.4428975 *	0.0000000
9 C	4.3641274	2.9133276 *	2.4748227 *	1.4002263 *
10 C	3.8868423	2.5027901 *	2.8440464 *	2.4420797 *
11 C	2.6279906 *	1.4672011 *	2.4971867 *	2.8608292 *
12 N	3.1076383	2.5401053 *	3.8465015	4.3168804
13 C	4.3773084	3.7334630	4.9193074	5.1242729
14 C	5.4437765	5.0400961	6.3132354	6.5785977
15 C	5.6790173	5.6061407	6.9949936	7.4802882
16 C	7.0284416	7.0110307	8.4021523	8.8634699
17 C	8.0481689	7.8471054	9.1678066	9.4473781
18 C	7.9215819	7.4913898	8.6993700	8.7902795
19 C	6.7336182	6.1838442	7.3399278	7.3908251
20 O	4.7918721	5.0166167	6.4543167	7.1779947
21 N	1.5101059 *	2.5889802 *	3.8808992	5.1030012
22 H	3.9450928	3.5230984	2.1982702 *	2.6763674 *
23 H	3.4659704	4.0243159	3.4826196	4.6637641
24 H	2.1863332 *	3.5092156	3.9519897	5.3936941
25 H	4.6658833	3.5162544	2.1943579 *	1.1046092 *
26 H	5.4685655	4.0178524	3.4807442	2.1829083 *
27 H	4.8073136	3.5061137	3.9438837	3.4246855

28 H	4.9147809	4.0198317	4.9703345	4.8884942
29 H	7.4498075	7.6125518	9.0388984	9.6177189
30 H	9.0910340	8.9366097	10.2673111	10.5509603
31 H	8.8860845	8.3682287	9.5054328	9.4755140
32 H	6.9300336	6.1860794	7.1854668	7.0415193
33 H	5.4531199	5.8358574	7.2707220	8.0632782
34 H	2.1060750 *	2.9536737 *	4.2148008	5.3409714
35 H	2.0936148 *	3.4240548	4.5669672	5.8902562

C C C N

1 CO	5.3596097	4.1928613	2.9185559 *	1.9339473 *
2 C	3.7715281	4.2845577	3.8361459	5.0660314
3 C	4.9478094	5.1753093	4.3822271	5.3359395
4 C	5.1761971	5.0027846	3.8939157	4.5053823
5 C	4.3641274	3.8868423	2.6279906 *	3.1076383
6 C	2.9133276 *	2.5027901 *	1.4672011 *	2.5401053 *
7 C	2.4748227 *	2.8440464 *	2.4971867 *	3.8465015
8 C	1.4002263 *	2.4420797 *	2.8608292 *	4.3168804
9 C	0.0000000	1.4289755 *	2.4843213 *	3.8005162
10 C	1.4289755 *	0.0000000	1.4153578 *	2.4727890 *
11 C	2.4843213 *	1.4153578 *	0.0000000	1.4577371 *
12 N	3.8005162	2.4727890 *	1.4577371 *	0.0000000
13 C	4.3068906	2.8939645 *	2.4354294 *	1.3328950 *
14 C	5.7378686	4.3171565	3.8368840	2.5173436 *
15 C	6.7964766	5.3747934	4.6350655	3.1838758
16 C	8.1229801	6.6946167	6.0288192	4.5834424
17 C	8.5462410	7.1338392	6.7031199	5.3302580
18 C	7.7669363	6.4082873	6.2127839	4.9902668
19 C	6.3704103	5.0172149	4.8654375	3.7366386
20 O	6.7416469	5.3945651	4.3721247	2.9876780 *
21 N	5.3841538	4.5671972	3.1579773	2.9133906 *
22 H	4.0725015	4.8852929	4.6940832	6.0148739
23 H	5.9203163	6.2449021	5.4829739	6.4142974
24 H	6.2656103	6.0070298	4.8058345	5.1908909
25 H	2.1810881 *	3.4519380	3.9652616	5.4214890
26 H	1.1046472 *	2.1982077 *	3.4763898	4.6705352
27 H	2.1751786 *	1.1043319 *	2.1928543 *	2.6974172 *
28 H	3.8804050	2.5690938 *	2.6244254 *	2.0913557 *
29 H	8.9708304	7.5517118	6.7684706	5.3141598
30 H	9.6367591	8.2277118	7.8062494	6.4255015
31 H	8.3685731	7.0739998	7.0384851	5.9124673
32 H	5.9154526	4.6727462	4.7997703	3.9409952
33 H	7.6778089	6.3483335	5.3002790	3.9523390
34 H	5.5481766	4.7072205	3.3579511	3.0466287
35 H	6.3020821	5.5544240	4.1505317	3.8906435

	C	C	C	C
1 CO	2.8504531 *	3.2638281	3.0283818	4.3139598
2 C	6.2275681	7.5688912	8.1123113	9.5127591
3 C	6.5943656	7.7994767	8.1164263	9.4769074
4 C	5.7836360	6.8371367	6.9895307	8.3056925
5 C	4.3773084	5.4437765	5.6790173	7.0284416
6 C	3.7334630	5.0400961	5.6061407	7.0110307
7 C	4.9193074	6.3132354	6.9949936	8.4021523
8 C	5.1242729	6.5785977	7.4802882	8.8634699
9 C	4.3068906	5.7378686	6.7964766	8.1229801
10 C	2.8939645 *	4.3171565	5.3747934	6.6946167
11 C	2.4354294 *	3.8368840	4.6350655	6.0288192
12 N	1.3328950 *	2.5173436 *	3.1838758	4.5834424
13 C	0.0000000	1.4651206 *	2.6136602 *	3.8859295
14 C	1.4651206 *	0.0000000	1.4371018 *	2.4963236 *
15 C	2.6136602 *	1.4371018 *	0.0000000	1.4073172 *
16 C	3.8859295	2.4963236 *	1.4073172 *	0.0000000
17 C	4.3388215	2.8802091 *	2.4459639 *	1.4295844 *
18 C	3.7821870	2.4992554 *	2.8320665 *	2.4737965 *
19 C	2.4550065 *	1.4427147 *	2.4467872 *	2.8399008 *
20 O	3.0631739	2.5025048 *	1.4668952 *	2.4673063 *
21 N	4.0279544	4.7546227	4.7033921	5.9537625
22 H	7.1159652	8.5011347	9.1191956	10.5246468
23 H	7.6825871	8.8615428	9.1159999	10.4560410
24 H	6.4465681	7.3475363	7.3102427	8.5451495
25 H	6.2058248	7.6629433	8.5830219	9.9638453
26 H	4.9591840	6.3259547	7.4843524	8.7485224
27 H	2.6231308 *	3.8884935	5.0788362	6.2906123
28 H	1.1071019 *	2.1676489 *	3.5305647	4.6602382
29 H	4.8042452	3.5009051	2.1966782 *	1.1071338 *
30 H	5.4451200	3.9869084	3.4458522	2.1955520 *
31 H	4.6393288	3.4935104	3.9367986	3.4792650
32 H	2.6121923 *	2.1930878 *	3.4482017	3.9451496
33 H	4.0426351	3.3359398	2.0479997 *	2.5142386 *
34 H	3.9359001	4.6213335	4.6725733	5.8758454
35 H	4.9829482	5.5682546	5.3058096	6.4473231

	C	C	C	O
1 CO	5.4731482	5.6333710	4.7034373	1.9660869 *
2 C	10.3800882	10.0036180	8.6700161	7.3943382
3 C	10.4831636	10.2818682	9.0257295	7.1993064
4 C	9.3849149	9.3116171	8.1385605	5.9820422
5 C	8.0481689	7.9215819	6.7336182	4.7918721

6 C	7.8471054	7.4913898	6.1838442	5.0166167
7 C	9.1678066	8.6993700	7.3399278	6.4543167
8 C	9.4473781	8.7902795	7.3908251	7.1779947
9 C	8.5462410	7.7669363	6.3704103	6.7416469
10 C	7.1338392	6.4082873	5.0172149	5.3945651
11 C	6.7031199	6.2127839	4.8654375	4.3721247
12 N	5.3302580	4.9902668	3.7366386	2.9876780 *
13 C	4.3388215	3.7821870	2.4550065 *	3.0631739
14 C	2.8802091 *	2.4992554 *	1.4427147 *	2.5025048 *
15 C	2.4459639 *	2.8320665 *	2.4467872 *	1.4668952 *
16 C	1.4295844 *	2.4737965 *	2.8399008 *	2.4673063 *
17 C	0.0000000	1.4230079 *	2.4508763 *	3.7792376
18 C	1.4230079 *	0.0000000	1.4143394 *	4.2988111
19 C	2.4508763 *	1.4143394 *	0.0000000	3.7963181
20 O	3.7792376	4.2988111	3.7963181	0.0000000
21 N	7.0704513	7.1376383	6.1091898	3.6948895
22 H	11.3434834	10.8962905	9.5350263	8.4493576
23 H	11.5044074	11.3468677	10.1067105	8.1281841
24 H	9.7107880	9.7773904	8.6947357	6.1745595
25 H	10.5267674	9.8316283	8.4273659	8.2711426
26 H	9.0287842	8.1283256	6.7582208	7.5765898
27 H	6.5488635	5.7037877	4.3432782	5.3663694
28 H	4.8281455	3.9639508	2.5496404 *	4.1524685
29 H	2.1980741 *	3.4723336	3.9466880	2.6996943 *
30 H	1.1067741 *	2.2004718 *	3.4574940	4.6606989
31 H	2.2026596 *	1.1048772 *	2.1849799 *	5.4035019
32 H	3.4534539	2.1850297 *	1.1052706 *	4.6881890
33 H	3.9373300	4.7412032	4.4934757	0.9929404 *
34 H	6.8894475	6.8866151	5.8663012	3.8810374
35 H	7.6599086	7.8762699	6.9462079	4.1289000

N H H H

1 CO	1.9776402 *	6.5277638	6.1813062	4.3760029
2 C	4.3413569	1.1054668 *	2.1852627 *	3.4399908
3 C	3.8185824	2.1809981 *	1.1025033 *	2.1946024 *
4 C	2.4794315 *	3.4541028	2.2016771 *	1.1084341 *
5 C	1.5101059 *	3.9450928	3.4659704	2.1863332 *
6 C	2.5889802 *	3.5230984	4.0243159	3.5092156
7 C	3.8808992	2.1982702 *	3.4826196	3.9519897
8 C	5.1030012	2.6763674 *	4.6637641	5.3936941
9 C	5.3841538	4.0725015	5.9203163	6.2656103
10 C	4.5671972	4.8852929	6.2449021	6.0070298
11 C	3.1579773	4.6940832	5.4829739	4.8058345
12 N	2.9133906 *	6.0148739	6.4142974	5.1908909
13 C	4.0279544	7.1159652	7.6825871	6.4465681

14 C	4.7546227	8.5011347	8.8615428	7.3475363
15 C	4.7033921	9.1191956	9.1159999	7.3102427
16 C	5.9537625	10.5246468	10.4560410	8.5451495
17 C	7.0704513	11.3434834	11.5044074	9.7107880
18 C	7.1376383	10.8962905	11.3468677	9.7773904
19 C	6.1091898	9.5350263	10.1067105	8.6947357
20 O	3.6948895	8.4493576	8.1281841	6.1745595
21 N	0.0000000	5.4443962	4.6795264	2.6650974 *
22 H	5.4443962	0.0000000	2.5305775 *	4.3603815
23 H	4.6795264	2.5305775 *	0.0000000	2.5177136 *
24 H	2.6650974 *	4.3603815	2.5177136 *	0.0000000
25 H	6.0427592	2.3922964 *	4.7717395	5.9683644
26 H	6.4681309	4.7684682	6.8392630	7.3463380
27 H	5.2710514	5.9542508	7.3293650	6.9675454
28 H	4.7945900	7.1363091	8.0250939	7.0569479
29 H	6.2591404	11.0974513	10.8049387	8.7489266
30 H	8.0552988	12.4388687	12.5451233	10.6834755
31 H	8.1576565	11.6969975	12.2815453	10.7882313
32 H	6.5055876	9.3501695	10.1767382	8.9908407
33 H	4.2569550	9.1874553	8.6657979	6.5790733
34 H	1.0453811 *	5.8116851	5.1640323	3.2196400
35 H	1.0393607 *	5.8340002	4.6044507	2.2365672 *

H H H H

1 CO	6.5818943	6.3326903	4.5381860	3.8681831
2 C	2.6729465 *	4.6602843	5.3809654	6.3590527
3 C	4.0727431	5.9214192	6.2556640	6.9241724
4 C	4.8847638	6.2497573	6.0050950	6.2892925
5 C	4.6658833	5.4685655	4.8073136	4.9147809
6 C	3.5162544	4.0178524	3.5061137	4.0198317
7 C	2.1943579 *	3.4807442	3.9438837	4.9703345
8 C	1.1046092 *	2.1829083 *	3.4246855	4.8884942
9 C	2.1810881 *	1.1046472 *	2.1751786 *	3.8804050
10 C	3.4519380	2.1982077 *	1.1043319 *	2.5690938 *
11 C	3.9652616	3.4763898	2.1928543 *	2.6244254 *
12 N	5.4214890	4.6705352	2.6974172 *	2.0913557 *
13 C	6.2058248	4.9591840	2.6231308 *	1.1071019 *
14 C	7.6629433	6.3259547	3.8884935	2.1676489 *
15 C	8.5830219	7.4843524	5.0788362	3.5305647
16 C	9.9638453	8.7485224	6.2906123	4.6602382
17 C	10.5267674	9.0287842	6.5488635	4.8281455
18 C	9.8316283	8.1283256	5.7037877	3.9639508
19 C	8.4273659	6.7582208	4.3432782	2.5496404 *
20 O	8.2711426	7.5765898	5.3663694	4.1524685
21 N	6.0427592	6.4681309	5.2710514	4.7945900

22 H	2.3922964 *	4.7684682	5.9542508	7.1363091
23 H	4.7717395	6.8392630	7.3293650	8.0250939
24 H	5.9683644	7.3463380	6.9675454	7.0569479
25 H	0.0000000	2.5288541 *	4.3428555	5.9062157
26 H	2.5288541 *	0.0000000	2.4939151 *	4.3518842
27 H	4.3428555	2.4939151 *	0.0000000	2.0678880 *
28 H	5.9062157	4.3518842	2.0678880 *	0.0000000
29 H	10.7206949	9.6528389	7.2242909	5.6641500
30 H	11.6290969	10.0941300	7.6139788	5.9077610
31 H	10.4789454	8.6113993	6.2750814	4.6120183
32 H	8.0179937	6.1616686	3.8897577	2.2155824 *
33 H	9.1457090	8.5225650	6.3222425	5.1226177
34 H	6.2794576	6.5978140	5.3640716	4.6050697
35 H	6.7587788	7.3985561	6.2772163	5.8007964

H H H H

1 CO	4.6619955	6.4597900	6.6978221	5.2717852
2 C	10.0537805	11.4677593	10.8480434	8.5701947
3 C	9.8823922	11.5372539	11.2042443	9.0800310
4 C	8.6372951	10.4074738	10.2852140	8.3311893
5 C	7.4498075	9.0910340	8.8860845	6.9300336
6 C	7.6125518	8.9366097	8.3682287	6.1860794
7 C	9.0388984	10.2673111	9.5054328	7.1854668
8 C	9.6177189	10.5509603	9.4755140	7.0415193
9 C	8.9708304	9.6367591	8.3685731	5.9154526
10 C	7.5517118	8.2277118	7.0739998	4.6727462
11 C	6.7684706	7.8062494	7.0384851	4.7997703
12 N	5.3141598	6.4255015	5.9124673	3.9409952
13 C	4.8042452	5.4451200	4.6393288	2.6121923 *
14 C	3.5009051	3.9869084	3.4935104	2.1930878 *
15 C	2.1966782 *	3.4458522	3.9367986	3.4482017
16 C	1.1071338 *	2.1955520 *	3.4792650	3.9451496
17 C	2.1980741 *	1.1067741 *	2.2026596 *	3.4534539
18 C	3.4723336	2.2004718 *	1.1048772 *	2.1850297 *
19 C	3.9466880	3.4574940	2.1849799 *	1.1052706 *
20 O	2.6996943 *	4.6606989	5.4035019	4.6881890
21 N	6.2591404	8.0552988	8.1576565	6.5055876
22 H	11.0974513	12.4388687	11.6969975	9.3501695
23 H	10.8049387	12.5451233	12.2815453	10.1767382
24 H	8.7489266	10.6834755	10.7882313	8.9908407
25 H	10.7206949	11.6290969	10.4789454	8.0179937
26 H	9.6528389	10.0941300	8.6113993	6.1616686
27 H	7.2242909	7.6139788	6.2750814	3.8897577
28 H	5.6641500	5.9077610	4.6120183	2.2155824 *
29 H	0.0000000	2.5188365 *	4.3893932	5.0518989

30 H	2.5188365 *	0.0000000	2.5467627 *	4.3727356
31 H	4.3893932	2.5467627 *	0.0000000	2.5121970 *
32 H	5.0518989	4.3727356	2.5121970 *	0.0000000
33 H	2.3150301 *	4.6393314	5.8287335	5.4698692
34 H	6.2421998	7.8676741	7.8612268	6.2160042
35 H	6.5897685	8.5827640	8.9235152	7.4236953

H H H

1 CO	2.6690015 *	2.4855202 *	2.6032038 *
2 C	8.1185749	4.7421150	4.7504125
3 C	7.8020908	4.3063320	3.9346470
4 C	6.5272605	3.0504839	2.5012472 *
5 C	5.4531199	2.1060750 *	2.0936148 *
6 C	5.8358574	2.9536737 *	3.4240548
7 C	7.2707220	4.2148008	4.5669672
8 C	8.0632782	5.3409714	5.8902562
9 C	7.6778089	5.5481766	6.3020821
10 C	6.3483335	4.7072205	5.5544240
11 C	5.3002790	3.3579511	4.1505317
12 N	3.9523390	3.0466287	3.8906435
13 C	4.0426351	3.9359001	4.9829482
14 C	3.3359398	4.6213335	5.5682546
15 C	2.0479997 *	4.6725733	5.3058096
16 C	2.5142386 *	5.8758454	6.4473231
17 C	3.9373300	6.8894475	7.6599086
18 C	4.7412032	6.8866151	7.8762699
19 C	4.4934757	5.8663012	6.9462079
20 O	0.9929404 *	3.8810374	4.1289000
21 N	4.2569550	1.0453811 *	1.0393607 *
22 H	9.1874553	5.8116851	5.8340002
23 H	8.6657979	5.1640323	4.6044507
24 H	6.5790733	3.2196400	2.2365672 *
25 H	9.1457090	6.2794576	6.7587788
26 H	8.5225650	6.5978140	7.3985561
27 H	6.3222425	5.3640716	6.2772163
28 H	5.1226177	4.6050697	5.8007964
29 H	2.3150301 *	6.2421998	6.5897685
30 H	4.6393314	7.8676741	8.5827640
31 H	5.8287335	7.8612268	8.9235152
32 H	5.4698692	6.2160042	7.4236953
33 H	0.0000000	4.4899862	4.4811501
34 H	4.4899862	0.0000000	1.6694568 *
35 H	4.4811501	1.6694568 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.82 , TOTAL = 5076.4 SECONDS (84.6 MIN)
WALL CLOCK TIME: STEP = 0.82 , TOTAL = 4693.4 SECONDS (78.2 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.92 , TOTAL = 5077.3 SECONDS (84.6 MIN)
WALL CLOCK TIME: STEP = 0.93 , TOTAL = 4694.4 SECONDS (78.2 MIN)
CPU UTILIZATION: STEP = 99.33%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

		NONZERO BLOCKS				
ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD	
-----START SECOND ORDER SCF-----						
1	0	-284.634965562	-284.634965562	0.013748944	0.001290204	196979518
11400561						
2	1	-284.635101952	-0.000136389	0.003726091	0.000183989	158984342
14610224						
3	2	-284.635098020	0.000003932	0.002288457	0.000411015	146767583
15592592						
4	3	-284.635105360	-0.000007340	0.000576859	0.000043906	142127281
15950025						
5	4	-284.635105197	0.000000163	0.000336186	0.000116498	129936682
16936238						
6	5	-284.635105507	-0.000000310	0.000226723	0.000030271	123941678
17436167						
7	6	-284.635105492	0.000000014	0.000127995	0.000039152	120731458
17602095						
8	7	-284.635105567	-0.000000075	0.000143094	0.000020060	139050529
16232536						
9	8	-284.635105594	-0.000000027	0.000389841	0.000018584	157031602
14870301						
-----DISABLING FDIFF OPTION-----						
10	9	-284.635105601	-0.000000007	0.000341159	0.000023080	196975404
11400683						
11	10	-284.635105637	-0.000000035	0.000406155	0.000023826	196975830
11400672						

12 11	-284.635105669	-0.000000032	0.000205777	0.000024883	196976501
11400670					
13 12	-284.635105690	-0.000000022	0.000255646	0.000016480	196976530
11400666					
14 13	-284.635105706	-0.000000016	0.000124823	0.000007198	196976564
11400674					
15 14	-284.635105712	-0.000000005	0.000060161	0.000005154	196976630
11400659					
16 15	-284.635105714	-0.000000002	0.000019719	0.000003907	196976571
11400667					
17 16	-284.635105714	-0.000000001	0.000028127	0.000003737	196976601
11400666					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 57.0 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 18.5 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.2 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6351057144 AFTER 17 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5991349095
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999985839

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 60.19 , TOTAL = 5137.5 SECONDS (85.6 MIN)
WALL CLOCK TIME: STEP = 55.28 , TOTAL = 4749.6 SECONDS (79.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.96 , TOTAL = 5141.4 SECONDS (85.7 MIN)

WALL CLOCK TIME: STEP = 3.93 , TOTAL = 4753.6 SECONDS (79.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.89 , TOTAL = 5144.3 SECONDS (85.7 MIN)

WALL CLOCK TIME: STEP = 2.69 , TOTAL = 4756.3 SECONDS (79.3 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 51 ENERGY= -284.6351057

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0007700	0.0002039	-0.0001687
2 C	6.0	-0.0000073	0.0019055	-0.0000546
3 C	6.0	0.0014750	-0.0004799	0.0002502
4 C	6.0	-0.0001150	-0.0005379	0.0000575
5 C	6.0	0.0003396	0.0002552	-0.0001680
6 C	6.0	0.0005067	-0.0003219	-0.0001186
7 C	6.0	0.0001678	-0.0000097	-0.0002085
8 C	6.0	-0.0008067	0.0002336	-0.0000392
9 C	6.0	0.0002120	-0.0009393	-0.0001639
10 C	6.0	0.0002125	-0.0001658	0.0000351
11 C	6.0	-0.0005087	-0.0004739	0.0001824
12 N	7.0	-0.0001927	-0.0001896	0.0000910
13 C	6.0	0.0003420	0.0005315	-0.0000806
14 C	6.0	-0.0006108	-0.0006019	0.0000230
15 C	6.0	-0.0000569	0.0001210	0.0005689
16 C	6.0	0.0000765	0.0008942	-0.0001638
17 C	6.0	0.0005474	0.0002451	-0.0000822
18 C	6.0	0.0000982	-0.0001973	-0.0003346
19 C	6.0	0.0000711	-0.0005184	-0.0004777
20 O	8.0	0.0005280	-0.0008747	-0.0005394
21 N	7.0	0.0004822	0.0002594	0.0006754
22 H	1.0	0.0003005	0.0002365	-0.0003567
23 H	1.0	-0.0010331	0.0004326	0.0009064
24 H	1.0	0.0004655	-0.0003186	-0.0000640

25 H	1.0	-0.0001275	-0.0002148	-0.0009419
26 H	1.0	0.0001665	0.0003386	-0.0003287
27 H	1.0	-0.0001341	0.0003476	0.0006775
28 H	1.0	0.0003052	0.0002297	0.0006197
29 H	1.0	-0.0004267	-0.0002749	-0.0010333
30 H	1.0	-0.0011730	0.0001554	0.0004839
31 H	1.0	-0.0000266	0.0009445	0.0004615
32 H	1.0	0.0004734	-0.0003985	0.0001780
33 H	1.0	-0.0002918	-0.0011896	-0.0000266
34 H	1.0	-0.0009095	0.0005118	-0.0004622
35 H	1.0	-0.0011197	-0.0001393	0.0006026

MAXIMUM GRADIENT = 0.0019055 RMS GRADIENT = 0.0005293
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001077410
 PREDICTED ENERGY CHANGE WAS -0.0001843070 RATIO= 0.585
 GDIIS STEP HAS LENGTH = 0.155262
 RADIUS OF STEP TAKEN= 0.08326 CURRENT TRUST RADIUS= 0.08326

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 5144.4 SECONDS (85.7 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4756.3 SECONDS (79.3
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 52

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1389349006	-1.7720267733	0.9573202602
C	6.0	4.9903212799	0.6857553004	0.4738459725
C	6.0	5.2133216995	-0.6806706148	0.2486218086
C	6.0	4.0861956044	-1.5429944279	0.0391279154
C	6.0	2.7696909394	-1.0489293397	0.1073443289
C	6.0	2.4799110517	0.3340514091	0.4596030100
C	6.0	3.6500103152	1.2108501505	0.5909544620
C	6.0	3.4854056550	2.6190115281	0.8585933791
C	6.0	2.2169509540	3.1659869938	1.0856428141
C	6.0	1.0700168229	2.3147615655	1.0504234251
C	6.0	1.1690843981	0.9471548922	0.7011184094
N	7.0	-0.0414650408	0.1344875934	0.6880087711
C	6.0	-1.2374711363	0.6717352259	0.4469895046
C	6.0	-2.5503083671	0.0237540280	0.5090535513
C	6.0	-2.8570773399	-1.3463134703	0.8159379962

C	6.0	-4.1735422905	-1.8415492681	0.8574531796
C	6.0	-5.2603702629	-0.9448069349	0.6162357287
C	6.0	-5.0086618569	0.4218761728	0.3103326567
C	6.0	-3.6749307933	0.8883871059	0.2473750323
O	8.0	-1.7569073274	-2.2751899453	1.0956648041
N	7.0	1.6721799894	-2.0140469065	-0.2694449429
H	1.0	5.8408746693	1.3822825618	0.5823529614
H	1.0	6.2352455414	-1.0897610498	0.2065363659
H	1.0	4.2692841905	-2.6053394777	-0.2136380738
H	1.0	4.3879962263	3.2548568806	0.8990010408
H	1.0	2.0965433569	4.2382033786	1.3227193745
H	1.0	0.0965742418	2.7476868342	1.3409409002
H	1.0	-1.2711241224	1.7385402787	0.1536566771
H	1.0	-4.3806717614	-2.9081717730	1.0677428879
H	1.0	-6.2978907541	-1.3242733756	0.6712526430
H	1.0	-5.8428096706	1.1227693091	0.1308744326
H	1.0	-3.4741446814	1.9487962960	0.0089644527
H	1.0	-2.0984718769	-3.1725806930	1.3518490187
H	1.0	1.3253990689	-1.7901235173	-1.2296710460
H	1.0	2.0679033768	-2.9730649373	-0.3198967019

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4598892	5.2385793	4.0591132
2 C	5.4598892	0.0000000	1.4027027 *	2.4441253 *
3 C	5.2385793	1.4027027 *	0.0000000	1.4345394 *
4 C	4.0591132	2.4441253 *	1.4345394 *	0.0000000
5 C	2.8576575 *	2.8415935 *	2.4752586 *	1.4078133 *
6 C	3.1880177	2.5349671 *	2.9233042 *	2.5060428 *
7 C	4.6216263	1.4442550 *	2.4776975 *	2.8422579 *
8 C	5.5217598	2.4799761 *	3.7743425	4.2842462
9 C	5.3589735	3.7706004	4.9472838	5.1733717
10 C	4.1925435	4.2842607	5.1751787	5.0002334
11 C	2.9190403 *	3.8369042	4.3829698	3.8921219
12 N	1.9338743 *	5.0664223	5.3357593	4.5025076
13 C	2.8507725 *	6.2278661	6.5940185	5.7803811
14 C	3.2646288	7.5697147	7.7998712	6.8351091
15 C	3.0294076	8.1134454	8.1176517	6.9893602
16 C	4.3141936	9.5137174	9.4779497	8.3055440
17 C	5.4729451	10.3805436	10.4834694	9.3834522
18 C	5.6328994	10.0038009	10.2814574	9.3086358
19 C	4.7039766	8.6705791	9.0256842	8.1357277
20 O	1.9663494 *	7.3945216	7.2002824	5.9828281

21 N	1.9784760 *	4.3418285	3.8191583	2.4788261 *
22 H	6.5270503	1.1047013 *	2.1819659 *	3.4541623
23 H	6.1801429	2.1848911 *	1.1015691 *	2.2026942 *
24 H	4.3732526	3.4385802	2.1929982 *	1.1072439 *
25 H	6.5823615	2.6727954 *	4.0733932	4.8836301
26 H	6.3315570	4.6598738	5.9214284	6.2472851
27 H	4.5361625	5.3807226	6.2552298	6.0018115
28 H	3.8675862	6.3574032	6.9216788	6.2835071
29 H	4.6615301	10.0540806	9.8831893	8.6376849
30 H	6.4587183	11.4674721	11.5369343	10.4056076
31 H	6.6965756	10.8473654	11.2028702	10.2810437
32 H	5.2724043	8.5707976	9.0798460	8.3278003
33 H	2.6689311 *	8.1184133	7.8031437	6.5290811
34 H	2.4881631 *	4.7395781	4.3049016	3.0484293
35 H	2.6066636 *	4.7494757	3.9334389	2.4995007 *

C C C C

1 CO	2.8576575 *	3.1880177	4.6216263	5.5217598
2 C	2.8415935 *	2.5349671 *	1.4442550 *	2.4799761 *
3 C	2.4752586 *	2.9233042 *	2.4776975 *	3.7743425
4 C	1.4078133 *	2.5060428 *	2.8422579 *	4.2842462
5 C	0.0000000	1.4562604 *	2.4729424 *	3.8118779
6 C	1.4562604 *	0.0000000	1.4680468 *	2.5280932 *
7 C	2.4729424 *	1.4680468 *	0.0000000	1.4427903 *
8 C	3.8118779	2.5280932 *	1.4427903 *	0.0000000
9 C	4.3621221	2.9122041 *	2.4740525 *	1.3998968 *
10 C	3.8849333	2.5020158 *	2.8436066 *	2.4420217 *
11 C	2.6265683 *	1.4671374 *	2.4973315 *	2.8609871 *
12 N	3.1048744	2.5395536 *	3.8464225	4.3174964
13 C	4.3741734	3.7327094	4.9192322	5.1251213
14 C	5.4419126	5.0400235	6.3134663	6.5793148
15 C	5.6790020	5.6066073	6.9951335	7.4801546
16 C	7.0284705	7.0114167	8.4021509	8.8631872
17 C	8.0468438	7.8467807	9.1674630	9.4471231
18 C	7.9187906	7.4905753	8.6990708	8.7907438
19 C	6.7309697	6.1833977	7.3400812	7.3918243
20 O	4.7927637	5.0163079	6.4530587	7.1757408
21 N	1.5092887 *	2.5879540 *	3.8796986	5.1015182
22 H	3.9457058	3.5227734	2.1975781 *	2.6747040 *
23 H	3.4672143	4.0241548	3.4819578	4.6628094
24 H	2.1849993 *	3.5064410	3.9489458	5.3905463
25 H	4.6656412	3.5163851	2.1948757 *	1.1048085 *
26 H	5.4666294	4.0167578	3.4804608	2.1831477 *
27 H	4.8043322	3.5046664	3.9435079	3.4254043
28 H	4.9092075	4.0170209	4.9686266	4.8884293

29 H	7.4502909	7.6124531	9.0380044	9.6160633
30 H	9.0892709	8.9355829	10.2661597	10.5497621
31 H	8.8821166	8.3664699	9.5043707	9.4754376
32 H	6.9268695	6.1855684	7.1858793	7.0431810
33 H	5.4550615	5.8355944	7.2690078	8.0601197
34 H	2.1030830 *	2.9493497 *	4.2100282	5.3354427
35 H	2.0922090 *	3.4226289	4.5648502	5.8880787

C C C N

1 CO	5.3589735	4.1925435	2.9190403 *	1.9338743 *
2 C	3.7706004	4.2842607	3.8369042	5.0664223
3 C	4.9472838	5.1751787	4.3829698	5.3357593
4 C	5.1733717	5.0002334	3.8921219	4.5025076
5 C	4.3621221	3.8849333	2.6265683 *	3.1048744
6 C	2.9122041 *	2.5020158 *	1.4671374 *	2.5395536 *
7 C	2.4740525 *	2.8436066 *	2.4973315 *	3.8464225
8 C	1.3998968 *	2.4420217 *	2.8609871 *	4.3174964
9 C	0.0000000	1.4287348 *	2.4837671 *	3.8011241
10 C	1.4287348 *	0.0000000	1.4149828 *	2.4739303 *
11 C	2.4837671 *	1.4149828 *	0.0000000	1.4580912 *
12 N	3.8011241	2.4739303 *	1.4580912 *	0.0000000
13 C	4.3083874	2.8962335 *	2.4355589 *	1.3331001 *
14 C	5.7387145	4.3183969	3.8371136	2.5176540 *
15 C	6.7955397	5.3740601	4.6349929	3.1838358
16 C	8.1219390	6.6938083	6.0286791	4.5833934
17 C	8.5457184	7.1335199	6.7025825	5.3298217
18 C	7.7679296	6.4094527	6.2123409	4.9898172
19 C	6.3721601	5.0193584	4.8655750	3.7369233
20 O	6.7378080	5.3908443	4.3704234	2.9858787 *
21 N	5.3819875	4.5654393	3.1565510	2.9102401 *
22 H	4.0703471	4.8836146	4.6935131	6.0141563
23 H	5.9186917	6.2435973	5.4826660	6.4130879
24 H	6.2616621	6.0033788	4.8029402	5.1867310
25 H	2.1808646 *	3.4519118	3.9656071	5.4223011
26 H	1.1046951 *	2.1971641 *	3.4752796	4.6705910
27 H	2.1762696 *	1.1042713 *	2.1912476 *	2.6970698 *
28 H	3.8823794	2.5723846 *	2.6230941 *	2.0905929 *
29 H	8.9679625	7.5491283	6.7674035	5.3132560
30 H	9.6351796	8.2263241	7.8048700	6.4242608
31 H	8.3693526	7.0748559	7.0372350	5.9112350
32 H	5.9185606	4.6763203	4.8002020	3.9415868
33 H	7.6727557	6.3435876	5.2983578	3.9507799
34 H	5.5424340	4.7025666	3.3533678	3.0413716
35 H	6.2996599	5.5528969	4.1495145	3.8887262

	C	C	C	C
1 CO	2.8507725 *	3.2646288	3.0294076	4.3141936
2 C	6.2278661	7.5697147	8.1134454	9.5137174
3 C	6.5940185	7.7998712	8.1176517	9.4779497
4 C	5.7803811	6.8351091	6.9893602	8.3055440
5 C	4.3741734	5.4419126	5.6790020	7.0284705
6 C	3.7327094	5.0400235	5.6066073	7.0114167
7 C	4.9192322	6.3134663	6.9951335	8.4021509
8 C	5.1251213	6.5793148	7.4801546	8.8631872
9 C	4.3083874	5.7387145	6.7955397	8.1219390
10 C	2.8962335 *	4.3183969	5.3740601	6.6938083
11 C	2.4355589 *	3.8371136	4.6349929	6.0286791
12 N	1.3331001 *	2.5176540 *	3.1838358	4.5833934
13 C	0.0000000	1.4653577 *	2.6137651 *	3.8865915
14 C	1.4653577 *	0.0000000	1.4371396 *	2.4971238 *
15 C	2.6137651 *	1.4371396 *	0.0000000	1.4071467 *
16 C	3.8865915	2.4971238 *	1.4071467 *	0.0000000
17 C	4.3388443	2.8799364 *	2.4447710 *	1.4295201 *
18 C	3.7819286	2.4982980 *	2.8304500 *	2.4738351 *
19 C	2.4551973 *	1.4425123 *	2.4466374 *	2.8413661 *
20 O	3.0618559	2.5017477 *	1.4667763 *	2.4667618 *
21 N	4.0240246	4.7526940	4.7051138	5.9558479
22 H	7.1152077	8.5007603	9.1188907	10.5241303
23 H	7.6812877	8.8610039	9.1163329	10.4561820
24 H	6.4420495	7.3444713	7.3095966	8.5447019
25 H	6.2066670	7.6636907	8.5830507	9.9636852
26 H	4.9600656	6.3258886	7.4821129	8.7460756
27 H	2.6245764 *	3.8881659	5.0754827	6.2871888
28 H	1.1069100 *	2.1686658 *	3.5313152	4.6622314
29 H	4.8042459	3.5012216	2.1963941 *	1.1067104 *
30 H	5.4444643	3.9859579	3.4439246	2.1943339 *
31 H	4.6381573	3.4916212	3.9344986	3.4787289
32 H	2.6125580 *	2.1930231 *	3.4481483	3.9466200
33 H	4.0421353	3.3363177	2.0488862 *	2.5143566 *
34 H	3.9294074	4.6189201	4.6770282	5.8819290
35 H	4.9797774	5.5674017	5.3096022	6.4515211

	C	C	C	O
1 CO	5.4729451	5.6328994	4.7039766	1.9663494 *
2 C	10.3805436	10.0038009	8.6705791	7.3945216
3 C	10.4834694	10.2814574	9.0256842	7.2002824
4 C	9.3834522	9.3086358	8.1357277	5.9828281
5 C	8.0468438	7.9187906	6.7309697	4.7927637
6 C	7.8467807	7.4905753	6.1833977	5.0163079

7 C	9.1674630	8.6990708	7.3400812	6.4530587
8 C	9.4471231	8.7907438	7.3918243	7.1757408
9 C	8.5457184	7.7679296	6.3721601	6.7378080
10 C	7.1335199	6.4094527	5.0193584	5.3908443
11 C	6.7025825	6.2123409	4.8655750	4.3704234
12 N	5.3298217	4.9898172	3.7369233	2.9858787 *
13 C	4.3388443	3.7819286	2.4551973 *	3.0618559
14 C	2.8799364 *	2.4982980 *	1.4425123 *	2.5017477 *
15 C	2.4447710 *	2.8304500 *	2.4466374 *	1.4667763 *
16 C	1.4295201 *	2.4738351 *	2.8413661 *	2.4667618 *
17 C	0.0000000	1.4229394 *	2.4515866 *	3.7780979
18 C	1.4229394 *	0.0000000	1.4143672 *	4.2970711
19 C	2.4515866 *	1.4143672 *	0.0000000	3.7956066
20 O	3.7780979	4.2970711	3.7956066	0.0000000
21 N	7.0702162	7.1346697	6.1059659	3.7000487
22 H	11.3425805	10.8953576	9.5345003	8.4478924
23 H	11.5038275	11.3455398	10.1057574	8.1283638
24 H	9.7087781	9.7733752	8.6907543	6.1756179
25 H	10.5265430	9.8320645	8.4282613	8.2692161
26 H	9.0270091	8.1285436	6.7592565	7.5713228
27 H	6.5464924	5.7039446	4.3447822	5.3595565
28 H	4.8299499	3.9657711	2.5514369 *	4.1513124
29 H	2.1983015 *	3.4723567	3.9477757	2.6991824 *
30 H	1.1061060 *	2.2003210 *	3.4576665	4.6588516
31 H	2.2021995 *	1.1042006 *	2.1836223 *	5.4010689
32 H	3.4543190	2.1856465 *	1.1052702 *	4.6874174
33 H	3.9372204	4.7406837	4.4940566	0.9937841 *
34 H	6.8916101	6.8836678	5.8616877	3.8914122
35 H	7.6611859	7.8740453	6.9435404	4.1376347

N H H H

1 CO	1.9784760 *	6.5270503	6.1801429	4.3732526
2 C	4.3418285	1.1047013 *	2.1848911 *	3.4385802
3 C	3.8191583	2.1819659 *	1.1015691 *	2.1929982 *
4 C	2.4788261 *	3.4541623	2.2026942 *	1.1072439 *
5 C	1.5092887 *	3.9457058	3.4672143	2.1849993 *
6 C	2.5879540 *	3.5227734	4.0241548	3.5064410
7 C	3.8796986	2.1975781 *	3.4819578	3.9489458
8 C	5.1015182	2.6747040 *	4.6628094	5.3905463
9 C	5.3819875	4.0703471	5.9186917	6.2616621
10 C	4.5654393	4.8836146	6.2435973	6.0033788
11 C	3.1565510	4.6935131	5.4826660	4.8029402
12 N	2.9102401 *	6.0141563	6.4130879	5.1867310
13 C	4.0240246	7.1152077	7.6812877	6.4420495
14 C	4.7526940	8.5007603	8.8610039	7.3444713

15 C	4.7051138	9.1188907	9.1163329	7.3095966
16 C	5.9558479	10.5241303	10.4561820	8.5447019
17 C	7.0702162	11.3425805	11.5038275	9.7087781
18 C	7.1346697	10.8953576	11.3455398	9.7733752
19 C	6.1059659	9.5345003	10.1057574	8.6907543
20 O	3.7000487	8.4478924	8.1283638	6.1756179
21 N	0.0000000	5.4441371	4.6800032	2.6641493 *
22 H	5.4441371	0.0000000	2.5313566 *	4.3594298
23 H	4.6800032	2.5313566 *	0.0000000	2.5176435 *
24 H	2.6641493 *	4.3594298	2.5176435 *	0.0000000
25 H	6.0417109	2.3911621 *	4.7715346	5.9660674
26 H	6.4657331	4.7670162	6.8382692	7.3427022
27 H	5.2678254	5.9528793	7.3277667	6.9629817
28 H	4.7878977	7.1338087	8.0217000	7.0498455
29 H	6.2629502	11.0961080	10.8049060	8.7495933
30 H	8.0549815	12.4371610	12.5439413	10.6812615
31 H	8.1532166	11.6952837	12.2792684	10.7829461
32 H	6.5012534	9.3498288	10.1756633	8.9861224
33 H	4.2648107	9.1854301	8.6660674	6.5818561
34 H	1.0451951 *	5.8083656	5.1633121	3.2192172
35 H	1.0386809 *	5.8325311	4.6033364	2.2344105 *

H H H H

1 CO	6.5823615	6.3315570	4.5361625	3.8675862
2 C	2.6727954 *	4.6598738	5.3807226	6.3574032
3 C	4.0733932	5.9214284	6.2552298	6.9216788
4 C	4.8836301	6.2472851	6.0018115	6.2835071
5 C	4.6656412	5.4666294	4.8043322	4.9092075
6 C	3.5163851	4.0167578	3.5046664	4.0170209
7 C	2.1948757 *	3.4804608	3.9435079	4.9686266
8 C	1.1048085 *	2.1831477 *	3.4254043	4.8884293
9 C	2.1808646 *	1.1046951 *	2.1762696 *	3.8823794
10 C	3.4519118	2.1971641 *	1.1042713 *	2.5723846 *
11 C	3.9656071	3.4752796	2.1912476 *	2.6230941 *
12 N	5.4223011	4.6705910	2.6970698 *	2.0905929 *
13 C	6.2066670	4.9600656	2.6245764 *	1.1069100 *
14 C	7.6636907	6.3258886	3.8881659	2.1686658 *
15 C	8.5830507	7.4821129	5.0754827	3.5313152
16 C	9.9636852	8.7460756	6.2871888	4.6622314
17 C	10.5265430	9.0270091	6.5464924	4.8299499
18 C	9.8320645	8.1285436	5.7039446	3.9657711
19 C	8.4282613	6.7592565	4.3447822	2.5514369 *
20 O	8.2692161	7.5713228	5.3595565	4.1513124
21 N	6.0417109	6.4657331	5.2678254	4.7878977
22 H	2.3911621 *	4.7670162	5.9528793	7.1338087

23 H	4.7715346	6.8382692	7.3277667	8.0217000
24 H	5.9660674	7.3427022	6.9629817	7.0498455
25 H	0.0000000	2.5292813 *	4.3438272	5.9059629
26 H	2.5292813 *	0.0000000	2.4943633 *	4.3538727
27 H	4.3438272	2.4943633 *	0.0000000	2.0733112 *
28 H	5.9059629	4.3538727	2.0733112 *	0.0000000
29 H	10.7191853	9.6483163	7.2186637	5.6654014
30 H	11.6279183	10.0911883	7.6104221	5.9090706
31 H	10.4787979	8.6116056	6.2754202	4.6130252
32 H	8.0194276	6.1644061	3.8938953	2.2177563 *
33 H	9.1428274	8.5157925	6.3141044	5.1224290
34 H	6.2739599	6.5916679	5.3581507	4.5942351
35 H	6.7568893	7.3960394	6.2746730	5.7941851

H H H H

1 CO	4.6615301	6.4587183	6.6965756	5.2724043
2 C	10.0540806	11.4674721	10.8473654	8.5707976
3 C	9.8831893	11.5369343	11.2028702	9.0798460
4 C	8.6376849	10.4056076	10.2810437	8.3278003
5 C	7.4502909	9.0892709	8.8821166	6.9268695
6 C	7.6124531	8.9355829	8.3664699	6.1855684
7 C	9.0380044	10.2661597	9.5043707	7.1858793
8 C	9.6160633	10.5497621	9.4754376	7.0431810
9 C	8.9679625	9.6351796	8.3693526	5.9185606
10 C	7.5491283	8.2263241	7.0748559	4.6763203
11 C	6.7674035	7.8048700	7.0372350	4.8002020
12 N	5.3132560	6.4242608	5.9112350	3.9415868
13 C	4.8042459	5.4444643	4.6381573	2.6125580 *
14 C	3.5012216	3.9859579	3.4916212	2.1930231 *
15 C	2.1963941 *	3.4439246	3.9344986	3.4481483
16 C	1.1067104 *	2.1943339 *	3.4787289	3.9466200
17 C	2.1983015 *	1.1061060 *	2.2021995 *	3.4543190
18 C	3.4723567	2.2003210 *	1.1042006 *	2.1856465 *
19 C	3.9477757	3.4576665	2.1836223 *	1.1052702 *
20 O	2.6991824 *	4.6588516	5.4010689	4.6874174
21 N	6.2629502	8.0549815	8.1532166	6.5012534
22 H	11.0961080	12.4371610	11.6952837	9.3498288
23 H	10.8049060	12.5439413	12.2792684	10.1756633
24 H	8.7495933	10.6812615	10.7829461	8.9861224
25 H	10.7191853	11.6279183	10.4787979	8.0194276
26 H	9.6483163	10.0911883	8.6116056	6.1644061
27 H	7.2186637	7.6104221	6.2754202	3.8938953
28 H	5.6654014	5.9090706	4.6130252	2.2177563 *
29 H	0.0000000	2.5182667 *	4.3890837	5.0530132
30 H	2.5182667 *	0.0000000	2.5469836 *	4.3732314

31 H	4.3890837	2.5469836 *	0.0000000	2.5115247 *
32 H	5.0530132	4.3732314	2.5115247 *	0.0000000
33 H	2.3149654 *	4.6383801	5.8275961	5.4703123
34 H	6.2519906	7.8705194	7.8561597	6.2088130
35 H	6.5965048	8.5841367	8.9195534	7.4193776

H H H

1 CO	2.6689311 *	2.4881631 *	2.6066636 *
2 C	8.1184133	4.7395781	4.7494757
3 C	7.8031437	4.3049016	3.9334389
4 C	6.5290811	3.0484293	2.4995007 *
5 C	5.4550615	2.1030830 *	2.0922090 *
6 C	5.8355944	2.9493497 *	3.4226289
7 C	7.2690078	4.2100282	4.5648502
8 C	8.0601197	5.3354427	5.8880787
9 C	7.6727557	5.5424340	6.2996599
10 C	6.3435876	4.7025666	5.5528969
11 C	5.2983578	3.3533678	4.1495145
12 N	3.9507799	3.0413716	3.8887262
13 C	4.0421353	3.9294074	4.9797774
14 C	3.3363177	4.6189201	5.5674017
15 C	2.0488862 *	4.6770282	5.3096022
16 C	2.5143566 *	5.8819290	6.4515211
17 C	3.9372204	6.8916101	7.6611859
18 C	4.7406837	6.8836678	7.8740453
19 C	4.4940566	5.8616877	6.9435404
20 O	0.9937841 *	3.8914122	4.1376347
21 N	4.2648107	1.0451951 *	1.0386809 *
22 H	9.1854301	5.8083656	5.8325311
23 H	8.6660674	5.1633121	4.6033364
24 H	6.5818561	3.2192172	2.2344105 *
25 H	9.1428274	6.2739599	6.7568893
26 H	8.5157925	6.5916679	7.3960394
27 H	6.3141044	5.3581507	6.2746730
28 H	5.1224290	4.5942351	5.7941851
29 H	2.3149654 *	6.2519906	6.5965048
30 H	4.6383801	7.8705194	8.5841367
31 H	5.8275961	7.8561597	8.9195534
32 H	5.4703123	6.2088130	7.4193776
33 H	0.0000000	4.5053663	4.4936870
34 H	4.5053663	0.0000000	1.6668390 *
35 H	4.4936870	1.6668390 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.77 , TOTAL = 5145.1 SECONDS (85.8 MIN)
WALL CLOCK TIME: STEP = 0.80 , TOTAL = 4757.1 SECONDS (79.3 MIN)
CPU UTILIZATION: STEP = 96.09% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.93 , TOTAL = 5146.1 SECONDS (85.8 MIN)
WALL CLOCK TIME: STEP = 0.92 , TOTAL = 4758.0 SECONDS (79.3 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.635040819	-284.635040819	0.014392922	0.001216072	196997501
11398403						
2	1	-284.635170264	-0.000129444	0.002868116	0.000118400	157863066
14716047						
3	2	-284.635168730	0.000001533	0.001792157	0.000248448	144426114
15804544						
4	3	-284.635172686	-0.000003956	0.000439758	0.000034470	139105210
16205552						
5	4	-284.635172601	0.000000085	0.000313216	0.000089880	128778630
17042871						
6	5	-284.635172795	-0.000000194	0.000156631	0.000026517	121693012
17615681						
7	6	-284.635172776	0.000000019	0.000103278	0.000030179	120139952
17646217						
8	7	-284.635172821	-0.000000045	0.000103091	0.000013961	137315488
16358373						
9	8	-284.635172833	-0.000000011	0.000206658	0.000012393	135408410
16577400						
10	9	-284.635172853	-0.000000021	0.000244986	0.000016093	156710172
14994987						

-----DISABLING FDIFF OPTION-----

11	10	-284.635172838	0.000000015	0.000163464	0.000018542	196992682
11398635						
12	11	-284.635172852	-0.000000014	0.000154535	0.000016364	196992775
11398635						

13 12	-284.635172863	-0.000000012	0.000208710	0.000010981	196992755
11398635					
14 13	-284.635172874	-0.000000011	0.000101121	0.000007187	196992708
11398639					
15 14	-284.635172876	-0.000000002	0.000037662	0.000004724	196992771
11398634					
16 15	-284.635172878	-0.000000001	0.000020250	0.000002861	196992769
11398634					
17 16	-284.635172878	0.000000000	0.000017751	0.000002745	196992704
11398637					
18 17	-284.635172878	0.000000000	0.000043529	0.000002380	196992707
11398636					
19 18	-284.635172879	-0.000000001	0.000039888	0.000001910	196992730
11398637					
20 19	-284.635172879	0.000000000	0.000030457	0.000002110	196992742
11398635					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 67.0 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 21.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.3, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.5 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6351728791 AFTER 20 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6005760328
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999952258

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 70.72 , TOTAL = 5216.8 SECONDS (86.9 MIN)
WALL CLOCK TIME: STEP = 64.97 , TOTAL = 4823.0 SECONDS (80.4 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.68 , TOTAL = 5220.5 SECONDS (87.0 MIN)
 WALL CLOCK TIME: STEP = 3.65 , TOTAL = 4826.6 SECONDS (80.4 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
 USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.07 , TOTAL = 5223.5 SECONDS (87.1 MIN)
 WALL CLOCK TIME: STEP = 2.91 , TOTAL = 4829.6 SECONDS (80.5 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 52 ENERGY= -284.6351729

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0007360	0.0002894	0.0000293
2 C	6.0	0.0006634	0.0028914	0.0001539
3 C	6.0	0.0027127	-0.0015522	-0.0000006
4 C	6.0	-0.0007500	-0.0009263	-0.0002706
5 C	6.0	-0.0003067	0.0002958	-0.0002002
6 C	6.0	0.0006891	-0.0007037	-0.0001937
7 C	6.0	-0.0002138	-0.0000717	-0.0001793
8 C	6.0	-0.0009550	0.0001554	-0.0001249
9 C	6.0	0.0005246	-0.0014096	-0.0002354
10 C	6.0	0.0007517	0.0000136	0.0002660
11 C	6.0	-0.0006919	0.0000593	0.0002943
12 N	7.0	-0.0001673	-0.0006223	-0.0001296
13 C	6.0	0.0001453	0.0007861	-0.0001783
14 C	6.0	-0.0007719	-0.0006791	0.0000216
15 C	6.0	-0.0004137	0.0002049	0.0003387
16 C	6.0	-0.0000092	0.0003559	-0.0000679
17 C	6.0	0.0002273	0.0002415	-0.0000535
18 C	6.0	-0.0000852	-0.0002455	-0.0004278
19 C	6.0	0.0000867	-0.0002896	-0.0005160
20 O	8.0	0.0004435	-0.0000367	-0.0006448
21 N	7.0	0.0006463	-0.0000631	0.0009978

22 H	1.0	-0.0001561	-0.0000046	-0.0003782
23 H	1.0	-0.0015521	0.0008204	0.0010454
24 H	1.0	0.0003833	0.0004850	0.0002094
25 H	1.0	-0.0000366	-0.0000857	-0.0009691
26 H	1.0	0.0000422	0.0003515	-0.0003425
27 H	1.0	-0.0001694	0.0001412	0.0005770
28 H	1.0	0.0004669	0.0000528	0.0006131
29 H	1.0	-0.0003484	-0.0000315	-0.0010175
30 H	1.0	-0.0006977	0.0002017	0.0005232
31 H	1.0	0.0004072	0.0007260	0.0005224
32 H	1.0	0.0005361	-0.0003655	0.0002888
33 H	1.0	-0.0004639	-0.0018705	0.0002013
34 H	1.0	-0.0004443	0.0004464	-0.0004139
35 H	1.0	-0.0012293	0.0004393	0.0002614

MAXIMUM GRADIENT = 0.0028914 RMS GRADIENT = 0.0006785
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000671647
 PREDICTED ENERGY CHANGE WAS -0.0001541851 RATIO= 0.436
 GDIIS STEP HAS LENGTH = 0.207909
 RADIUS OF STEP TAKEN= 0.08326 CURRENT TRUST RADIUS= 0.08326

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 5223.6 SECONDS (87.1 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4829.6 SECONDS (80.5 MIN)
 CPU UTILIZATION: STEP = 91.74% , TOTAL = 100.00%

INSERCH= 53

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1383734049	-1.7727590844	0.9534201050
C	6.0	4.9906659352	0.6842039181	0.4763835916
C	6.0	5.2132206093	-0.6813509402	0.2486391301
C	6.0	4.0850849607	-1.5417164488	0.0360075929
C	6.0	2.7687277402	-1.0476757567	0.1040239934
C	6.0	2.4795747914	0.3343560079	0.4585946993
C	6.0	3.6503643162	1.2099083711	0.5927206793
C	6.0	3.4864962712	2.6176400891	0.8624434330
C	6.0	2.2176419995	3.1639279027	1.0916511493
C	6.0	1.0704898514	2.3135584370	1.0541697339
C	6.0	1.1689312855	0.9469519036	0.6999010220
N	7.0	-0.0414143702	0.1340961836	0.6830935185

C	6.0	-1.2371904295	0.6709522075	0.4394039725
C	6.0	-2.5504396369	0.0231792934	0.5033678213
C	6.0	-2.8573489132	-1.3452674589	0.8172291389
C	6.0	-4.1734262868	-1.8409309232	0.8633112239
C	6.0	-5.2601619971	-0.9455390758	0.6186720023
C	6.0	-5.0087665726	0.4194571667	0.3057310939
C	6.0	-3.6755989316	0.8867143413	0.2396428706
O	8.0	-1.7570847775	-2.2714862148	1.1047306062
N	7.0	1.6713222153	-2.0109291725	-0.2758731670
H	1.0	5.8404189736	1.3810645335	0.5880077000
H	1.0	6.2352835684	-1.0913303576	0.2081144173
H	1.0	4.2675479294	-2.6034756706	-0.2175334491
H	1.0	4.3886978825	3.2535216852	0.9028487280
H	1.0	2.0972865107	4.2353228578	1.3313962004
H	1.0	0.0965513171	2.7448236932	1.3445259202
H	1.0	-1.2697995631	1.7367642150	0.1426751522
H	1.0	-4.3798802455	-2.9060679059	1.0817202696
H	1.0	-6.2972754450	-1.3250014983	0.6780777125
H	1.0	-5.8433533456	1.1190663694	0.1241397444
H	1.0	-3.4758273112	1.9468348165	-0.0014094900
H	1.0	-2.0979725210	-3.1660859757	1.3710398672
H	1.0	1.3260143009	-1.7824902177	-1.2352522013
H	1.0	2.0688434835	-2.9691322913	-0.3327277822

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4597595	5.2385076	4.0585168
2 C	5.4597595	0.0000000	1.4021905 *	2.4430983 *
3 C	5.2385076	1.4021905 *	0.0000000	1.4346188 *
4 C	4.0585168	2.4430983 *	1.4346188 *	0.0000000
5 C	2.8576185 *	2.8416665 *	2.4760155 *	1.4076572 *
6 C	3.1884181	2.5354070 *	2.9237923 *	2.5051728 *
7 C	4.6217409	1.4444057 *	2.4774531 *	2.8408363 *
8 C	5.5221199	2.4798677 *	3.7738143	4.2827038
9 C	5.3584834	3.7705765	4.9467494	5.1715390
10 C	4.1924912	4.2844385	5.1749956	4.9987581
11 C	2.9194433 *	3.8372715	4.3830678	3.8907810
12 N	1.9342950 *	5.0662787	5.3352501	4.5005627
13 C	2.8509846 *	6.2279803	6.5933995	5.7779968
14 C	3.2646068	7.5700697	7.7997224	6.8335577
15 C	3.0291334	8.1133388	8.1177689	6.9890119
16 C	4.3132799	9.5134960	9.4779527	8.3052374
17 C	5.4717944	10.3805482	10.4832468	9.3823540

18	C	5.6319058	10.0043922	10.2812480	9.3068302
19	C	4.7041112	8.6718627	9.0260746	8.1343075
20	O	1.9658040 *	7.3934474	7.2004569	5.9837848
21	N	1.9793481 *	4.3413909	3.8194156	2.4786449 *
22	H	6.5263660	1.1046062 *	2.1822251 *	3.4537733
23	H	6.1799789	2.1848486 *	1.1019701 *	2.2035931 *
24	H	4.3716478	3.4370420	2.1922995 *	1.1067558 *
25	H	6.5826525	2.6731315 *	4.0732113	4.8824075
26	H	6.3306599	4.6597357	5.9207339	6.2452828
27	H	4.5346739	5.3807233	6.2545939	5.9995873
28	H	3.8674297	6.3570963	6.9201199	6.2796976
29	H	4.6599856	10.0530403	9.8828626	8.6377431
30	H	6.4570796	11.4671360	11.5364736	10.4044523
31	H	6.6956266	10.8484632	11.2028938	10.2791741
32	H	5.2734737	8.5734492	9.0812685	8.3269913
33	H	2.6677723 *	8.1162761	7.8030274	6.5307800
34	H	2.4901550 *	4.7375045	4.3040462	3.0473832
35	H	2.6100191 *	4.7474807	3.9317984	2.4977413 *

C C C C

1	CO	2.8576185 *	3.1884181	4.6217409	5.5221199
2	C	2.8416665 *	2.5354070 *	1.4444057 *	2.4798677 *
3	C	2.4760155 *	2.9237923 *	2.4774531 *	3.7738143
4	C	1.4076572 *	2.5051728 *	2.8408363 *	4.2827038
5	C	0.0000000	1.4557959 *	2.4724064 *	3.8111589
6	C	1.4557959 *	0.0000000	1.4681042 *	2.5279183 *
7	C	2.4724064 *	1.4681042 *	0.0000000	1.4426752 *
8	C	3.8111589	2.5279183 *	1.4426752 *	0.0000000
9	C	4.3608151	2.9113307 *	2.4738264 *	1.4003420 *
10	C	3.8839006	2.5014940 *	2.8437178 *	2.4426035 *
11	C	2.6254443 *	1.4667273 *	2.4976276 *	2.8615951 *
12	N	3.1030316	2.5388757 *	3.8463969	4.3181374
13	C	4.3719037	3.7320248	4.9195702	5.1265751
14	C	5.4405650	5.0398294	6.3139749	6.5806350
15	C	5.6789049	5.6064702	6.9949738	7.4800436
16	C	7.0284617	7.0112832	8.4019366	8.8630283
17	C	8.0460155	7.8464821	9.1675573	9.4477352
18	C	7.9172333	7.4903849	8.6998692	8.7926917
19	C	6.7297551	6.1837855	7.3415840	7.3945650
20	O	4.7939654	5.0156943	6.4515710	7.1733814
21	N	1.5088001 *	2.5870983 *	3.8787701	5.1004191
22	H	3.9456694	3.5224452	2.1967376 *	2.6730855 *
23	H	3.4683930	4.0250056	3.4821587	4.6626645
24	H	2.1841187 *	3.5049753	3.9470654	5.3885473
25	H	4.6650534	3.5161969	2.1949194 *	1.1045115 *

26 H	5.4651029	4.0156530	3.4800611	2.1832815 *
27 H	4.8023353	3.5034311	3.9434456	3.4264130
28 H	4.9055380	4.0155152	4.9687152	4.8904354
29 H	7.4506448	7.6118826	9.0368805	9.6145365
30 H	9.0883916	8.9350288	10.2658945	10.5499101
31 H	8.8804908	8.3665264	9.5057086	9.4782335
32 H	6.9262311	6.1869626	7.1887870	7.0477068
33 H	5.4569004	5.8343457	7.2662565	8.0558332
34 H	2.1011985 *	2.9463294 *	4.2069629	5.3318999
35 H	2.0910728 *	3.4216847	4.5631178	5.8864420

C C C N

1 CO	5.3584834	4.1924912	2.9194433 *	1.9342950 *
2 C	3.7705765	4.2844385	3.8372715	5.0662787
3 C	4.9467494	5.1749956	4.3830678	5.3352501
4 C	5.1715390	4.9987581	3.8907810	4.5005627
5 C	4.3608151	3.8839006	2.6254443 *	3.1030316
6 C	2.9113307 *	2.5014940 *	1.4667273 *	2.5388757 *
7 C	2.4738264 *	2.8437178 *	2.4976276 *	3.8463969
8 C	1.4003420 *	2.4426035 *	2.8615951 *	4.3181374
9 C	0.0000000	1.4284576 *	2.4835952 *	3.8013334
10 C	1.4284576 *	0.0000000	1.4152069 *	2.4746887 *
11 C	2.4835952 *	1.4152069 *	0.0000000	1.4580650 *
12 N	3.8013334	2.4746887 *	1.4580650 *	0.0000000
13 C	4.3100141	2.8985307 *	2.4358687 *	1.3332214 *
14 C	5.7397719	4.3197627	3.8374081	2.5178983 *
15 C	6.7943861	5.3731802	4.6345407	3.1837080
16 C	8.1207453	6.6928966	6.0282483	4.5833103
17 C	8.5456995	7.1336195	6.7023399	5.3296425
18 C	7.7698630	6.4113289	6.2126944	4.9898318
19 C	6.3751007	5.0224194	4.8667175	3.7376972
20 O	6.7336729	5.3870557	4.3685010	2.9846490 *
21 N	5.3803098	4.5641217	3.1549314	2.9076137 *
22 H	4.0690013	4.8825276	4.6929491	6.0133131
23 H	5.9185559	6.2437306	5.4830989	6.4128163
24 H	6.2593149	6.0013027	4.8009007	5.1838774
25 H	2.1810908 *	3.4520912	3.9658982	5.4226380
26 H	1.1044683 *	2.1964390 *	3.4747681	4.6705886
27 H	2.1768371 *	1.1040166 *	2.1904070 *	2.6967435 *
28 H	3.8858204	2.5769106 *	2.6233018 *	2.0903414 *
29 H	8.9650570	7.5466411	6.7661553	5.3126064
30 H	9.6345913	8.2258452	7.8042611	6.4237675
31 H	8.3724060	7.0776405	7.0379869	5.9114373
32 H	5.9238239	4.6816379	4.8026435	3.9433181
33 H	7.6662678	6.3376702	5.2952968	3.9489117

34 H	5.5386398	4.6994000	3.3495294	3.0369746
35 H	6.2980492	5.5522082	4.1487202	3.8878153

	C	C	C	C
--	---	---	---	---

1 CO	2.8509846 *	3.2646068	3.0291334	4.3132799
2 C	6.2279803	7.5700697	8.1133388	9.5134960
3 C	6.5933995	7.7997224	8.1177689	9.4779527
4 C	5.7779968	6.8335577	6.9890119	8.3052374
5 C	4.3719037	5.4405650	5.6789049	7.0284617
6 C	3.7320248	5.0398294	5.6064702	7.0112832
7 C	4.9195702	6.3139749	6.9949738	8.4019366
8 C	5.1265751	6.5806350	7.4800436	8.8630283
9 C	4.3100141	5.7397719	6.7943861	8.1207453
10 C	2.8985307 *	4.3197627	5.3731802	6.6928966
11 C	2.4358687 *	3.8374081	4.6345407	6.0282483
12 N	1.3332214 *	2.5178983 *	3.1837080	4.5833103
13 C	0.0000000	1.4657164 *	2.6139639 *	3.8872529
14 C	1.4657164 *	0.0000000	1.4371321 *	2.4977093 *
15 C	2.6139639 *	1.4371321 *	0.0000000	1.4070769 *
16 C	3.8872529	2.4977093 *	1.4070769 *	0.0000000
17 C	4.3392950	2.8799836 *	2.4439146 *	1.4291849 *
18 C	3.7823147	2.4978927 *	2.8292192 *	2.4734679 *
19 C	2.4560728 *	1.4426459 *	2.4464018 *	2.8419787 *
20 O	3.0611915	2.5013074 *	1.4666695 *	2.4662456 *
21 N	4.0203924	4.7505881	4.7060430	5.9571575
22 H	7.1146959	8.5004426	9.1179271	10.5230292
23 H	7.6809506	8.8610518	9.1165493	10.4562146
24 H	6.4386015	7.3419323	7.3087603	8.5439888
25 H	6.2076618	7.6646152	8.5826212	9.9631813
26 H	4.9617663	6.3268588	7.4803588	8.7442440
27 H	2.6266054 *	3.8886317	5.0727127	6.2843792
28 H	1.1068273 *	2.1694496 *	3.5318912	4.6637182
29 H	4.8045960	3.5016901	2.1963960 *	1.1067260 *
30 H	5.4447458	3.9858366	3.4427995	2.1934516 *
31 H	4.6386350	3.4911407	3.9331332	3.4780188
32 H	2.6141324 *	2.1935344 *	3.4482781	3.9473479
33 H	4.0412564	3.3360147	2.0490825 *	2.5142260 *
34 H	3.9235025	4.6162904	4.6802106	5.8865296
35 H	4.9775760	5.5669346	5.3128815	6.4551746

	C	C	C	O
--	---	---	---	---

1 CO	5.4717944	5.6319058	4.7041112	1.9658040 *
2 C	10.3805482	10.0043922	8.6718627	7.3934474
3 C	10.4832468	10.2812480	9.0260746	7.2004569

4 C	9.3823540	9.3068302	8.1343075	5.9837848
5 C	8.0460155	7.9172333	6.7297551	4.7939654
6 C	7.8464821	7.4903849	6.1837855	5.0156943
7 C	9.1675573	8.6998692	7.3415840	6.4515710
8 C	9.4477352	8.7926917	7.3945650	7.1733814
9 C	8.5456995	7.7698630	6.3751007	6.7336729
10 C	7.1336195	6.4113289	5.0224194	5.3870557
11 C	6.7023399	6.2126944	4.8667175	4.3685010
12 N	5.3296425	4.9898318	3.7376972	2.9846490 *
13 C	4.3392950	3.7823147	2.4560728 *	3.0611915
14 C	2.8799836 *	2.4978927 *	1.4426459 *	2.5013074 *
15 C	2.4439146 *	2.8292192 *	2.4464018 *	1.4666695 *
16 C	1.4291849 *	2.4734679 *	2.8419787 *	2.4662456 *
17 C	0.0000000	1.4227953 *	2.4518678 *	3.7770278
18 C	1.4227953 *	0.0000000	1.4142252 *	4.2956968
19 C	2.4518678 *	1.4142252 *	0.0000000	3.7951685
20 O	3.7770278	4.2956968	3.7951685	0.0000000
21 N	7.0697058	7.1322246	6.1034138	3.7051223
22 H	11.3418218	10.8953750	9.5352156	8.4457204
23 H	11.5036986	11.3455133	10.1063963	8.1286309
24 H	9.7069691	9.7704626	8.6881539	6.1769571
25 H	10.5267927	9.8336570	8.4305695	8.2666265
26 H	9.0267023	8.1307325	6.7624929	7.5661165
27 H	6.5452287	5.7053216	4.3476953	5.3532078
28 H	4.8315956	3.9675886	2.5534013 *	4.1507914
29 H	2.1984046 *	3.4722866	3.9484559	2.6985699 *
30 H	1.1059499 *	2.2004620 *	3.4579040	4.6573809
31 H	2.2016516 *	1.1040668 *	2.1832287 *	5.3995367
32 H	3.4545880	2.1856625 *	1.1053825 *	4.6874144
33 H	3.9365376	4.7395912	4.4937907	0.9936970 *
34 H	6.8931299	6.8813262	5.8579948	3.9012993
35 H	7.6625330	7.8729113	6.9421740	4.1461698

N H H H

1 CO	1.9793481 *	6.5263660	6.1799789	4.3716478
2 C	4.3413909	1.1046062 *	2.1848486 *	3.4370420
3 C	3.8194156	2.1822251 *	1.1019701 *	2.1922995 *
4 C	2.4786449 *	3.4537733	2.2035931 *	1.1067558 *
5 C	1.5088001 *	3.9456694	3.4683930	2.1841187 *
6 C	2.5870983 *	3.5224452	4.0250056	3.5049753
7 C	3.8787701	2.1967376 *	3.4821587	3.9470654
8 C	5.1004191	2.6730855 *	4.6626645	5.3885473
9 C	5.3803098	4.0690013	5.9185559	6.2593149
10 C	4.5641217	4.8825276	6.2437306	6.0013027
11 C	3.1549314	4.6929491	5.4830989	4.8009007

12 N	2.9076137 *	6.0133131	6.4128163	5.1838774
13 C	4.0203924	7.1146959	7.6809506	6.4386015
14 C	4.7505881	8.5004426	8.8610518	7.3419323
15 C	4.7060430	9.1179271	9.1165493	7.3087603
16 C	5.9571575	10.5230292	10.4562146	8.5439888
17 C	7.0697058	11.3418218	11.5036986	9.7069691
18 C	7.1322246	10.8953750	11.3455133	9.7704626
19 C	6.1034138	9.5352156	10.1063963	8.6881539
20 O	3.7051223	8.4457204	8.1286309	6.1769571
21 N	0.0000000	5.4436458	4.6807744	2.6636259 *
22 H	5.4436458	0.0000000	2.5323849 *	4.3588279
23 H	4.6807744	2.5323849 *	0.0000000	2.5178846 *
24 H	2.6636259 *	4.3588279	2.5178846 *	0.0000000
25 H	6.0405264	2.3901286 *	4.7718208	5.9644238
26 H	6.4637779	4.7655490	6.8379833	7.3401896
27 H	5.2652428	5.9518211	7.3274513	6.9599963
28 H	4.7823201	7.1330254	8.0205158	7.0448314
29 H	6.2658906	11.0940422	10.8045436	8.7497221
30 H	8.0547544	12.4360175	12.5435443	10.6795182
31 H	8.1502903	11.6959118	12.2795104	10.7798137
32 H	6.4986440	9.3520026	10.1774271	8.9839799
33 H	4.2725043	9.1819266	8.6660351	6.5848270
34 H	1.0449067 *	5.8062212	5.1635195	3.2190664
35 H	1.0389460 *	5.8306730	4.6019423	2.2318772 *

H H H H

1 CO	6.5826525	6.3306599	4.5346739	3.8674297
2 C	2.6731315 *	4.6597357	5.3807233	6.3570963
3 C	4.0732113	5.9207339	6.2545939	6.9201199
4 C	4.8824075	6.2452828	5.9995873	6.2796976
5 C	4.6650534	5.4651029	4.8023353	4.9055380
6 C	3.5161969	4.0156530	3.5034311	4.0155152
7 C	2.1949194 *	3.4800611	3.9434456	4.9687152
8 C	1.1045115 *	2.1832815 *	3.4264130	4.8904354
9 C	2.1810908 *	1.1044683 *	2.1768371 *	3.8858204
10 C	3.4520912	2.1964390 *	1.1040166 *	2.5769106 *
11 C	3.9658982	3.4747681	2.1904070 *	2.6233018 *
12 N	5.4226380	4.6705886	2.6967435 *	2.0903414 *
13 C	6.2076618	4.9617663	2.6266054 *	1.1068273 *
14 C	7.6646152	6.3268588	3.8886317	2.1694496 *
15 C	8.5826212	7.4803588	5.0727127	3.5318912
16 C	9.9631813	8.7442440	6.2843792	4.6637182
17 C	10.5267927	9.0267023	6.5452287	4.8315956
18 C	9.8336570	8.1307325	5.7053216	3.9675886
19 C	8.4305695	6.7624929	4.3476953	2.5534013 *

20	O	8.2666265	7.5661165	5.3532078	4.1507914
21	N	6.0405264	6.4637779	5.2652428	4.7823201
22	H	2.3901286 *	4.7655490	5.9518211	7.1330254
23	H	4.7718208	6.8379833	7.3274513	8.0205158
24	H	5.9644238	7.3401896	6.9599963	7.0448314
25	H	0.0000000	2.5294570 *	4.3446950	5.9073692
26	H	2.5294570 *	0.0000000	2.4949352 *	4.3581099
27	H	4.3446950	2.4949352 *	0.0000000	2.0802750 *
28	H	5.9073692	4.3581099	2.0802750 *	0.0000000
29	H	10.7172992	9.6444538	7.2138812	5.6665949
30	H	11.6277007	10.0902281	7.6084592	5.9107173
31	H	10.4812766	8.6152356	6.2781284	4.6151152
32	H	8.0234575	6.1703441	3.9000279	2.2206865 *
33	H	9.1382415	8.5077978	6.3051956	5.1217859
34	H	6.2700018	6.5876110	5.3538216	4.5849848
35	H	6.7549831	7.3942066	6.2731499	5.7894738

H H H H

1	CO	4.6599856	6.4570796	6.6956266	5.2734737
2	C	10.0530403	11.4671360	10.8484632	8.5734492
3	C	9.8828626	11.5364736	11.2028938	9.0812685
4	C	8.6377431	10.4044523	10.2791741	8.3269913
5	C	7.4506448	9.0883916	8.8804908	6.9262311
6	C	7.6118826	8.9350288	8.3665264	6.1869626
7	C	9.0368805	10.2658945	9.5057086	7.1887870
8	C	9.6145365	10.5499101	9.4782335	7.0477068
9	C	8.9650570	9.6345913	8.3724060	5.9238239
10	C	7.5466411	8.2258452	7.0776405	4.6816379
11	C	6.7661553	7.8042611	7.0379869	4.8026435
12	N	5.3126064	6.4237675	5.9114373	3.9433181
13	C	4.8045960	5.4447458	4.6386350	2.6141324 *
14	C	3.5016901	3.9858366	3.4911407	2.1935344 *
15	C	2.1963960 *	3.4427995	3.9331332	3.4482781
16	C	1.1067260 *	2.1934516 *	3.4780188	3.9473479
17	C	2.1984046 *	1.1059499 *	2.2016516 *	3.4545880
18	C	3.4722866	2.2004620 *	1.1040668 *	2.1856625 *
19	C	3.9484559	3.4579040	2.1832287 *	1.1053825 *
20	O	2.6985699 *	4.6573809	5.3995367	4.6874144
21	N	6.2658906	8.0547544	8.1502903	6.4986440
22	H	11.0940422	12.4360175	11.6959118	9.3520026
23	H	10.8045436	12.5435443	12.2795104	10.1774271
24	H	8.7497221	10.6795182	10.7798137	8.9839799
25	H	10.7172992	11.6277007	10.4812766	8.0234575
26	H	9.6444538	10.0902281	8.6152356	6.1703441
27	H	7.2138812	7.6084592	6.2781284	3.9000279

28 H	5.6665949	5.9107173	4.6151152	2.2206865 *
29 H	0.0000000	2.5177575 *	4.3886695	5.0538249
30 H	2.5177575 *	0.0000000	2.5468334 *	4.3734638
31 H	4.3886695	2.5468334 *	0.0000000	2.5112034 *
32 H	5.0538249	4.3734638	2.5112034 *	0.0000000
33 H	2.3148257 *	4.6372334	5.8262482	5.4702888
34 H	6.2600336	7.8730346	7.8528218	6.2038630
35 H	6.6023237	8.5858511	8.9176765	7.4175386

H H H

1 CO	2.6677723 *	2.4901550 *	2.6100191 *
2 C	8.1162761	4.7375045	4.7474807
3 C	7.8030274	4.3040462	3.9317984
4 C	6.5307800	3.0473832	2.4977413 *
5 C	5.4569004	2.1011985 *	2.0910728 *
6 C	5.8343457	2.9463294 *	3.4216847
7 C	7.2662565	4.2069629	4.5631178
8 C	8.0558332	5.3318999	5.8864420
9 C	7.6662678	5.5386398	6.2980492
10 C	6.3376702	4.6994000	5.5522082
11 C	5.2952968	3.3495294	4.1487202
12 N	3.9489117	3.0369746	3.8878153
13 C	4.0412564	3.9235025	4.9775760
14 C	3.3360147	4.6162904	5.5669346
15 C	2.0490825 *	4.6802106	5.3128815
16 C	2.5142260 *	5.8865296	6.4551746
17 C	3.9365376	6.8931299	7.6625330
18 C	4.7395912	6.8813262	7.8729113
19 C	4.4937907	5.8579948	6.9421740
20 O	0.9936970 *	3.9012993	4.1461698
21 N	4.2725043	1.0449067 *	1.0389460 *
22 H	9.1819266	5.8062212	5.8306730
23 H	8.6660351	5.1635195	4.6019423
24 H	6.5848270	3.2190664	2.2318772 *
25 H	9.1382415	6.2700018	6.7549831
26 H	8.5077978	6.5876110	7.3942066
27 H	6.3051956	5.3538216	6.2731499
28 H	5.1217859	4.5849848	5.7894738
29 H	2.3148257 *	6.2600336	6.6023237
30 H	4.6372334	7.8730346	8.5858511
31 H	5.8262482	7.8528218	8.9176765
32 H	5.4702888	6.2038630	7.4175386
33 H	0.0000000	4.5200422	4.5059927
34 H	4.5200422	0.0000000	1.6656725 *
35 H	4.5059927	1.6656725 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.84 , TOTAL = 5224.4 SECONDS (87.1 MIN)
WALL CLOCK TIME: STEP = 0.83 , TOTAL = 4830.4 SECONDS (80.5 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.95 , TOTAL = 5225.3 SECONDS (87.1 MIN)
WALL CLOCK TIME: STEP = 0.95 , TOTAL = 4831.4 SECONDS (80.5 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.635123035	-284.635123035	0.010356530	0.001157865	197006162
11397580						
2	1	-284.635248871	-0.000125836	0.001688530	0.000106969	156814793
14834828						
3	2	-284.635249468	-0.000000597	0.001192502	0.000141462	141142486
16097043						
4	3	-284.635250478	-0.000001010	0.000577774	0.000050865	135987754
16477857						
5	4	-284.635250580	-0.000000102	0.000456578	0.000062603	129995327
16968719						
6	5	-284.635250668	-0.000000088	0.000263140	0.000050659	124148660
17410187						
7	6	-284.635250711	-0.000000043	0.000174873	0.000022758	121932435
17582179						
8	7	-284.635250718	-0.000000007	0.000138382	0.000013769	116593663
17909400						
9	8	-284.635250746	-0.000000028	0.000103313	0.000011289	114158038
18170582						
10	9	-284.635250775	-0.000000029	0.000108043	0.000011794	112209826
18310564						
11	10	-284.635250788	-0.000000013	0.000215774	0.000013346	133557209
16769956						

12 11 -284.635250801 -0.000000012 0.000145086 0.000014393 159393728
14742273
13 12 -284.635250808 -0.000000008 0.000122402 0.000013382 154832330
15115811
14 13 -284.635250815 -0.000000007 0.000169045 0.000009445 154128707
15134641
-----DISABLING FDIFF OPTION-----
15 14 -284.635250776 0.000000039 0.000067225 0.000002911 197002543
11397898
16 15 -284.635250777 -0.000000001 0.000030706 0.000001976 197002559
11397895
17 16 -284.635250778 -0.000000001 0.000013615 0.000000995 197002586
11397894

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 55.3 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 18.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.1 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6352507779 AFTER 17 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6013011478
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999919228

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 58.38 , TOTAL = 5283.7 SECONDS (88.1 MIN)
WALL CLOCK TIME: STEP = 53.70 , TOTAL = 4885.1 SECONDS (81.4
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 4.03 , TOTAL = 5287.8 SECONDS (88.1 MIN)

WALL CLOCK TIME: STEP = 4.00 , TOTAL = 4889.1 SECONDS (81.5 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.81 , TOTAL = 5290.6 SECONDS (88.2 MIN)

WALL CLOCK TIME: STEP = 2.65 , TOTAL = 4891.7 SECONDS (81.5 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 53 ENERGY= -284.6352508

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0005425	0.0002499	0.0002031
2 C	6.0	0.0008668	0.0023536	0.0001231
3 C	6.0	0.0025693	-0.0012013	-0.0000225
4 C	6.0	-0.0009016	-0.0008557	-0.0004065
5 C	6.0	-0.0005698	0.0002111	-0.0002144
6 C	6.0	0.0005057	-0.0008222	-0.0002161
7 C	6.0	-0.0002153	-0.0000857	-0.0001429
8 C	6.0	-0.0003373	0.0002111	-0.0002277
9 C	6.0	0.0001925	-0.0014079	-0.0001469
10 C	6.0	0.0009224	0.0004367	0.0005378
11 C	6.0	-0.0006937	-0.0000084	0.0002497
12 N	7.0	-0.0000752	-0.0007153	-0.0002805
13 C	6.0	0.0001138	0.0009047	-0.0002532
14 C	6.0	-0.0007572	-0.0008244	-0.0000236
15 C	6.0	-0.0005945	0.0002120	0.0000837
16 C	6.0	-0.0001706	0.0003298	-0.0001512
17 C	6.0	0.0003200	0.0003139	-0.0000558
18 C	6.0	0.0001007	-0.0003733	-0.0004129
19 C	6.0	-0.0001543	-0.0002480	-0.0004831
20 O	8.0	0.0002082	0.0000759	-0.0004753
21 N	7.0	0.0004201	0.0003059	0.0010357
22 H	1.0	-0.0002894	0.0000493	-0.0003557
23 H	1.0	-0.0012583	0.0007637	0.0010963
24 H	1.0	0.0003252	0.0008152	0.0003410

25 H	1.0	-0.0002006	-0.0001810	-0.0010411
26 H	1.0	0.0000285	0.0001835	-0.0003764
27 H	1.0	-0.0000420	-0.0000418	0.0004770
28 H	1.0	0.0005341	-0.0000764	0.0005756
29 H	1.0	-0.0003425	-0.0000501	-0.0009303
30 H	1.0	-0.0005627	0.0001567	0.0005897
31 H	1.0	0.0004773	0.0006512	0.0005151
32 H	1.0	0.0005176	-0.0002600	0.0003799
33 H	1.0	-0.0003776	-0.0018121	0.0002284
34 H	1.0	-0.0001099	0.0003843	-0.0002662
35 H	1.0	-0.0009923	0.0003552	0.0000463

MAXIMUM GRADIENT = 0.0025693 RMS GRADIENT = 0.0006352
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000778987
 PREDICTED ENERGY CHANGE WAS -0.0000852606 RATIO= 0.914
 GDIIS STEP HAS LENGTH = 0.297189
 RADIUS OF STEP TAKEN= 0.16652 CURRENT TRUST RADIUS= 0.16652

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 5290.6 SECONDS (88.2 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4891.7 SECONDS (81.5
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 54

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1368148310	-1.7724455110	0.9445807446
C	6.0	4.9906901661	0.6801656427	0.4817272008
C	6.0	5.2123113828	-0.6833202554	0.2482617643
C	6.0	4.0830562327	-1.5396567210	0.0293325354
C	6.0	2.7671316444	-1.0449112898	0.0970689531
C	6.0	2.4789105862	0.3354769433	0.4558333183
C	6.0	3.6512503866	1.2079211399	0.5962632908
C	6.0	3.4890388673	2.6150296946	0.8712680846
C	6.0	2.2197396133	3.1608737401	1.1041651709
C	6.0	1.0714648536	2.3120897597	1.0600072200
C	6.0	1.1686378510	0.9477117614	0.6959832245
N	7.0	-0.0415434446	0.1354109611	0.6718824312
C	6.0	-1.2370200790	0.6708001913	0.4230331599
C	6.0	-2.5506385206	0.0229691526	0.4909493461
C	6.0	-2.8567224250	-1.3426203386	0.8182084996

C	6.0	-4.1717202261	-1.8400007150	0.8727140208
C	6.0	-5.2596730512	-0.9483209784	0.6232208370
C	6.0	-5.0101070396	0.4138777285	0.2985544090
C	6.0	-3.6779889045	0.8832976768	0.2251187016
O	8.0	-1.7562029347	-2.2626802478	1.1224621167
N	7.0	1.6697038579	-2.0059462882	-0.2883242605
H	1.0	5.8396362792	1.3772768308	0.6005069041
H	1.0	6.2352247536	-1.0957597172	0.2099408140
H	1.0	4.2631422030	-2.6009090198	-0.2268361487
H	1.0	4.3913806384	3.2499357357	0.9128047354
H	1.0	2.1003431033	4.2301127134	1.3506855819
H	1.0	0.0966089757	2.7407921223	1.3500631689
H	1.0	-1.2691259050	1.7349483209	0.1195888315
H	1.0	-4.3758797033	-2.9024178801	1.1062324940
H	1.0	-6.2956480810	-1.3285073854	0.6912583005
H	1.0	-5.8470562332	1.1098521656	0.1141067836
H	1.0	-3.4819332115	1.9430089937	-0.0211490286
H	1.0	-2.0959582983	-3.1499475419	1.4127374313
H	1.0	1.3272504632	-1.7709327274	-1.2458503133
H	1.0	2.0708783682	-2.9620696575	-0.3535133233

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4579887	5.2375299	4.0576707
2 C	5.4579887	0.0000000	1.4009696 *	2.4405064 *
3 C	5.2375299	1.4009696 *	0.0000000	1.4340360 *
4 C	4.0576707	2.4405064 *	1.4340360 *	0.0000000
5 C	2.8576474 *	2.8404339 *	2.4763908 *	1.4074867 *
6 C	3.1886711	2.5354521 *	2.9244681 *	2.5042589 *
7 C	4.6211652	1.4442103 *	2.4768550 *	2.8384945 *
8 C	5.5220213	2.4799995 *	3.7731840	4.2805527
9 C	5.3573950	3.7708764	4.9463000	5.1693521
10 C	4.1916968	4.2846133	5.1747485	4.9967914
11 C	2.9198827 *	3.8373911	4.3831513	3.8891207
12 N	1.9354825 *	5.0652040	5.3341134	4.4978934
13 C	2.8511197 *	6.2279939	6.5922730	5.7744551
14 C	3.2636943	7.5699162	7.7987905	6.8308708
15 C	3.0268771	8.1109042	8.1159610	6.9872510
16 C	4.3096639	9.5107241	9.4756477	8.3031821
17 C	5.4685039	10.3798813	10.4820455	9.3802437
18 C	5.6292241	10.0060185	10.2812553	9.3045363
19 C	4.7035439	8.6748549	9.0273067	8.1328262
20 O	1.9635397 *	7.3886027	7.1985274	5.9845336

21 N	1.9809912 *	4.3401759	3.8193366	2.4784272 *
22 H	6.5239030	1.1048901 *	2.1825841 *	3.4525809
23 H	6.1796604	2.1855537 *	1.1035971 *	2.2048794 *
24 H	4.3686550	3.4346527	2.1917543 *	1.1064853 *
25 H	6.5822985	2.6737087 *	4.0725971	4.8801417
26 H	6.3285914	4.6595406	5.9195868	6.2423845
27 H	4.5315942	5.3807267	6.2537127	5.9965268
28 H	3.8676986	6.3583809	6.9190757	6.2751126
29 H	4.6548234	10.0477631	9.8789633	8.6354171
30 H	6.4527384	11.4656052	11.5345413	10.4019341
31 H	6.6935820	10.8524892	11.2046007	10.2778508
32 H	5.2756586	8.5809676	9.0862576	8.3282996
33 H	2.6649500 *	8.1090772	7.8007089	6.5335340
34 H	2.4930157 *	4.7342579	4.3022053	3.0453317
35 H	2.6155029 *	4.7422364	3.9272679	2.4937300 *

C C C C

1 CO	2.8576474 *	3.1886711	4.6211652	5.5220213
2 C	2.8404339 *	2.5354521 *	1.4442103 *	2.4799995 *
3 C	2.4763908 *	2.9244681 *	2.4768550 *	3.7731840
4 C	1.4074867 *	2.5042589 *	2.8384945 *	4.2805527
5 C	0.0000000	1.4550790 *	2.4710554 *	3.8099478
6 C	1.4550790 *	0.0000000	1.4680804 *	2.5277076 *
7 C	2.4710554 *	1.4680804 *	0.0000000	1.4428772 *
8 C	3.8099478	2.5277076 *	1.4428772 *	0.0000000
9 C	4.3591867	2.9103902 *	2.4741082 *	1.4011807 *
10 C	3.8822664	2.5005855 *	2.8442117 *	2.4437797 *
11 C	2.6238192 *	1.4660553 *	2.4982030 *	2.8626796 *
12 N	3.1003592	2.5375957 *	3.8461309	4.3189438
13 C	4.3684264	3.7311738	4.9207414	5.1299684
14 C	5.4382157	5.0393708	6.3149528	6.5833975
15 C	5.6777115	5.6050251	6.9934420	7.4789368
16 C	7.0271942	7.0098062	8.4003049	8.8619709
17 C	8.0446106	7.8461349	9.1681330	9.4498125
18 C	7.9154345	7.4910793	8.7027724	8.7982130
19 C	6.7285931	6.1855273	7.3458068	7.4015331
20 O	4.7953048	5.0130830	6.4468993	7.1671273
21 N	1.5087955 *	2.5866675 *	3.8778816	5.0998091
22 H	3.9447091	3.5214705	2.1949333 *	2.6703281 *
23 H	3.4703019	4.0272568	3.4832620	4.6635661
24 H	2.1826798 *	3.5031247	3.9445014	5.3861940
25 H	4.6636167	3.5157410	2.1949521 *	1.1041067 *
26 H	5.4627868	4.0140082	3.4796707	2.1833026 *
27 H	4.7992954	3.5015067	3.9437778	3.4283584
28 H	4.9009695	4.0148920	4.9714263	4.8969069

29 H	7.4492518	7.6088851	9.0327057	9.6101186
30 H	9.0866641	8.9340444	10.2656360	10.5510183
31 H	8.8796131	8.3688803	9.5110421	9.4869133
32 H	6.9276587	6.1921991	7.1974899	7.0599201
33 H	5.4600188	5.8303752	7.2586539	8.0448956
34 H	2.0985226 *	2.9426196 *	4.2033235	5.3284318
35 H	2.0888488 *	3.4198459	4.5594380	5.8834774

C C C N

1 CO	5.3573950	4.1916968	2.9198827 *	1.9354825 *
2 C	3.7708764	4.2846133	3.8373911	5.0652040
3 C	4.9463000	5.1747485	4.3831513	5.3341134
4 C	5.1693521	4.9967914	3.8891207	4.4978934
5 C	4.3591867	3.8822664	2.6238192 *	3.1003592
6 C	2.9103902 *	2.5005855 *	1.4660553 *	2.5375957 *
7 C	2.4741082 *	2.8442117 *	2.4982030 *	3.8461309
8 C	1.4011807 *	2.4437797 *	2.8626796 *	4.3189438
9 C	0.0000000	1.4286074 *	2.4838505 *	3.8018015
10 C	1.4286074 *	0.0000000	1.4154446 *	2.4753503 *
11 C	2.4838505 *	1.4154446 *	0.0000000	1.4577216 *
12 N	3.8018015	2.4753503 *	1.4577216 *	0.0000000
13 C	4.3143475	2.9032172 *	2.4368775 *	1.3333162 *
14 C	5.7427334	4.3224452	3.8379949	2.5181219 *
15 C	6.7921791	5.3708498	4.6329349	3.1829578
16 C	8.1186867	6.6907342	6.0267735	4.5826788
17 C	8.5474208	7.1347297	6.7024932	5.3297016
18 C	7.7759680	6.4162712	6.2144844	4.9903449
19 C	6.3830461	5.0294927	4.8698720	3.7393406
20 O	6.7248340	5.3784874	4.3638509	2.9822677 *
21 N	5.3793676	4.5630388	3.1534147	2.9044406 *
22 H	4.0667606	4.8806223	4.6916807	6.0112894
23 H	5.9196864	6.2450354	5.4847348	6.4130328
24 H	6.2566124	5.9983604	4.7979435	5.1793301
25 H	2.1818743 *	3.4529791	3.9665247	5.4230180
26 H	1.1037662 *	2.1958817 *	3.4743152	4.6706567
27 H	2.1782144 *	1.1037491 *	2.1891102 *	2.6957422 *
28 H	3.8954892	2.5876329 *	2.6257692 *	2.0905757 *
29 H	8.9591129	7.5410072	6.7626532	5.3107000
30 H	9.6351888	8.2258298	7.8036376	6.4231812
31 H	8.3821298	7.0856218	7.0416499	5.9130896
32 H	5.9378952	4.6945238	4.8096472	3.9476556
33 H	7.6515966	6.3238311	5.2879236	3.9450053
34 H	5.5355058	4.6961131	3.3446828	3.0307494
35 H	6.2958258	5.5510022	4.1475139	3.8869202

	C	C	C	C
1 CO	2.8511197 *	3.2636943	3.0268771	4.3096639
2 C	6.2279939	7.5699162	8.1109042	9.5107241
3 C	6.5922730	7.7987905	8.1159610	9.4756477
4 C	5.7744551	6.8308708	6.9872510	8.3031821
5 C	4.3684264	5.4382157	5.6777115	7.0271942
6 C	3.7311738	5.0393708	5.6050251	7.0098062
7 C	4.9207414	6.3149528	6.9934420	8.4003049
8 C	5.1299684	6.5833975	7.4789368	8.8619709
9 C	4.3143475	5.7427334	6.7921791	8.1186867
10 C	2.9032172 *	4.3224452	5.3708498	6.6907342
11 C	2.4368775 *	3.8379949	4.6329349	6.0267735
12 N	1.3333162 *	2.5181219 *	3.1829578	4.5826788
13 C	0.0000000	1.4662507 *	2.6140890 *	3.8882900
14 C	1.4662507 *	0.0000000	1.4372267 *	2.4988611 *
15 C	2.6140890 *	1.4372267 *	0.0000000	1.4069745 *
16 C	3.8882900	2.4988611 *	1.4069745 *	0.0000000
17 C	4.3408945	2.8809319 *	2.4428802 *	1.4286290 *
18 C	3.7838723	2.4977611 *	2.8270817 *	2.4723511 *
19 C	2.4581811 *	1.4428271 *	2.4455971 *	2.8424469 *
20 O	3.0600750	2.5008258 *	1.4663641 *	2.4649048 *
21 N	4.0149776	4.7471102	4.7066921	5.9580016
22 H	7.1140475	8.4995802	9.1143782	10.5191364
23 H	7.6811838	8.8612591	9.1156148	10.4545524
24 H	6.4325886	7.3367268	7.3053324	8.5401930
25 H	6.2105323	7.6670011	8.5811140	9.9617145
26 H	4.9666123	6.3301527	7.4773915	8.7414823
27 H	2.6311248 *	3.8900588	5.0674740	6.2793439
28 H	1.1070323 *	2.1704967 *	3.5326988	4.6661024
29 H	4.8049025	3.5025659	2.1963071 *	1.1067711 *
30 H	5.4459979	3.9864407	3.4412970	2.1921727 *
31 H	4.6411890	3.4913743	3.9309639	3.4761858
32 H	2.6182911 *	2.1945632 *	3.4482995	3.9479057
33 H	4.0392329	3.3352403	2.0490628 *	2.5132397 *
34 H	3.9144240	4.6122207	4.6850207	5.8933661
35 H	4.9742296	5.5661470	5.3175932	6.4600859

	C	C	C	O
1 CO	5.4685039	5.6292241	4.7035439	1.9635397 *
2 C	10.3798813	10.0060185	8.6748549	7.3886027
3 C	10.4820455	10.2812553	9.0273067	7.1985274
4 C	9.3802437	9.3045363	8.1328262	5.9845336
5 C	8.0446106	7.9154345	6.7285931	4.7953048
6 C	7.8461349	7.4910793	6.1855273	5.0130830

7 C	9.1681330	8.7027724	7.3458068	6.4468993
8 C	9.4498125	8.7982130	7.4015331	7.1671273
9 C	8.5474208	7.7759680	6.3830461	6.7248340
10 C	7.1347297	6.4162712	5.0294927	5.3784874
11 C	6.7024932	6.2144844	4.8698720	4.3638509
12 N	5.3297016	4.9903449	3.7393406	2.9822677 *
13 C	4.3408945	3.7838723	2.4581811 *	3.0600750
14 C	2.8809319 *	2.4977611 *	1.4428271 *	2.5008258 *
15 C	2.4428802 *	2.8270817 *	2.4455971 *	1.4663641 *
16 C	1.4286290 *	2.4723511 *	2.8424469 *	2.4649048 *
17 C	0.0000000	1.4224193 *	2.4525572 *	3.7750609
18 C	1.4224193 *	0.0000000	1.4143149 *	4.2930966
19 C	2.4525572 *	1.4143149 *	0.0000000	3.7941618
20 O	3.7750609	4.2930966	3.7941618	0.0000000
21 N	7.0686456	7.1288041	6.0999322	3.7139020
22 H	11.3403522	10.8966161	9.5378258	8.4391053
23 H	11.5032697	11.3465565	10.1088428	8.1275651
24 H	9.7024561	9.7651485	8.6836353	6.1779868
25 H	10.5286303	9.8391310	8.4373344	8.2598835
26 H	9.0285779	8.1381282	6.7717939	7.5552229
27 H	6.5442809	5.7095315	4.3546957	5.3403605
28 H	4.8350849	3.9714224	2.5571598 *	4.1501847
29 H	2.1983825 *	3.4716574	3.9490575	2.6967080 *
30 H	1.1056288 *	2.2006222 *	3.4585412	4.6545868
31 H	2.2000665 *	1.1040314 *	2.1836904 *	5.3968357
32 H	3.4547591	2.1853531 *	1.1054744 *	4.6876234
33 H	3.9344106	4.7365090	4.4922518	0.9934469 *
34 H	6.8962075	6.8790030	5.8532991	3.9189800
35 H	7.6646055	7.8716305	6.9405432	4.1610336

N H H H

1 CO	1.9809912 *	6.5239030	6.1796604	4.3686550
2 C	4.3401759	1.1048901 *	2.1855537 *	3.4346527
3 C	3.8193366	2.1825841 *	1.1035971 *	2.1917543 *
4 C	2.4784272 *	3.4525809	2.2048794 *	1.1064853 *
5 C	1.5087955 *	3.9447091	3.4703019	2.1826798 *
6 C	2.5866675 *	3.5214705	4.0272568	3.5031247
7 C	3.8778816	2.1949333 *	3.4832620	3.9445014
8 C	5.0998091	2.6703281 *	4.6635661	5.3861940
9 C	5.3793676	4.0667606	5.9196864	6.2566124
10 C	4.5630388	4.8806223	6.2450354	5.9983604
11 C	3.1534147	4.6916807	5.4847348	4.7979435
12 N	2.9044406 *	6.0112894	6.4130328	5.1793301
13 C	4.0149776	7.1140475	7.6811838	6.4325886
14 C	4.7471102	8.4995802	8.8612591	7.3367268

15 C	4.7066921	9.1143782	9.1156148	7.3053324
16 C	5.9580016	10.5191364	10.4545524	8.5401930
17 C	7.0686456	11.3403522	11.5032697	9.7024561
18 C	7.1288041	10.8966161	11.3465565	9.7651485
19 C	6.0999322	9.5378258	10.1088428	8.6836353
20 O	3.7139020	8.4391053	8.1275651	6.1779868
21 N	0.0000000	5.4428445	4.6819535	2.6615191 *
22 H	5.4428445	0.0000000	2.5347469 *	4.3584163
23 H	4.6819535	2.5347469 *	0.0000000	2.5189994 *
24 H	2.6615191 *	4.3584163	2.5189994 *	0.0000000
25 H	6.0394148	2.3878496 *	4.7727191	5.9621817
26 H	6.4622160	4.7627465	6.8383815	7.3368340
27 H	5.2621732	5.9500732	7.3281384	6.9556007
28 H	4.7746629	7.1339828	8.0209943	7.0374469
29 H	6.2687742	11.0873041	10.8010597	8.7464667
30 H	8.0539020	12.4336089	12.5422730	10.6747345
31 H	8.1468910	11.6998668	12.2823215	10.7750686
32 H	6.4965371	9.3593892	10.1838439	8.9819648
33 H	4.2874889	9.1721939	8.6645841	6.5899775
34 H	1.0437250 *	5.8036096	5.1636613	3.2166304
35 H	1.0389237 *	5.8261152	4.5980838	2.2254224 *

H H H H

1 CO	6.5822985	6.3285914	4.5315942	3.8676986
2 C	2.6737087 *	4.6595406	5.3807267	6.3583809
3 C	4.0725971	5.9195868	6.2537127	6.9190757
4 C	4.8801417	6.2423845	5.9965268	6.2751126
5 C	4.6636167	5.4627868	4.7992954	4.9009695
6 C	3.5157410	4.0140082	3.5015067	4.0148920
7 C	2.1949521 *	3.4796707	3.9437778	4.9714263
8 C	1.1041067 *	2.1833026 *	3.4283584	4.8969069
9 C	2.1818743 *	1.1037662 *	2.1782144 *	3.8954892
10 C	3.4529791	2.1958817 *	1.1037491 *	2.5876329 *
11 C	3.9665247	3.4743152	2.1891102 *	2.6257692 *
12 N	5.4230180	4.6706567	2.6957422 *	2.0905757 *
13 C	6.2105323	4.9666123	2.6311248 *	1.1070323 *
14 C	7.6670011	6.3301527	3.8900588	2.1704967 *
15 C	8.5811140	7.4773915	5.0674740	3.5326988
16 C	9.9617145	8.7414823	6.2793439	4.6661024
17 C	10.5286303	9.0285779	6.5442809	4.8350849
18 C	9.8391310	8.1381282	5.7095315	3.9714224
19 C	8.4373344	6.7717939	4.3546957	2.5571598 *
20 O	8.2598835	7.5552229	5.3403605	4.1501847
21 N	6.0394148	6.4622160	5.2621732	4.7746629
22 H	2.3878496 *	4.7627465	5.9500732	7.1339828

23 H	4.7727191	6.8383815	7.3281384	8.0209943
24 H	5.9621817	7.3368340	6.9556007	7.0374469
25 H	0.0000000	2.5300869 *	4.3468938	5.9131813
26 H	2.5300869 *	0.0000000	2.4966030 *	4.3697558
27 H	4.3468938	2.4966030 *	0.0000000	2.0954762 *
28 H	5.9131813	4.3697558	2.0954762 *	0.0000000
29 H	10.7123164	9.6371267	7.2047503	5.6683816
30 H	11.6285772	10.0908756	7.6061930	5.9141772
31 H	10.4901604	8.6270684	6.2860727	4.6204135
32 H	8.0355086	6.1866455	3.9144150	2.2270188 *
33 H	9.1265549	8.4898813	6.2858645	5.1203606
34 H	6.2656050	6.5842401	5.3487294	4.5713014
35 H	6.7510964	7.3913902	6.2707691	5.7828567

H H H H

1 CO	4.6548234	6.4527384	6.6935820	5.2756586
2 C	10.0477631	11.4656052	10.8524892	8.5809676
3 C	9.8789633	11.5345413	11.2046007	9.0862576
4 C	8.6354171	10.4019341	10.2778508	8.3282996
5 C	7.4492518	9.0866641	8.8796131	6.9276587
6 C	7.6088851	8.9340444	8.3688803	6.1921991
7 C	9.0327057	10.2656360	9.5110421	7.1974899
8 C	9.6101186	10.5510183	9.4869133	7.0599201
9 C	8.9591129	9.6351888	8.3821298	5.9378952
10 C	7.5410072	8.2258298	7.0856218	4.6945238
11 C	6.7626532	7.8036376	7.0416499	4.8096472
12 N	5.3107000	6.4231812	5.9130896	3.9476556
13 C	4.8049025	5.4459979	4.6411890	2.6182911 *
14 C	3.5025659	3.9864407	3.4913743	2.1945632 *
15 C	2.1963071 *	3.4412970	3.9309639	3.4482995
16 C	1.1067711 *	2.1921727 *	3.4761858	3.9479057
17 C	2.1983825 *	1.1056288 *	2.2000665 *	3.4547591
18 C	3.4716574	2.2006222 *	1.1040314 *	2.1853531 *
19 C	3.9490575	3.4585412	2.1836904 *	1.1054744 *
20 O	2.6967080 *	4.6545868	5.3968357	4.6876234
21 N	6.2687742	8.0539020	8.1468910	6.4965371
22 H	11.0873041	12.4336089	11.6998668	9.3593892
23 H	10.8010597	12.5422730	12.2823215	10.1838439
24 H	8.7464667	10.6747345	10.7750686	8.9819648
25 H	10.7123164	11.6285772	10.4901604	8.0355086
26 H	9.6371267	10.0908756	8.6270684	6.1866455
27 H	7.2047503	7.6061930	6.2860727	3.9144150
28 H	5.6683816	5.9141772	4.6204135	2.2270188 *
29 H	0.0000000	2.5169244 *	4.3871386	5.0545317
30 H	2.5169244 *	0.0000000	2.5455718 *	4.3734809

31 H	4.3871386	2.5455718 *	0.0000000	2.5112251 *
32 H	5.0545317	4.3734809	2.5112251 *	0.0000000
33 H	2.3137108 *	4.6341742	5.8226344	5.4694756
34 H	6.2720209	7.8776083	7.8497823	6.1985082
35 H	6.6102274	8.5882966	8.9158793	7.4164667

H H H

1 CO	2.6649500 *	2.4930157 *	2.6155029 *
2 C	8.1090772	4.7342579	4.7422364
3 C	7.8007089	4.3022053	3.9272679
4 C	6.5335340	3.0453317	2.4937300 *
5 C	5.4600188	2.0985226 *	2.0888488 *
6 C	5.8303752	2.9426196 *	3.4198459
7 C	7.2586539	4.2033235	4.5594380
8 C	8.0448956	5.3284318	5.8834774
9 C	7.6515966	5.5355058	6.2958258
10 C	6.3238311	4.6961131	5.5510022
11 C	5.2879236	3.3446828	4.1475139
12 N	3.9450053	3.0307494	3.8869202
13 C	4.0392329	3.9144240	4.9742296
14 C	3.3352403	4.6122207	5.5661470
15 C	2.0490628 *	4.6850207	5.3175932
16 C	2.5132397 *	5.8933661	6.4600859
17 C	3.9344106	6.8962075	7.6646055
18 C	4.7365090	6.8790030	7.8716305
19 C	4.4922518	5.8532991	6.9405432
20 O	0.9934469 *	3.9189800	4.1610336
21 N	4.2874889	1.0437250 *	1.0389237 *
22 H	9.1721939	5.8036096	5.8261152
23 H	8.6645841	5.1636613	4.5980838
24 H	6.5899775	3.2166304	2.2254224 *
25 H	9.1265549	6.2656050	6.7510964
26 H	8.4898813	6.5842401	7.3913902
27 H	6.2858645	5.3487294	6.2707691
28 H	5.1203606	4.5713014	5.7828567
29 H	2.3137108 *	6.2720209	6.6102274
30 H	4.6341742	7.8776083	8.5882966
31 H	5.8226344	7.8497823	8.9158793
32 H	5.4694756	6.1985082	7.4164667
33 H	0.0000000	4.5484205	4.5296211
34 H	4.5484205	0.0000000	1.6637473 *
35 H	4.5296211	1.6637473 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.79 , TOTAL = 5291.4 SECONDS (88.2 MIN)
WALL CLOCK TIME: STEP = 0.79 , TOTAL = 4892.5 SECONDS (81.5 MIN)
CPU UTILIZATION: STEP = 99.88%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.92 , TOTAL = 5292.3 SECONDS (88.2 MIN)
WALL CLOCK TIME: STEP = 0.97 , TOTAL = 4893.5 SECONDS (81.6 MIN)
CPU UTILIZATION: STEP = 94.55%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.634886232	-284.634886232	0.021148073	0.002244742	197032684
11396074						
2	1	-284.635387431	-0.000501199	0.003526730	0.000237366	162548424
14373690						
3	2	-284.635389632	-0.000002201	0.002220709	0.000402241	148138552
15549334						
4	3	-284.635394076	-0.000004444	0.001173650	0.000090592	143099921
15924715						
5	4	-284.635394540	-0.000000464	0.001028386	0.000059005	136469499
16463874						
6	5	-284.635394777	-0.000000237	0.000438550	0.000049573	129960962
16919042						
7	6	-284.635394898	-0.000000121	0.000243105	0.000040532	127845807
17166217						
8	7	-284.635394944	-0.000000046	0.000220615	0.000032124	123002035
17474375						
9	8	-284.635394998	-0.000000054	0.000310339	0.000026619	119801281
17796238						
10	9	-284.635395036	-0.000000038	0.000248346	0.000027373	144798597
15899533						
11	10	-284.635395093	-0.000000057	0.000380010	0.000028725	140903721
16214632						
12	11	-284.635395132	-0.000000039	0.000274559	0.000027425	164656991
14314734						

13 12	-284.635395174	-0.000000042	0.000525713	0.000023184	158194792
14868114					
-----DISABLING FDIFF OPTION-----					
14 13	-284.635395232	-0.000000058	0.000256928	0.000014001	197021541
11396903					
15 14	-284.635395251	-0.000000019	0.000102282	0.000011454	197021662
11396897					
16 15	-284.635395256	-0.000000005	0.000065433	0.000004875	197021654
11396888					
17 16	-284.635395258	-0.000000002	0.000036375	0.000004889	197021749
11396895					
18 17	-284.635395258	-0.000000001	0.000051706	0.000004447	197021793
11396889					
19 18	-284.635395259	-0.000000001	0.000087283	0.000003351	197021797
11396893					
20 19	-284.635395261	-0.000000001	0.000092235	0.000003188	197021671
11396894					
21 20	-284.635395262	-0.000000001	0.000080091	0.000004941	197021685
11396895					
22 21	-284.635395263	-0.000000001	0.000126192	0.000005047	197021577
11396901					
23 22	-284.635395264	-0.000000002	0.000045495	0.000002633	197021694
11396896					
24 23	-284.635395265	-0.000000001	0.000019372	0.000001110	197021671
11396893					
25 24	-284.635395265	0.000000000	0.000011235	0.000000915	197021740
11396893					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 83.3 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 27.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.0
TIME TO SOLVE SCF EQUATIONS= 3.0 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6353952650 AFTER 25 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6023692574
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999858428

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 87.72 , TOTAL = 5380.0 SECONDS (89.7 MIN)
WALL CLOCK TIME: STEP = 80.51 , TOTAL = 4974.0 SECONDS (82.9 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.77 , TOTAL = 5383.8 SECONDS (89.7 MIN)
WALL CLOCK TIME: STEP = 3.74 , TOTAL = 4977.8 SECONDS (83.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.87 , TOTAL = 5386.7 SECONDS (89.8 MIN)
WALL CLOCK TIME: STEP = 2.71 , TOTAL = 4980.5 SECONDS (83.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 54 ENERGY= -284.6353953

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000496	0.0001154	0.0005308
2 C	6.0	0.0006483	0.0007985	-0.0000360
3 C	6.0	0.0012736	-0.0001513	-0.0000107
4 C	6.0	-0.0006533	-0.0002127	-0.0004540
5 C	6.0	-0.0006320	0.0002694	-0.0001213
6 C	6.0	0.0001479	-0.0008188	-0.0002109
7 C	6.0	0.0001580	-0.0003784	-0.0001703
8 C	6.0	0.0006216	0.0004415	-0.0003591
9 C	6.0	-0.0002765	-0.0007647	0.0001332
10 C	6.0	0.0009482	0.0007025	0.0008659

11	C	6.0	-0.0006616	-0.0002030	0.0001595
12	N	7.0	0.0001381	-0.0005371	-0.0005069
13	C	6.0	0.0000902	0.0006514	-0.0002982
14	C	6.0	-0.0005621	-0.0008278	-0.0002429
15	C	6.0	-0.0007104	0.0001168	-0.0004313
16	C	6.0	-0.0003891	0.0003743	-0.0004048
17	C	6.0	0.0003020	0.0004541	-0.0000914
18	C	6.0	0.0003739	-0.0006544	-0.0002428
19	C	6.0	-0.0003048	-0.0002130	-0.0003414
20	O	8.0	-0.0001222	0.0002580	-0.0001434
21	N	7.0	-0.0001445	0.0003956	0.0003564
22	H	1.0	-0.0003066	0.0003415	-0.0002560
23	H	1.0	-0.0001934	0.0003432	0.0011240
24	H	1.0	0.0001873	0.0009955	0.0004435
25	H	1.0	-0.0004009	-0.0003500	-0.0011976
26	H	1.0	0.0000808	-0.0003049	-0.0004367
27	H	1.0	0.0001145	-0.0002831	0.0003636
28	H	1.0	0.0005348	-0.0001242	0.0004264
29	H	1.0	-0.0003523	-0.0000644	-0.0007546
30	H	1.0	-0.0003121	0.0001159	0.0007114
31	H	1.0	0.0003929	0.0004808	0.0004703
32	H	1.0	0.0003982	-0.0001464	0.0005463
33	H	1.0	-0.0002308	-0.0015904	0.0003026
34	H	1.0	0.0005325	0.0002204	0.0004663
35	H	1.0	-0.0006408	0.0005495	-0.0001897

MAXIMUM GRADIENT = 0.0015904 RMS GRADIENT = 0.0004980
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001444871
 PREDICTED ENERGY CHANGE WAS -0.0001763220 RATIO= 0.819
 GDIIS STEP HAS LENGTH = 0.261552
 RADIUS OF STEP TAKEN= 0.23549 CURRENT TRUST RADIUS= 0.23549

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 5386.7 SECONDS (89.8 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 4980.5 SECONDS (83.0
 MIN)
 CPU UTILIZATION: STEP = 91.31%, TOTAL = 100.00%

1NSERCH= 55

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1355820065	-1.7722477347	0.9316190362

C	6.0	4.9902609892	0.6746145098	0.4891743784
C	6.0	5.2104997100	-0.6864826940	0.2477553789
C	6.0	4.0800032394	-1.5374586617	0.0204301064
C	6.0	2.7650043959	-1.0416661316	0.0873341004
C	6.0	2.4779521921	0.3375102734	0.4518859294
C	6.0	3.6517030527	1.2059012058	0.6010851291
C	6.0	3.4919221013	2.6116056481	0.8839883180
C	6.0	2.2221948948	3.1570280452	1.1212452301
C	6.0	1.0720665251	2.3099432507	1.0672426256
C	6.0	1.1688094511	0.9492249168	0.6904426528
N	7.0	-0.0417252570	0.1371018840	0.6573270923
C	6.0	-1.2367158323	0.6704042476	0.4008346078
C	6.0	-2.5502146124	0.0230438034	0.4744013247
C	6.0	-2.8550794594	-1.3388567665	0.8206849421
C	6.0	-4.1687502304	-1.8391982152	0.8871212529
C	6.0	-5.2587534834	-0.9523380641	0.6303207147
C	6.0	-5.0118273812	0.4068090544	0.2888491462
C	6.0	-3.6808741765	0.8788631198	0.2047304721
O	8.0	-1.7542442840	-2.2501159218	1.1464357136
N	7.0	1.6679799589	-1.9995701575	-0.3060090707
H	1.0	5.8384868109	1.3714269230	0.6184061759
H	1.0	6.2341059897	-1.1019912878	0.2116304314
H	1.0	4.2559757770	-2.5981956322	-0.2401581149
H	1.0	4.3950967077	3.2453568319	0.9286399259
H	1.0	2.1037332417	4.2236141064	1.3782856926
H	1.0	0.0961821068	2.7347235199	1.3579152298
H	1.0	-1.2686043959	1.7322463958	0.0874230137
H	1.0	-4.3694466934	-2.8972841376	1.1413810596
H	1.0	-6.2929271829	-1.3331591849	0.7089626058
H	1.0	-5.8518898246	1.0968809919	0.0991933477
H	1.0	-3.4895576527	1.9375729630	-0.0514322256
H	1.0	-2.0932726013	-3.1261020941	1.4712550763
H	1.0	1.3281519980	-1.7548374242	-1.2620011949
H	1.0	2.0741689186	-2.9532625831	-0.3835131040

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4544294	5.2346294	4.0551017
2 C	5.4544294	0.0000000	1.3997763 *	2.4375311 *
3 C	5.2346294	1.3997763 *	0.0000000	1.4331291 *
4 C	4.0551017	2.4375311 *	1.4331291 *	0.0000000
5 C	2.8566464 *	2.8388134 *	2.4763557 *	1.4069500 *
6 C	3.1887177	2.5350987 *	2.9252430 *	2.5036434 *

7 C	4.6197111	1.4444815 *	2.4770559 *	2.8366573 *
8 C	5.5213638	2.4804903 *	3.7730211	4.2785870
9 C	5.3560873	3.7714825	4.9462637	5.1673447
10 C	4.1904272	4.2849400	5.1746263	4.9945972
11 C	2.9209824 *	3.8365885	4.3825531	3.8868446
12 N	1.9370828 *	5.0634060	5.3321579	4.4942671
13 C	2.8515754 *	6.2276048	6.5902324	5.7694773
14 C	3.2627631	7.5685887	7.7963763	6.8264959
15 C	3.0239362	8.1063760	8.1121765	6.9839260
16 C	4.3050829	9.5060561	9.4714239	8.2996466
17 C	5.4646032	10.3783040	10.4796134	9.3769243
18 C	5.6264789	10.0076781	10.2807075	9.3012693
19 C	4.7034130	8.6782032	9.0282162	8.1304241
20 O	1.9611088 *	7.3806769	7.1944586	5.9844977
21 N	1.9828369 *	4.3383328	3.8184159	2.4774919 *
22 H	6.5195027	1.1053214 *	2.1832869 *	3.4512976
23 H	6.1773475	2.1864376 *	1.1053154 *	2.2059801 *
24 H	4.3626708	3.4325482	2.1917623 *	1.1063614 *
25 H	6.5817802	2.6750825 *	4.0728182	4.8784683
26 H	6.3264121	4.6602532	5.9193874	6.2401422
27 H	4.5272586	5.3805918	6.2524676	5.9925986
28 H	3.8685767	6.3602976	6.9177125	6.2692155
29 H	4.6481169	10.0393208	9.8722633	8.6312722
30 H	6.4473332	11.4625389	11.5308167	10.3977642
31 H	6.6913863	10.8573767	11.2062000	10.2756240
32 H	5.2792800	8.5903809	9.0920943	8.3294214
33 H	2.6630662 *	8.0985417	7.7970369	6.5374319
34 H	2.4968973 *	4.7307394	4.3003919	3.0437754
35 H	2.6234496 *	4.7356804	3.9208879	2.4881805 *

C C C C

1 CO	2.8566464 *	3.1887177	4.6197111	5.5213638
2 C	2.8388134 *	2.5350987 *	1.4444815 *	2.4804903 *
3 C	2.4763557 *	2.9252430 *	2.4770559 *	3.7730211
4 C	1.4069500 *	2.5036434 *	2.8366573 *	4.2785870
5 C	0.0000000	1.4551373 *	2.4701687 *	3.8091288
6 C	1.4551373 *	0.0000000	1.4676697 *	2.5271243 *
7 C	2.4701687 *	1.4676697 *	0.0000000	1.4427644 *
8 C	3.8091288	2.5271243 *	1.4427644 *	0.0000000
9 C	4.3580554	2.9091466 *	2.4740566 *	1.4021354 *
10 C	3.8806629	2.4991339 *	2.8444220 *	2.4454618 *
11 C	2.6220651 *	1.4645678 *	2.4977246 *	2.8631839 *
12 N	3.0971144	2.5359700 *	3.8453749	4.3198620
13 C	4.3638552	3.7299039	4.9217371	5.1343663
14 C	5.4346096	5.0380410	6.3149809	6.5860329

15 C	5.6755148	5.6024500	6.9901528	7.4762684
16 C	7.0251456	7.0075775	8.3972577	8.8597723
17 C	8.0426056	7.8455186	9.1681561	9.4520032
18 C	7.9131410	7.4918744	8.7059060	8.8050596
19 C	6.7269284	6.1875109	7.3505605	7.4103167
20 O	4.7964211	5.0089615	6.4393888	7.1573373
21 N	1.5085628 *	2.5869683 *	3.8772444	5.0995883
22 H	3.9435200	3.5199298	2.1931078 *	2.6673851 *
23 H	3.4718517	4.0297120	3.4852328	4.6650230
24 H	2.1801447 *	3.5012372	3.9425865	5.3841910
25 H	4.6629993	3.5154387	2.1952917 *	1.1042458 *
26 H	5.4614111	4.0124879	3.4794888	2.1840260 *
27 H	4.7956342	3.4986210	3.9435794	3.4308621
28 H	4.8953642	4.0143254	4.9749687	4.9061595
29 H	7.4467930	7.6043520	9.0259012	9.6028765
30 H	9.0839152	8.9322757	10.2642163	10.5515439
31 H	8.8783101	8.3718160	9.5174607	9.4982691
32 H	6.9292617	6.1987663	7.2082402	7.0760435
33 H	5.4647018	5.8251026	7.2476337	8.0287342
34 H	2.0961545 *	2.9389400 *	4.1995182	5.3247532
35 H	2.0864208 *	3.4190815	4.5559512	5.8808454

C C C N

1 CO	5.3560873	4.1904272	2.9209824 *	1.9370828 *
2 C	3.7714825	4.2849400	3.8365885	5.0634060
3 C	4.9462637	5.1746263	4.3825531	5.3321579
4 C	5.1673447	4.9945972	3.8868446	4.4942671
5 C	4.3580554	3.8806629	2.6220651 *	3.0971144
6 C	2.9091466 *	2.4991339 *	1.4645678 *	2.5359700 *
7 C	2.4740566 *	2.8444220 *	2.4977246 *	3.8453749
8 C	1.4021354 *	2.4454618 *	2.8631839 *	4.3198620
9 C	0.0000000	1.4294279 *	2.4838692 *	3.8026975
10 C	1.4294279 *	0.0000000	1.4152356 *	2.4758438 *
11 C	2.4838692 *	1.4152356 *	0.0000000	1.4580928 *
12 N	3.8026975	2.4758438 *	1.4580928 *	0.0000000
13 C	4.3204575	2.9090658 *	2.4388862 *	1.3334925 *
14 C	5.7459687	4.3246145	3.8387010	2.5177351 *
15 C	6.7883747	5.3662844	4.6307627	3.1812107
16 C	8.1154957	6.6868512	6.0252410	4.5815830
17 C	8.5494143	7.1353109	6.7032173	5.3296334
18 C	7.7838079	6.4219609	6.2173760	4.9910353
19 C	6.3934544	5.0380912	4.8744537	3.7414514
20 O	6.7119229	5.3654864	4.3575170	2.9783817 *
21 N	5.3790997	4.5621090	3.1523768	2.9011163 *
22 H	4.0643309	4.8786299	4.6892782	6.0084913

23 H	5.9213238	6.2466008	5.4857979	6.4124921
24 H	6.2539814	5.9946978	4.7938300	5.1727716
25 H	2.1832089 *	3.4549586	3.9671009	5.4240436
26 H	1.1034984 *	2.1961831 *	3.4740229	4.6714404
27 H	2.1804321 *	1.1033038 *	2.1872481 *	2.6939711 *
28 H	3.9095359	2.6024067 *	2.6301600 *	2.0915327 *
29 H	8.9501307	7.5319838	6.7580514	5.3076341
30 H	9.6353029	8.2245785	7.8030208	6.4219825
31 H	8.3952153	7.0957601	7.0470984	5.9152939
32 H	5.9570429	4.7115293	4.8195015	3.9536798
33 H	7.6304319	6.3034266	5.2781756	3.9395210
34 H	5.5322327	4.6918438	3.3390688	3.0232134
35 H	6.2945898	5.5506970	4.1475855	3.8872495

C C C C

1 CO	2.8515754 *	3.2627631	3.0239362	4.3050829
2 C	6.2276048	7.5685887	8.1063760	9.5060561
3 C	6.5902324	7.7963763	8.1121765	9.4714239
4 C	5.7694773	6.8264959	6.9839260	8.2996466
5 C	4.3638552	5.4346096	5.6755148	7.0251456
6 C	3.7299039	5.0380410	5.6024500	7.0075775
7 C	4.9217371	6.3149809	6.9901528	8.3972577
8 C	5.1343663	6.5860329	7.4762684	8.8597723
9 C	4.3204575	5.7459687	6.7883747	8.1154957
10 C	2.9090658 *	4.3246145	5.3662844	6.6868512
11 C	2.4388862 *	3.8387010	4.6307627	6.0252410
12 N	1.3334925 *	2.5177351 *	3.1812107	4.5815830
13 C	0.0000000	1.4662083 *	2.6139061 *	3.8899107
14 C	1.4662083 *	0.0000000	1.4379249 *	2.5015876 *
15 C	2.6139061 *	1.4379249 *	0.0000000	1.4072975 *
16 C	3.8899107	2.5015876 *	1.4072975 *	0.0000000
17 C	4.3431260	2.8830303 *	2.4419836 *	1.4284868 *
18 C	3.7859596	2.4982479 *	2.8252009 *	2.4725002 *
19 C	2.4608580 *	1.4434473 *	2.4453258 *	2.8445628 *
20 O	3.0582993	2.5004908 *	1.4657233 *	2.4629122 *
21 N	4.0081977	4.7426968	4.7078709	5.9595888
22 H	7.1131753	8.4975988	9.1084932	10.5130925
23 H	7.6805184	8.8599685	9.1126475	10.4507980
24 H	6.4237277	7.3284186	7.2992074	8.5336302
25 H	6.2150038	7.6698751	8.5785618	9.9596134
26 H	4.9738628	6.3341162	7.4727387	8.7374473
27 H	2.6370503 *	3.8906580	5.0589147	6.2715273
28 H	1.1075886 *	2.1710943 *	3.5335889	4.6696445
29 H	4.8052900	3.5046801	2.1965541 *	1.1065591 *
30 H	5.4474290	3.9877566	3.4396673	2.1908774 *

31 H	4.6446422	3.4921292	3.9286436	3.4748166
32 H	2.6240347 *	2.1964262 *	3.4493685	3.9504665
33 H	4.0364526	3.3346114	2.0488624 *	2.5109642 *
34 H	3.9019696	4.6062656	4.6914866	5.9026924
35 H	4.9707264	5.5659087	5.3248370	6.4675877

C C C O

1 CO	5.4646032	5.6264789	4.7034130	1.9611088 *
2 C	10.3783040	10.0076781	8.6782032	7.3806769
3 C	10.4796134	10.2807075	9.0282162	7.1944586
4 C	9.3769243	9.3012693	8.1304241	5.9844977
5 C	8.0426056	7.9131410	6.7269284	4.7964211
6 C	7.8455186	7.4918744	6.1875109	5.0089615
7 C	9.1681561	8.7059060	7.3505605	6.4393888
8 C	9.4520032	8.8050596	7.4103167	7.1573373
9 C	8.5494143	7.7838079	6.3934544	6.7119229
10 C	7.1353109	6.4219609	5.0380912	5.3654864
11 C	6.7032173	6.2173760	4.8744537	4.3575170
12 N	5.3296334	4.9910353	3.7414514	2.9783817 *
13 C	4.3431260	3.7859596	2.4608580 *	3.0582993
14 C	2.8830303 *	2.4982479 *	1.4434473 *	2.5004908 *
15 C	2.4419836 *	2.8252009 *	2.4453258 *	1.4657233 *
16 C	1.4284868 *	2.4725002 *	2.8445628 *	2.4629122 *
17 C	0.0000000	1.4229744 *	2.4544099 *	3.7725571
18 C	1.4229744 *	0.0000000	1.4146899 *	4.2902859
19 C	2.4544099 *	1.4146899 *	0.0000000	3.7933127
20 O	3.7725571	4.2902859	3.7933127	0.0000000
21 N	7.0677468	7.1249101	6.0956110	3.7261224
22 H	11.3379349	10.8980922	9.5410681	8.4287575
23 H	11.5014571	11.3469581	10.1109180	8.1243948
24 H	9.6951871	9.7571552	8.6764884	6.1779080
25 H	10.5312136	9.8466698	8.4466350	8.2499728
26 H	9.0308440	8.1477651	6.7842667	7.5396900
27 H	6.5421061	5.7143546	4.3635086	5.3214120
28 H	4.8397336	3.9760627	2.5614585 *	4.1492847
29 H	2.1988325 *	3.4722465	3.9510422	2.6940928 *
30 H	1.1048640 *	2.2011818 *	3.4597852	4.6510036
31 H	2.1984553 *	1.1035731 *	2.1844859 *	5.3934964
32 H	3.4563603	2.1854827 *	1.1059330 *	4.6885966
33 H	3.9309910	4.7326004	4.4904688	0.9938811 *
34 H	6.9001602	6.8755502	5.8461974	3.9429730
35 H	7.6683316	7.8710543	6.9391454	4.1823326

N H H H

1 CO	1.9828369 *	6.5195027	6.1773475	4.3626708
2 C	4.3383328	1.1053214 *	2.1864376 *	3.4325482
3 C	3.8184159	2.1832869 *	1.1053154 *	2.1917623 *
4 C	2.4774919 *	3.4512976	2.2059801 *	1.1063614 *
5 C	1.5085628 *	3.9435200	3.4718517	2.1801447 *
6 C	2.5869683 *	3.5199298	4.0297120	3.5012372
7 C	3.8772444	2.1931078 *	3.4852328	3.9425865
8 C	5.0995883	2.6673851 *	4.6650230	5.3841910
9 C	5.3790997	4.0643309	5.9213238	6.2539814
10 C	4.5621090	4.8786299	6.2466008	5.9946978
11 C	3.1523768	4.6892782	5.4857979	4.7938300
12 N	2.9011163 *	6.0084913	6.4124921	5.1727716
13 C	4.0081977	7.1131753	7.6805184	6.4237277
14 C	4.7426968	8.4975988	8.8599685	7.3284186
15 C	4.7078709	9.1084932	9.1126475	7.2992074
16 C	5.9595888	10.5130925	10.4507980	8.5336302
17 C	7.0677468	11.3379349	11.5014571	9.6951871
18 C	7.1249101	10.8980922	11.3469581	9.7571552
19 C	6.0956110	9.5410681	10.1109180	8.6764884
20 O	3.7261224	8.4287575	8.1243948	6.1779080
21 N	0.0000000	5.4416259	4.6822116	2.6571434 *
22 H	5.4416259	0.0000000	2.5376719 *	4.3588275
23 H	4.6822116	2.5376719 *	0.0000000	2.5210592 *
24 H	2.6571434 *	4.3588275	2.5210592 *	0.0000000
25 H	6.0391045	2.3856306 *	4.7744626	5.9609185
26 H	6.4617917	4.7603333	6.8398199	7.3340709
27 H	5.2585862	5.9480681	7.3286055	6.9496582
28 H	4.7649524	7.1360269	8.0211591	7.0271633
29 H	6.2730654	11.0768815	10.7945747	8.7404815
30 H	8.0529692	12.4295693	12.5390326	10.6667943
31 H	8.1425205	11.7051212	12.2849085	10.7674369
32 H	6.4935429	9.3691845	10.1910641	8.9778674
33 H	4.3098449	9.1579433	8.6619232	6.5970126
34 H	1.0436944 *	5.8010844	5.1639309	3.2136534
35 H	1.0394833 *	5.8203841	4.5920015	2.2151533 *

H H H H

1 CO	6.5817802	6.3264121	4.5272586	3.8685767
2 C	2.6750825 *	4.6602532	5.3805918	6.3602976
3 C	4.0728182	5.9193874	6.2524676	6.9177125
4 C	4.8784683	6.2401422	5.9925986	6.2692155
5 C	4.6629993	5.4614111	4.7956342	4.8953642
6 C	3.5154387	4.0124879	3.4986210	4.0143254
7 C	2.1952917 *	3.4794888	3.9435794	4.9749687
8 C	1.1042458 *	2.1840260 *	3.4308621	4.9061595

9 C	2.1832089 *	1.1034984 *	2.1804321 *	3.9095359
10 C	3.4549586	2.1961831 *	1.1033038 *	2.6024067 *
11 C	3.9671009	3.4740229	2.1872481 *	2.6301600 *
12 N	5.4240436	4.6714404	2.6939711 *	2.0915327 *
13 C	6.2150038	4.9738628	2.6370503 *	1.1075886 *
14 C	7.6698751	6.3341162	3.8906580	2.1710943 *
15 C	8.5785618	7.4727387	5.0589147	3.5335889
16 C	9.9596134	8.7374473	6.2715273	4.6696445
17 C	10.5312136	9.0308440	6.5421061	4.8397336
18 C	9.8466698	8.1477651	5.7143546	3.9760627
19 C	8.4466350	6.7842667	4.3635086	2.5614585 *
20 O	8.2499728	7.5396900	5.3214120	4.1492847
21 N	6.0391045	6.4617917	5.2585862	4.7649524
22 H	2.3856306 *	4.7603333	5.9480681	7.1360269
23 H	4.7744626	6.8398199	7.3286055	8.0211591
24 H	5.9609185	7.3340709	6.9496582	7.0271633
25 H	0.0000000	2.5317020 *	4.3503667	5.9223863
26 H	2.5317020 *	0.0000000	2.4994943 *	4.3870150
27 H	4.3503667	2.4994943 *	0.0000000	2.1170151 *
28 H	5.9223863	4.3870150	2.1170151 *	0.0000000
29 H	10.7048829	9.6262856	7.1908440	5.6708556
30 H	11.6294850	10.0910668	7.6019423	5.9183479
31 H	10.5026027	8.6431751	6.2965442	4.6271301
32 H	8.0522428	6.2092657	3.9343664	2.2347423 *
33 H	9.1098220	8.4641497	6.2574623	5.1184586
34 H	6.2615494	6.5813770	5.3420847	4.5523448
35 H	6.7476910	7.3900181	6.2688269	5.7749380

H H H H

1 CO	4.6481169	6.4473332	6.6913863	5.2792800
2 C	10.0393208	11.4625389	10.8573767	8.5903809
3 C	9.8722633	11.5308167	11.2062000	9.0920943
4 C	8.6312722	10.3977642	10.2756240	8.3294214
5 C	7.4467930	9.0839152	8.8783101	6.9292617
6 C	7.6043520	8.9322757	8.3718160	6.1987663
7 C	9.0259012	10.2642163	9.5174607	7.2082402
8 C	9.6028765	10.5515439	9.4982691	7.0760435
9 C	8.9501307	9.6353029	8.3952153	5.9570429
10 C	7.5319838	8.2245785	7.0957601	4.7115293
11 C	6.7580514	7.8030208	7.0470984	4.8195015
12 N	5.3076341	6.4219825	5.9152939	3.9536798
13 C	4.8052900	5.4474290	4.6446422	2.6240347 *
14 C	3.5046801	3.9877566	3.4921292	2.1964262 *
15 C	2.1965541 *	3.4396673	3.9286436	3.4493685
16 C	1.1065591 *	2.1908774 *	3.4748166	3.9504665

17 C	2.1988325 *	1.1048640 *	2.1984553 *	3.4563603
18 C	3.4722465	2.2011818 *	1.1035731 *	2.1854827 *
19 C	3.9510422	3.4597852	2.1844859 *	1.1059330 *
20 O	2.6940928 *	4.6510036	5.3934964	4.6885966
21 N	6.2730654	8.0529692	8.1425205	6.4935429
22 H	11.0768815	12.4295693	11.7051212	9.3691845
23 H	10.7945747	12.5390326	12.2849085	10.1910641
24 H	8.7404815	10.6667943	10.7674369	8.9778674
25 H	10.7048829	11.6294850	10.5026027	8.0522428
26 H	9.6262856	10.0910668	8.6431751	6.2092657
27 H	7.1908440	7.6019423	6.2965442	3.9343664
28 H	5.6708556	5.9183479	4.6271301	2.2347423 *
29 H	0.0000000	2.5165949 *	4.3860173	5.0569607
30 H	2.5165949 *	0.0000000	2.5439001 *	4.3743308
31 H	4.3860173	2.5439001 *	0.0000000	2.5119841 *
32 H	5.0569607	4.3743308	2.5119841 *	0.0000000
33 H	2.3113076 *	4.6295607	5.8175032	5.4689116
34 H	6.2884069	7.8831059	7.8446255	6.1894829
35 H	6.6218289	8.5922369	8.9139820	7.4152278

H H H

1 CO	2.6630662 *	2.4968973 *	2.6234496 *
2 C	8.0985417	4.7307394	4.7356804
3 C	7.7970369	4.3003919	3.9208879
4 C	6.5374319	3.0437754	2.4881805 *
5 C	5.4647018	2.0961545 *	2.0864208 *
6 C	5.8251026	2.9389400 *	3.4190815
7 C	7.2476337	4.1995182	4.5559512
8 C	8.0287342	5.3247532	5.8808454
9 C	7.6304319	5.5322327	6.2945898
10 C	6.3034266	4.6918438	5.5506970
11 C	5.2781756	3.3390688	4.1475855
12 N	3.9395210	3.0232134	3.8872495
13 C	4.0364526	3.9019696	4.9707264
14 C	3.3346114	4.6062656	5.5659087
15 C	2.0488624 *	4.6914866	5.3248370
16 C	2.5109642 *	5.9026924	6.4675877
17 C	3.9309910	6.9001602	7.6683316
18 C	4.7326004	6.8755502	7.8710543
19 C	4.4904688	5.8461974	6.9391454
20 O	0.9938811 *	3.9429730	4.1823326
21 N	4.3098449	1.0436944 *	1.0394833 *
22 H	9.1579433	5.8010844	5.8203841
23 H	8.6619232	5.1639309	4.5920015
24 H	6.5970126	3.2136534	2.2151533 *

25 H	9.1098220	6.2615494	6.7476910
26 H	8.4641497	6.5813770	7.3900181
27 H	6.2574623	5.3420847	6.2688269
28 H	5.1184586	4.5523448	5.7749380
29 H	2.3113076 *	6.2884069	6.6218289
30 H	4.6295607	7.8831059	8.5922369
31 H	5.8175032	7.8446255	8.9139820
32 H	5.4689116	6.1894829	7.4152278
33 H	0.0000000	4.5888128	4.5648228
34 H	4.5888128	0.0000000	1.6626802 *
35 H	4.5648228	1.6626802 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.84 , TOTAL = 5387.5 SECONDS (89.8 MIN)
WALL CLOCK TIME: STEP = 0.84 , TOTAL = 4981.3 SECONDS (83.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.12 , TOTAL = 5388.6 SECONDS (89.8 MIN)
WALL CLOCK TIME: STEP = 1.12 , TOTAL = 4982.4 SECONDS (83.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.634521770	-284.634521770	0.026867325	0.002935459	197073072
11393904						
2	1	-284.635503569	-0.000981799	0.005793688	0.000311161	165234178
14156329						
3	2	-284.635508937	-0.000005368	0.002667394	0.000514489	151680850
15285731						
4	3	-284.635516400	-0.000007463	0.001935085	0.000158429	145631254
15730058						
5	4	-284.635517031	-0.000000631	0.001657609	0.000228336	141533318
16103219						

6 5	-284.635517915	-0.000000884	0.001029953	0.000118523	136137248
16501221					
7 6	-284.635518197	-0.000000283	0.000786988	0.000059089	134731373
16626714					
8 7	-284.635518431	-0.000000233	0.000495926	0.000051943	129241899
16975458					
9 8	-284.635518563	-0.000000133	0.000322292	0.000041947	127412938
17183952					
10 9	-284.635518693	-0.000000130	0.000449197	0.000036094	124488958
17429323					
11 10	-284.635518828	-0.000000135	0.000712698	0.000041238	146036613
15819716					
12 11	-284.635518948	-0.000000120	0.000465966	0.000043138	168783729
14005119					
13 12	-284.635519041	-0.000000094	0.000660404	0.000037643	164020496
14392005					
-----DISABLING FDIFF OPTION-----					
14 13	-284.635519115	-0.000000074	0.000539904	0.000023131	197051989
11395483					
15 14	-284.635519177	-0.000000062	0.000151495	0.000020847	197051961
11395469					
16 15	-284.635519191	-0.000000014	0.000127403	0.000008332	197052013
11395461					
17 16	-284.635519195	-0.000000004	0.000066759	0.000007530	197052130
11395461					
18 17	-284.635519198	-0.000000003	0.000077657	0.000006555	197052035
11395462					
19 18	-284.635519200	-0.000000002	0.000089881	0.000005279	197052123
11395459					
20 19	-284.635519203	-0.000000003	0.000194552	0.000003928	197052021
11395462					
21 20	-284.635519206	-0.000000003	0.000096341	0.000007596	197052017
11395460					
22 21	-284.635519208	-0.000000002	0.000103952	0.000007516	197051981
11395463					
23 22	-284.635519211	-0.000000003	0.000149107	0.000004341	197051975
11395464					
24 23	-284.635519214	-0.000000002	0.000060037	0.000002933	197051876
11395464					
25 24	-284.635519214	0.000000000	0.000028802	0.000002100	197051651
11395470					
26 25	-284.635519214	0.000000000	0.000014021	0.000001441	197051861
11395466					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 87.8 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 28.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 3.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6355192145 AFTER 26 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6014915093
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999750192

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 92.11 , TOTAL = 5480.8 SECONDS (91.3 MIN)
WALL CLOCK TIME: STEP = 84.33 , TOTAL = 5066.8 SECONDS (84.4
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.80 , TOTAL = 5484.6 SECONDS (91.4 MIN)
WALL CLOCK TIME: STEP = 3.79 , TOTAL = 5070.6 SECONDS (84.5
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.83 , TOTAL = 5487.4 SECONDS (91.5 MIN)
WALL CLOCK TIME: STEP = 2.66 , TOTAL = 5073.2 SECONDS (84.6
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 55 ENERGY= -284.6355192

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0006911	-0.0000412	0.0008512
2 C	6.0	0.0005129	-0.0010289	-0.0002733
3 C	6.0	-0.0002513	0.0007236	-0.0000592
4 C	6.0	-0.0003252	0.0007762	-0.0003728
5 C	6.0	-0.0004761	-0.0002562	-0.0001469
6 C	6.0	-0.0004820	-0.0001684	-0.0000152
7 C	6.0	0.0000493	-0.0002365	-0.0001473
8 C	6.0	0.0014290	0.0001887	-0.0005848
9 C	6.0	-0.0003608	-0.0001049	0.0003603
10 C	6.0	0.0004398	0.0004440	0.0010970
11 C	6.0	0.0001794	0.0000048	0.0000973
12 N	7.0	0.0001397	-0.0004544	-0.0006721
13 C	6.0	-0.0003033	-0.0000157	-0.0003039
14 C	6.0	0.0004254	-0.0003305	-0.0005943
15 C	6.0	-0.0005287	-0.0002409	-0.0010236
16 C	6.0	-0.0006620	-0.0004531	-0.0005260
17 C	6.0	-0.0004073	0.0000848	-0.0000086
18 C	6.0	0.0003147	-0.0000295	-0.0001575
19 C	6.0	-0.0004506	-0.0000987	-0.0001193
20 O	8.0	-0.0004414	0.0010529	-0.0000007
21 N	7.0	-0.0005125	0.0006128	0.0005558
22 H	1.0	-0.0002986	0.0007297	-0.0000760
23 H	1.0	0.0009103	-0.0001244	0.0011243
24 H	1.0	-0.0000905	0.0010696	0.0005054
25 H	1.0	-0.0003001	-0.0002968	-0.0013542
26 H	1.0	0.0000847	-0.0005197	-0.0003772
27 H	1.0	0.0003799	-0.0006116	0.0002629
28 H	1.0	0.0004293	-0.0000224	0.0001516
29 H	1.0	-0.0003266	0.0000938	-0.0005462
30 H	1.0	0.0002399	0.0001616	0.0007969
31 H	1.0	0.0004878	0.0000644	0.0004301
32 H	1.0	0.0002930	0.0001922	0.0006261
33 H	1.0	-0.0003547	-0.0018096	0.0006224
34 H	1.0	0.0009589	0.0002555	0.0004228
35 H	1.0	-0.0000112	0.0003891	-0.0005450

MAXIMUM GRADIENT = 0.0018096 RMS GRADIENT = 0.0005385
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001239495
 PREDICTED ENERGY CHANGE WAS -0.0000968881 RATIO= 1.279

NR STEP HAS LENGTH = 0.122051
RADIUS OF STEP TAKEN= 0.12205 CURRENT TRUST RADIUS= 0.33303

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 5487.4 SECONDS (91.5 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5073.2 SECONDS (84.6 MIN)
CPU UTILIZATION: STEP = 93.14%, TOTAL = 100.00%

1NSERCH= 56

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1347721056	-1.7682905020	0.9244126882
C	6.0	4.9890809528	0.6704079749	0.4932849506
C	6.0	5.2085558380	-0.6898126450	0.2446841875
C	6.0	4.0770242058	-1.5375332152	0.0154058207
C	6.0	2.7629103619	-1.0393328952	0.0839469107
C	6.0	2.4769980576	0.3388484648	0.4494612423
C	6.0	3.6518793818	1.2040737190	0.6043251639
C	6.0	3.4943204478	2.6093582820	0.8929885824
C	6.0	2.2252878263	3.1565108242	1.1290014766
C	6.0	1.0731583033	2.3117604581	1.0656391169
C	6.0	1.1679777846	0.9525909167	0.6848094545
N	7.0	-0.0427093899	0.1420058740	0.6478312914
C	6.0	-1.2376749340	0.6738614179	0.3890869571
C	6.0	-2.5514484341	0.0257784835	0.4664600238
C	6.0	-2.8526793608	-1.3347266985	0.8186252337
C	6.0	-4.1638060001	-1.8389125285	0.8886812441
C	6.0	-5.2570724286	-0.9573242946	0.6310672230
C	6.0	-5.0150062347	0.4006791191	0.2887959913
C	6.0	-3.6853571244	0.8777022624	0.1999229295
O	8.0	-1.7507585112	-2.2394488392	1.1559619464
N	7.0	1.6680443801	-2.0001702524	-0.3113064234
H	1.0	5.8374294567	1.3651525589	0.6292201603
H	1.0	6.2314303787	-1.1072061585	0.2049862987
H	1.0	4.2483328400	-2.5983913335	-0.2475847091
H	1.0	4.3997657667	3.2407240037	0.9427408147
H	1.0	2.1084677661	4.2214206379	1.3928866955
H	1.0	0.0962006154	2.7364397714	1.3532820228
H	1.0	-1.2720005612	1.7343033521	0.0711818318
H	1.0	-4.3600467152	-2.8957342920	1.1511997621
H	1.0	-6.2898082411	-1.3410188108	0.7120085701
H	1.0	-5.8594264579	1.0856561582	0.0997486392

H	1.0	-3.5004023826	1.9366746121	-0.0571406399
H	1.0	-2.0894403358	-3.1062344602	1.4987339533
H	1.0	1.3323007369	-1.7584318391	-1.2665271632
H	1.0	2.0796969054	-2.9502751262	-0.3849352472

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C	
1	CO	0.0000000	5.4495354	5.2314842	4.0522702
2	C	5.4495354	0.0000000	1.4000613 *	2.4362308 *
3	C	5.2314842	1.4000613 *	0.0000000	1.4323277 *
4	C	4.0522702	2.4362308 *	1.4323277 *	0.0000000
5	C	2.8539223 *	2.8366542 *	2.4757186 *	1.4070525 *
6	C	3.1861632	2.5342480 *	2.9260016 *	2.5038562 *
7	C	4.6159992	1.4440350 *	2.4777790 *	2.8361916 *
8	C	5.5182752	2.4806451 *	3.7740469	4.2785984
9	C	5.3540434	3.7713917	4.9473336	5.1675016
10	C	4.1889533	4.2843993	5.1754150	4.9943230
11	C	2.9202944 *	3.8362923	4.3837736	3.8873346
12	N	1.9383573 *	5.0618186	5.3320011	4.4936643
13	C	2.8520678 *	6.2276286	6.5904742	5.7685293
14	C	3.2625427	7.5680810	7.7960837	6.8252504
15	C	3.0206017	8.1005936	8.1073322	6.9790460
16	C	4.2993067	9.4988614	9.4644772	8.2924497
17	C	5.4603759	10.3755557	10.4761744	9.3723552
18	C	5.6239359	10.0098117	10.2816506	9.3003455
19	C	4.7031426	8.6818724	9.0311015	8.1315419
20	O	1.9572509 *	7.3710137	7.1877573	5.9796827
21	N	1.9828499 *	4.3368928	3.8159382	2.4746632 *
22	H	6.5135171	1.1049179 *	2.1831702 *	3.4498376
23	H	6.1744513	2.1877980 *	1.1054708 *	2.2051277 *
24	H	4.3570664	3.4325857	2.1924939 *	1.1063140 *
25	H	6.5788094	2.6750378 *	4.0731490	4.8780995
26	H	6.3238898	4.6601402	5.9202304	6.2400495
27	H	4.5252637	5.3803680	6.2533488	5.9919708
28	H	3.8697772	6.3648398	6.9212754	6.2705735
29	H	4.6396075	10.0277819	9.8613394	8.6208412
30	H	6.4422752	11.4589275	11.5262673	10.3920685
31	H	6.6899551	10.8635820	11.2104205	10.2772218
32	H	5.2824906	8.6010306	9.1014003	8.3362328
33	H	2.6583942 *	8.0857541	7.7892544	6.5334808
34	H	2.4968759 *	4.7295077	4.2954697	3.0373764
35	H	2.6256832 *	4.7270638	3.9109934	2.4789976 *

	C	C	C	C
1 CO	2.8539223 *	3.1861632	4.6159992	5.5182752
2 C	2.8366542 *	2.5342480 *	1.4440350 *	2.4806451 *
3 C	2.4757186 *	2.9260016 *	2.4777790 *	3.7740469
4 C	1.4070525 *	2.5038562 *	2.8361916 *	4.2785984
5 C	0.0000000	1.4542113 *	2.4685892 *	3.8082091
6 C	1.4542113 *	0.0000000	1.4672913 *	2.5272270 *
7 C	2.4685892 *	1.4672913 *	0.0000000	1.4432519 *
8 C	3.8082091	2.5272270 *	1.4432519 *	0.0000000
9 C	4.3573250	2.9093563 *	2.4743604 *	1.4019707 *
10 C	3.8792793	2.4985642 *	2.8442192 *	2.4454854 *
11 C	2.6215656 *	1.4647876 *	2.4978968 *	2.8635794 *
12 N	3.0959698	2.5351575 *	3.8444593	4.3195498
13 C	4.3626629	3.7302378	4.9229253	5.1372994
14 C	5.4335244	5.0382116	6.3157472	6.5884848
15 C	5.6711425	5.5984460	6.9857510	7.4730009
16 C	7.0189974	7.0025592	8.3919939	8.8562990
17 C	8.0390416	7.8440354	9.1674303	9.4539254
18 C	7.9127482	7.4939819	8.7097593	8.8120346
19 C	6.7281965	6.1909009	7.3556168	7.4180013
20 O	4.7919413	5.0020682	6.4304469	7.1477926
21 N	1.5093592 *	2.5892435 *	3.8782937	5.1022901
22 H	3.9410076	3.5182542	2.1916193 *	2.6660423 *
23 H	3.4712949	4.0307076	3.4864838	4.6666872
24 H	2.1787741 *	3.5001254	3.9421121	5.3842454
25 H	4.6621572	3.5158558	2.1958606 *	1.1049566 *
26 H	5.4605079	4.0125095	3.4797027	2.1838569 *
27 H	4.7936428	3.4976467	3.9435940	3.4315067
28 H	4.8962973	4.0181314	4.9809617	4.9151707
29 H	7.4378607	7.5960611	9.0165657	9.5949883
30 H	9.0794928	8.9301611	10.2628575	10.5530757
31 H	8.8803446	8.3771113	9.5254165	9.5101777
32 H	6.9358210	6.2079795	7.2200676	7.0909376
33 H	5.4606787	5.8156624	7.2347409	8.0133209
34 H	2.0946426 *	2.9416888 *	4.2020201	5.3306124
35 H	2.0828661 *	3.4164894	4.5507151	5.8773951

	C	C	C	N
1 CO	5.3540434	4.1889533	2.9202944 *	1.9383573 *
2 C	3.7713917	4.2843993	3.8362923	5.0618186
3 C	4.9473336	5.1754150	4.3837736	5.3320011
4 C	5.1675016	4.9943230	3.8873346	4.4936643
5 C	4.3573250	3.8792793	2.6215656 *	3.0959698
6 C	2.9093563 *	2.4985642 *	1.4647876 *	2.5351575 *

7 C	2.4743604 *	2.8442192 *	2.4978968 *	3.8444593
8 C	1.4019707 *	2.4454854 *	2.8635794 *	4.3195498
9 C	0.0000000	1.4300421 *	2.4844464 *	3.8029694
10 C	1.4300421 *	0.0000000	1.4146957 *	2.4753907 *
11 C	2.4844464 *	1.4146957 *	0.0000000	1.4574563 *
12 N	3.8029694	2.4753907 *	1.4574563 *	0.0000000
13 C	4.3247119	2.9121103 *	2.4397350 *	1.3333273 *
14 C	5.7495787	4.3269508	3.8393735	2.5179706 *
15 C	6.7862581	5.3637753	4.6276789	3.1789685
16 C	8.1137247	6.6846986	6.0217916	4.5788081
17 C	8.5532037	7.1377580	6.7031287	5.3290140
18 C	7.7924586	6.4281774	6.2201869	4.9919489
19 C	6.4024901	5.0447454	4.8780716	3.7430941
20 O	6.7026899	5.3568807	4.3508762	2.9743831 *
21 N	5.3829701	4.5653713	3.1561229	2.9044005 *
22 H	4.0627962	4.8769671	4.6879714	6.0060359
23 H	5.9230283	6.2480258	5.4873989	6.4126026
24 H	6.2535270	5.9929860	4.7924337	5.1695832
25 H	2.1840648 *	3.4560663	3.9681904	5.4244457
26 H	1.1033201 *	2.1967609 *	3.4743550	4.6716481
27 H	2.1816906 *	1.1034207 *	2.1857902 *	2.6922192 *
28 H	3.9208013	2.6119288 *	2.6345982 *	2.0926282 *
29 H	8.9440927	7.5262899	6.7517540	5.3028904
30 H	9.6389064	8.2268540	7.8025610	6.4210377
31 H	8.4089479	7.1061247	7.0529719	5.9181980
32 H	5.9731451	4.7242757	4.8283210	3.9589724
33 H	7.6141684	6.2884235	5.2675715	3.9324557
34 H	5.5400943	4.6981507	3.3443028	3.0277194
35 H	6.2933326	5.5503427	4.1482465	3.8901693

C C C C

1 CO	2.8520678 *	3.2625427	3.0206017	4.2993067
2 C	6.2276286	7.5680810	8.1005936	9.4988614
3 C	6.5904742	7.7960837	8.1073322	9.4644772
4 C	5.7685293	6.8252504	6.9790460	8.2924497
5 C	4.3626629	5.4335244	5.6711425	7.0189974
6 C	3.7302378	5.0382116	5.5984460	7.0025592
7 C	4.9229253	6.3157472	6.9857510	8.3919939
8 C	5.1372994	6.5884848	7.4730009	8.8562990
9 C	4.3247119	5.7495787	6.7862581	8.1137247
10 C	2.9121103 *	4.3269508	5.3637753	6.6846986
11 C	2.4397350 *	3.8393735	4.6276789	6.0217916
12 N	1.3333273 *	2.5179706 *	3.1789685	4.5788081
13 C	0.0000000	1.4669693 *	2.6128851 *	3.8891992
14 C	1.4669693 *	0.0000000	1.4372664 *	2.5010078 *

15 C	2.6128851 *	1.4372664 *	0.0000000	1.4064723 *
16 C	3.8891992	2.5010078 *	1.4064723 *	0.0000000
17 C	4.3445227	2.8833987 *	2.4410483 *	1.4278635 *
18 C	3.7885246	2.4982458 *	2.8227664 *	2.4698532 *
19 C	2.4634290 *	1.4431095 *	2.4435603 *	2.8431140 *
20 O	3.0559334	2.4995544 *	1.4651102 *	2.4606232 *
21 N	4.0105113	4.7448402	4.7070696	5.9562113
22 H	7.1128510	8.4966868	9.1018247	10.5051446
23 H	7.6807310	8.8595137	9.1076544	10.4433602
24 H	6.4194447	7.3234659	7.2909551	8.5224403
25 H	6.2190075	7.6734671	8.5760197	9.9569268
26 H	4.9789016	6.3384934	7.4708454	8.7363196
27 H	2.6387735 *	3.8915528	5.0553088	6.2687606
28 H	1.1076006 *	2.1707807 *	3.5321612	4.6689095
29 H	4.8033358	3.5035886	2.1953375 *	1.1064803 *
30 H	5.4486761	3.9879522	3.4387878	2.1906613 *
31 H	4.6490729	3.4929266	3.9262660	3.4714040
32 H	2.6294014 *	2.1968603 *	3.4479817	3.9483847
33 H	4.0306260	3.3299469	2.0453170 *	2.5062446 *
34 H	3.9066461	4.6119582	4.6948317	5.9041163
35 H	4.9737744	5.5703928	5.3279349	6.4682729

C C C O

1 CO	5.4603759	5.6239359	4.7031426	1.9572509 *
2 C	10.3755557	10.0098117	8.6818724	7.3710137
3 C	10.4761744	10.2816506	9.0311015	7.1877573
4 C	9.3723552	9.3003455	8.1315419	5.9796827
5 C	8.0390416	7.9127482	6.7281965	4.7919413
6 C	7.8440354	7.4939819	6.1909009	5.0020682
7 C	9.1674303	8.7097593	7.3556168	6.4304469
8 C	9.4539254	8.8120346	7.4180013	7.1477926
9 C	8.5532037	7.7924586	6.4024901	6.7026899
10 C	7.1377580	6.4281774	5.0447454	5.3568807
11 C	6.7031287	6.2201869	4.8780716	4.3508762
12 N	5.3290140	4.9919489	3.7430941	2.9743831 *
13 C	4.3445227	3.7885246	2.4634290 *	3.0559334
14 C	2.8833987 *	2.4982458 *	1.4431095 *	2.4995544 *
15 C	2.4410483 *	2.8227664 *	2.4435603 *	1.4651102 *
16 C	1.4278635 *	2.4698532 *	2.8431140 *	2.4606232 *
17 C	0.0000000	1.4212385 *	2.4542813 *	3.7700922
18 C	1.4212385 *	0.0000000	1.4154209 *	4.2869063
19 C	2.4542813 *	1.4154209 *	0.0000000	3.7912153
20 O	3.7700922	4.2869063	3.7912153	0.0000000
21 N	7.0663172	7.1265255	6.0993781	3.7280483
22 H	11.3349845	10.9005256	9.5449132	8.4173158

23 H	11.4973782	11.3473820	10.1134841	8.1179842
24 H	9.6859620	9.7514911	8.6733457	6.1715379
25 H	10.5344802	9.8555279	8.4560548	8.2405526
26 H	9.0360915	8.1584903	6.7949998	7.5294485
27 H	6.5439300	5.7195580	4.3686750	5.3112767
28 H	4.8413974	3.9794473	2.5641041 *	4.1468860
29 H	2.1983235 *	3.4697339	3.9495515	2.6905609 *
30 H	1.1046792 *	2.1994865 *	3.4594971	4.6483592
31 H	2.1951991 *	1.1036204 *	2.1862884 *	5.3900892
32 H	3.4546707	2.1847149 *	1.1053110 *	4.6875237
33 H	3.9248635	4.7245453	4.4839282	0.9917234 *
34 H	6.9038016	6.8825211	5.8546195	3.9503272
35 H	7.6702215	7.8751267	6.9448771	4.1895139

N H H H

1 CO	1.9828499 *	6.5135171	6.1744513	4.3570664
2 C	4.3368928	1.1049179 *	2.1877980 *	3.4325857
3 C	3.8159382	2.1831702 *	1.1054708 *	2.1924939 *
4 C	2.4746632 *	3.4498376	2.2051277 *	1.1063140 *
5 C	1.5093592 *	3.9410076	3.4712949	2.1787741 *
6 C	2.5892435 *	3.5182542	4.0307076	3.5001254
7 C	3.8782937	2.1916193 *	3.4864838	3.9421121
8 C	5.1022901	2.6660423 *	4.6666872	5.3842454
9 C	5.3829701	4.0627962	5.9230283	6.2535270
10 C	4.5653713	4.8769671	6.2480258	5.9929860
11 C	3.1561229	4.6879714	5.4873989	4.7924337
12 N	2.9044005 *	6.0060359	6.4126026	5.1695832
13 C	4.0105113	7.1128510	7.6807310	6.4194447
14 C	4.7448402	8.4966868	8.8595137	7.3234659
15 C	4.7070696	9.1018247	9.1076544	7.2909551
16 C	5.9562113	10.5051446	10.4433602	8.5224403
17 C	7.0663172	11.3349845	11.4973782	9.6859620
18 C	7.1265255	10.9005256	11.3473820	9.7514911
19 C	6.0993781	9.5449132	10.1134841	8.6733457
20 O	3.7280483	8.4173158	8.1179842	6.1715379
21 N	0.0000000	5.4400147	4.6785078	2.6494938 *
22 H	5.4400147	0.0000000	2.5392457 *	4.3593228
23 H	4.6785078	2.5392457 *	0.0000000	2.5221280 *
24 H	2.6494938 *	4.3593228	2.5221280 *	0.0000000
25 H	6.0416810	2.3838918 *	4.7753297	5.9611303
26 H	6.4657900	4.7588454	6.8413589	7.3334851
27 H	5.2608956	5.9469658	7.3302961	6.9471864
28 H	4.7682759	7.1408455	8.0245595	7.0248086
29 H	6.2672834	11.0641827	10.7830209	8.7263514
30 H	8.0504082	12.4257841	12.5336809	10.6561824

31 H	8.1458031	11.7121687	12.2885532	10.7638118
32 H	6.5020143	9.3804495	10.2001220	8.9803112
33 H	4.3148946	9.1424625	8.6548707	6.5935501
34 H	1.0409649 *	5.8005881	5.1566382	3.2010965
35 H	1.0380647 *	5.8113666	4.5805896	2.2012881 *

H H H H

1 CO	6.5788094	6.3238898	4.5252637	3.8697772
2 C	2.6750378 *	4.6601402	5.3803680	6.3648398
3 C	4.0731490	5.9202304	6.2533488	6.9212754
4 C	4.8780995	6.2400495	5.9919708	6.2705735
5 C	4.6621572	5.4605079	4.7936428	4.8962973
6 C	3.5158558	4.0125095	3.4976467	4.0181314
7 C	2.1958606 *	3.4797027	3.9435940	4.9809617
8 C	1.1049566 *	2.1838569 *	3.4315067	4.9151707
9 C	2.1840648 *	1.1033201 *	2.1816906 *	3.9208013
10 C	3.4560663	2.1967609 *	1.1034207 *	2.6119288 *
11 C	3.9681904	3.4743550	2.1857902 *	2.6345982 *
12 N	5.4244457	4.6716481	2.6922192 *	2.0926282 *
13 C	6.2190075	4.9789016	2.6387735 *	1.1076006 *
14 C	7.6734671	6.3384934	3.8915528	2.1707807 *
15 C	8.5760197	7.4708454	5.0553088	3.5321612
16 C	9.9569268	8.7363196	6.2687606	4.6689095
17 C	10.5344802	9.0360915	6.5439300	4.8413974
18 C	9.8555279	8.1584903	5.7195580	3.9794473
19 C	8.4560548	6.7949998	4.3686750	2.5641041 *
20 O	8.2405526	7.5294485	5.3112767	4.1468860
21 N	6.0416810	6.4657900	5.2608956	4.7682759
22 H	2.3838918 *	4.7588454	5.9469658	7.1408455
23 H	4.7753297	6.8413589	7.3302961	8.0245595
24 H	5.9611303	7.3334851	6.9471864	7.0248086
25 H	0.0000000	2.5326752 *	4.3524154	5.9327777
26 H	2.5326752 *	0.0000000	2.5011909 *	4.4000253
27 H	4.3524154	2.5011909 *	0.0000000	2.1260369 *
28 H	5.9327777	4.4000253	2.1260369 *	0.0000000
29 H	10.6973777	9.6204982	7.1847312	5.6691901
30 H	11.6323943	10.0963046	7.6038154	5.9200219
31 H	10.5169377	8.6598247	6.3060230	4.6331453
32 H	8.0692605	6.2275250	3.9451831	2.2412486 *
33 H	9.0941083	8.4456004	6.2397937	5.1124279
34 H	6.2675167	6.5904137	5.3474493	4.5575267
35 H	6.7434348	7.3888226	6.2685232	5.7781653

H H H H

1 CO	4.6396075	6.4422752	6.6899551	5.2824906
2 C	10.0277819	11.4589275	10.8635820	8.6010306
3 C	9.8613394	11.5262673	11.2104205	9.1014003
4 C	8.6208412	10.3920685	10.2772218	8.3362328
5 C	7.4378607	9.0794928	8.8803446	6.9358210
6 C	7.5960611	8.9301611	8.3771113	6.2079795
7 C	9.0165657	10.2628575	9.5254165	7.2200676
8 C	9.5949883	10.5530757	9.5101777	7.0909376
9 C	8.9440927	9.6389064	8.4089479	5.9731451
10 C	7.5262899	8.2268540	7.1061247	4.7242757
11 C	6.7517540	7.8025610	7.0529719	4.8283210
12 N	5.3028904	6.4210377	5.9181980	3.9589724
13 C	4.8033358	5.4486761	4.6490729	2.6294014 *
14 C	3.5035886	3.9879522	3.4929266	2.1968603 *
15 C	2.1953375 *	3.4387878	3.9262660	3.4479817
16 C	1.1064803 *	2.1906613 *	3.4714040	3.9483847
17 C	2.1983235 *	1.1046792 *	2.1951991 *	3.4546707
18 C	3.4697339	2.1994865 *	1.1036204 *	2.1847149 *
19 C	3.9495515	3.4594971	2.1862884 *	1.1053110 *
20 O	2.6905609 *	4.6483592	5.3900892	4.6875237
21 N	6.2672834	8.0504082	8.1458031	6.5020143
22 H	11.0641827	12.4257841	11.7121687	9.3804495
23 H	10.7830209	12.5336809	12.2885532	10.2001220
24 H	8.7263514	10.6561824	10.7638118	8.9803112
25 H	10.6973777	11.6323943	10.5169377	8.0692605
26 H	9.6204982	10.0963046	8.6598247	6.2275250
27 H	7.1847312	7.6038154	6.3060230	3.9451831
28 H	5.6691901	5.9200219	4.6331453	2.2412486 *
29 H	0.0000000	2.5167457 *	4.3823691	5.0548245
30 H	2.5167457 *	0.0000000	2.5394570 *	4.3721448
31 H	4.3823691	2.5394570 *	0.0000000	2.5127358 *
32 H	5.0548245	4.3721448	2.5127358 *	0.0000000
33 H	2.3066737 *	4.6236364	5.8087780	5.4628282
34 H	6.2882175	7.8857709	7.8534379	6.2025355
35 H	6.6206483	8.5931140	8.9192679	7.4247717

H H H

1 CO	2.6583942 *	2.4968759 *	2.6256832 *
2 C	8.0857541	4.7295077	4.7270638
3 C	7.7892544	4.2954697	3.9109934
4 C	6.5334808	3.0373764	2.4789976 *
5 C	5.4606787	2.0946426 *	2.0828661 *
6 C	5.8156624	2.9416888 *	3.4164894
7 C	7.2347409	4.2020201	4.5507151
8 C	8.0133209	5.3306124	5.8773951

9 C	7.6141684	5.5400943	6.2933326
10 C	6.2884235	4.6981507	5.5503427
11 C	5.2675715	3.3443028	4.1482465
12 N	3.9324557	3.0277194	3.8901693
13 C	4.0306260	3.9066461	4.9737744
14 C	3.3299469	4.6119582	5.5703928
15 C	2.0453170 *	4.6948317	5.3279349
16 C	2.5062446 *	5.9041163	6.4682729
17 C	3.9248635	6.9038016	7.6702215
18 C	4.7245453	6.8825211	7.8751267
19 C	4.4839282	5.8546195	6.9448771
20 O	0.9917234 *	3.9503272	4.1895139
21 N	4.3148946	1.0409649 *	1.0380647 *
22 H	9.1424625	5.8005881	5.8113666
23 H	8.6548707	5.1566382	4.5805896
24 H	6.5935501	3.2010965	2.2012881 *
25 H	9.0941083	6.2675167	6.7434348
26 H	8.4456004	6.5904137	7.3888226
27 H	6.2397937	5.3474493	6.2685232
28 H	5.1124279	4.5575267	5.7781653
29 H	2.3066737 *	6.2882175	6.6206483
30 H	4.6236364	7.8857709	8.5931140
31 H	5.8087780	7.8534379	8.9192679
32 H	5.4628282	6.2025355	7.4247717
33 H	0.0000000	4.6012556	4.5775800
34 H	4.6012556	0.0000000	1.6602096 *
35 H	4.5775800	1.6602096 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80 , TOTAL = 5488.2 SECONDS (91.5 MIN)
WALL CLOCK TIME: STEP = 0.82 , TOTAL = 5074.1 SECONDS (84.6 MIN)

CPU UTILIZATION: STEP = 97.88%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.93 , TOTAL = 5489.1 SECONDS (91.5 MIN)
WALL CLOCK TIME: STEP = 0.92 , TOTAL = 5075.0 SECONDS (84.6 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
 INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.635317705	-284.635317705	0.031102685	0.001370584	197112006
11392410						
2	1	-284.635594360	-0.000276655	0.005546449	0.000278643	161079066
14473848						
3	2	-284.635584992	0.000009368	0.003348524	0.000557483	150452545
15337676						
4	3	-284.635601500	-0.000016507	0.001220691	0.000206567	145503423
15734099						
5	4	-284.635599812	0.000001688	0.000942939	0.000402661	137336949
16403769						
6	5	-284.635602067	-0.000002255	0.000299988	0.000045440	133451457
16731010						
7	6	-284.635602080	-0.000000013	0.000165915	0.000043311	125047288
17277523						
8	7	-284.635602201	-0.000000121	0.000248302	0.000038105	118169509
17825102						
9	8	-284.635602277	-0.000000076	0.000496483	0.000031948	142204010
16050363						
10	9	-284.635602370	-0.000000093	0.000411805	0.000033966	164688039
14356606						
11	10	-284.635602456	-0.000000086	0.000661714	0.000036248	164275542
14340814						

-----DISABLING FDIFF OPTION-----

12	11	-284.635602555	-0.000000099	0.000607783	0.000035053	197117175
11392046						
13	12	-284.635602638	-0.000000083	0.000932299	0.000024420	197117158
11392029						
14	13	-284.635602737	-0.000000100	0.000376630	0.000013363	197117227
11392038						
15	14	-284.635602753	-0.000000016	0.000129255	0.000017008	197117085
11392047						
16	15	-284.635602766	-0.000000013	0.000085824	0.000007547	197117142
11392047						
17	16	-284.635602769	-0.000000003	0.000068137	0.000006113	197117151
11392043						
18	17	-284.635602772	-0.000000004	0.000127709	0.000004927	197117190
11392045						
19	18	-284.635602775	-0.000000002	0.000090954	0.000004238	197117175
11392046						
20	19	-284.635602777	-0.000000002	0.000044481	0.000004974	197117185
11392048						

21 20 -284.635602778 -0.000000001 0.000078608 0.000004613 197117196
11392047
22 21 -284.635602779 -0.000000002 0.000035688 0.000003409 197117176
11392050
23 22 -284.635602780 -0.000000001 0.000032667 0.000002694 197117319
11392048
24 23 -284.635602781 -0.000000001 0.000032508 0.000002546 197117318
11392047

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 80.2 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 26.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.1
TIME TO SOLVE SCF EQUATIONS= 3.8 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6356027807 AFTER 24 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6057585094
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999750222

SPIN SZ = 1.500
S-SQUARED = 3.759

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 84.70 , TOTAL = 5573.8 SECONDS (92.9 MIN)
WALL CLOCK TIME: STEP = 78.31 , TOTAL = 5153.3 SECONDS (85.9
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.72 , TOTAL = 5577.6 SECONDS (93.0 MIN)
WALL CLOCK TIME: STEP = 3.71 , TOTAL = 5157.0 SECONDS (86.0
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.

USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.04 , TOTAL = 5580.6 SECONDS (93.0 MIN)
WALL CLOCK TIME: STEP = 2.86 , TOTAL = 5159.9 SECONDS (86.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 56 ENERGY= -284.6356028

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0012711	-0.0001811	0.0009673
2 C	6.0	0.0002208	-0.0009600	-0.0002156
3 C	6.0	-0.0004472	0.0005771	-0.0001451
4 C	6.0	-0.0000484	0.0007607	-0.0003800
5 C	6.0	-0.0004946	0.0005080	0.0002482
6 C	6.0	-0.0001840	-0.0002746	-0.0000566
7 C	6.0	0.0001357	-0.0004812	-0.0002687
8 C	6.0	0.0009400	0.0001876	-0.0005555
9 C	6.0	-0.0000899	0.0002711	0.0004228
10 C	6.0	0.0005215	-0.0000305	0.0009234
11 C	6.0	-0.0001431	0.0002226	0.0001742
12 N	7.0	0.0003162	-0.0000585	-0.0006388
13 C	6.0	0.0001943	-0.0002398	-0.0003236
14 C	6.0	0.0000855	-0.0005747	-0.0007063
15 C	6.0	-0.0006891	-0.0003520	-0.0014243
16 C	6.0	-0.0003899	0.0001383	-0.0009078
17 C	6.0	-0.0001219	0.0009213	-0.0002816
18 C	6.0	0.0000770	-0.0012367	0.0004586
19 C	6.0	0.0000876	0.0001573	0.0000250
20 O	8.0	-0.0007910	0.0000031	0.0006301
21 N	7.0	-0.0008513	-0.0005104	-0.0015444
22 H	1.0	-0.0005734	0.0005853	0.0000335
23 H	1.0	0.0009604	-0.0003145	0.0009613
24 H	1.0	-0.0003652	0.0010518	0.0005147
25 H	1.0	0.0001301	-0.0000618	-0.0013850
26 H	1.0	0.0001380	-0.0006519	-0.0002719
27 H	1.0	0.0002957	-0.0007171	0.0002425
28 H	1.0	0.0002014	-0.0001664	0.0000190
29 H	1.0	-0.0002862	0.0002070	-0.0003750

30 H	1.0	0.0003189	0.0002460	0.0007709
31 H	1.0	0.0002393	-0.0002161	0.0003877
32 H	1.0	0.0000294	-0.0001785	0.0008126
33 H	1.0	0.0000941	-0.0000005	0.0000872
34 H	1.0	0.0017198	-0.0001599	0.0022823
35 H	1.0	0.0000407	0.0015291	-0.0004811

MAXIMUM GRADIENT = 0.0022823 RMS GRADIENT = 0.0006244
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000835662
 PREDICTED ENERGY CHANGE WAS -0.0000664790 RATIO= 1.257
 GDIIS STEP HAS LENGTH = 0.199549
 RADIUS OF STEP TAKEN= 0.17261 CURRENT TRUST RADIUS= 0.17261

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 5580.6 SECONDS (93.0 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5159.9 SECONDS (86.0 MIN)
 CPU UTILIZATION: STEP = 92.05% , TOTAL = 100.00%

INSERCH= 57

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1362345744	-1.7688850885	0.9132186814
C	6.0	4.9875595046	0.6669155285	0.4988976829
C	6.0	5.2062394429	-0.6924296544	0.2447277976
C	6.0	4.0746660029	-1.5380468561	0.0102243210
C	6.0	2.7617507108	-1.0378081748	0.0771665765
C	6.0	2.4765376583	0.3402131536	0.4465670692
C	6.0	3.6515575521	1.2036472917	0.6081000576
C	6.0	3.4947919864	2.6079224722	0.9032996728
C	6.0	2.2251352753	3.1547366668	1.1401482987
C	6.0	1.0721821835	2.3109101830	1.0686669490
C	6.0	1.1677410083	0.9534545157	0.6807439504
N	7.0	-0.0425155664	0.1433280848	0.6399335452
C	6.0	-1.2367872581	0.6738250189	0.3749832118
C	6.0	-2.5507293589	0.0261419284	0.4569731239
C	6.0	-2.8498337890	-1.3315369411	0.8233644746
C	6.0	-4.1600430212	-1.8378363203	0.9016902175
C	6.0	-5.2548646533	-0.9599810828	0.6371548180
C	6.0	-5.0152865787	0.3966050426	0.2818789003
C	6.0	-3.6864581604	0.8749630455	0.1854012858
O	8.0	-1.7472705726	-2.2307289741	1.1712529137

N	7.0	1.6676358469	-1.9960256163	-0.3255466648
H	1.0	5.8367493513	1.3594900031	0.6421072517
H	1.0	6.2286552979	-1.1114789832	0.2033273624
H	1.0	4.2423654665	-2.5989612952	-0.2577751411
H	1.0	4.4010835172	3.2377031856	0.9581886951
H	1.0	2.1091184736	4.2178911413	1.4131311201
H	1.0	0.0943733372	2.7324353772	1.3585694956
H	1.0	-1.2721659746	1.7319792367	0.0489901896
H	1.0	-4.3539187789	-2.8921960813	1.1787366505
H	1.0	-6.2873889788	-1.3440636883	0.7226874402
H	1.0	-5.8626546972	1.0770860564	0.0866070228
H	1.0	-3.5042131287	1.9325489739	-0.0827879758
H	1.0	-2.0870671250	-3.0869554259	1.5394744751
H	1.0	1.3303721831	-1.7471203830	-1.2803028770
H	1.0	2.0824452687	-2.9466373407	-0.4069135921

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4442759	5.2259531	4.0472123
2 C	5.4442759	0.0000000	1.4000866 *	2.4359875 *
3 C	5.2259531	1.4000866 *	0.0000000	1.4319633 *
4 C	4.0472123	2.4359875 *	1.4319633 *	0.0000000
5 C	2.8507528 *	2.8351657 *	2.4744471 *	1.4065797 *
6 C	3.1848199	2.5327265 *	2.9254678 *	2.5044500 *
7 C	4.6137340	1.4439208 *	2.4787462 *	2.8378448 *
8 C	5.5169240	2.4818146 *	3.7755918	4.2805256
9 C	5.3532284	3.7724586	4.9486815	5.1691111
10 C	4.1886623	4.2845694	5.1758434	4.9949655
11 C	2.9204765 *	3.8348645	4.3827519	3.8868224
12 N	1.9398958 *	5.0592183	5.3295504	4.4916299
13 C	2.8533698 *	6.2255839	6.5875801	5.7651506
14 C	3.2634425	7.5655897	7.7930712	6.8221796
15 C	3.0192634	8.0946788	8.1020735	6.9751373
16 C	4.2968463	9.4928739	9.4589007	8.2882458
17 C	5.4584327	10.3717482	10.4718805	9.3684227
18 C	5.6237094	10.0088508	10.2794441	9.2975218
19 C	4.7045330	8.6821740	9.0299673	8.1294743
20 O	1.9563929 *	7.3624956	7.1816513	5.9768505
21 N	1.9827562 *	4.3350729	3.8139600	2.4731116 *
22 H	6.5081565	1.1051207 *	2.1830775 *	3.4496280
23 H	6.1687696	2.1886908 *	1.1057353 *	2.2042955 *
24 H	4.3497775	3.4342131	2.1946355 *	1.1070168 *
25 H	6.5769967	2.6765372 *	4.0747082	4.8798538

26 H	6.3232644	4.6616170	5.9218726	6.2419826
27 H	4.5234915	5.3803976	6.2531207	5.9914759
28 H	3.8712445	6.3656061	6.9199573	6.2676300
29 H	4.6361411	10.0196144	9.8543376	8.6162743
30 H	6.4404747	11.4550680	11.5220036	10.3883308
31 H	6.6910022	10.8657890	11.2105578	10.2759475
32 H	5.2863506	8.6052536	9.1032831	8.3362519
33 H	2.6594316 *	8.0761804	7.7847571	6.5348817
34 H	2.4975939 *	4.7294971	4.2965612	3.0397896
35 H	2.6301303 *	4.7241875	3.9069398	2.4752928 *

C C C C

1 CO	2.8507528 *	3.1848199	4.6137340	5.5169240
2 C	2.8351657 *	2.5327265 *	1.4439208 *	2.4818146 *
3 C	2.4744471 *	2.9254678 *	2.4787462 *	3.7755918
4 C	1.4065797 *	2.5044500 *	2.8378448 *	4.2805256
5 C	0.0000000	1.4549041 *	2.4693662 *	3.8093566
6 C	1.4549041 *	0.0000000	1.4670662 *	2.5274398 *
7 C	2.4693662 *	1.4670662 *	0.0000000	1.4435051 *
8 C	3.8093566	2.5274398 *	1.4435051 *	0.0000000
9 C	4.3583619	2.9096049 *	2.4747738 *	1.4025445 *
10 C	3.8796430	2.4985735 *	2.8445264 *	2.4463444 *
11 C	2.6211257 *	1.4641900 *	2.4974423 *	2.8639067 *
12 N	3.0944626	2.5341238 *	3.8433665	4.3192745
13 C	4.3596661	3.7289681	4.9224963	5.1388416
14 C	5.4312694	5.0370788	6.3148809	6.5888638
15 C	5.6685949	5.5952621	6.9815175	7.4686014
16 C	7.0164886	6.9996600	8.3879629	8.8521903
17 C	8.0365270	7.8422835	9.1655054	9.4528969
18 C	7.9108633	7.4938463	8.7104492	8.8146200
19 C	6.7267976	6.1916623	7.3575255	7.4221884
20 O	4.7907575	4.9975463	6.4233501	7.1388771
21 N	1.5091209 *	2.5900759 *	3.8788591	5.1034205
22 H	3.9397732	3.5168429	2.1910059 *	2.6667526 *
23 H	3.4699815	4.0305040	3.4878480	4.6688239
24 H	2.1775227 *	3.5004274	3.9444424	5.3868914
25 H	4.6630043	3.5158330	2.1958449 *	1.1049891 *
26 H	5.4619690	4.0131820	3.4803533	2.1844950 *
27 H	4.7928730	3.4970248	3.9438505	3.4330192
28 H	4.8933629	4.0184399	4.9834518	4.9214845
29 H	7.4353859	7.5920799	9.0105056	9.5879836
30 H	9.0773024	8.9285744	10.2609268	10.5518662
31 H	8.8799344	8.3794202	9.5293341	9.5169457
32 H	6.9362028	6.2116930	7.2259033	7.1003219
33 H	5.4633674	5.8108880	7.2255479	7.9995940

34 H	2.0963520 *	2.9415534 *	4.2024989	5.3309691
35 H	2.0831270 *	3.4186436	4.5516182	5.8791595

	C	C	C	N
--	---	---	---	---

1 CO	5.3532284	4.1886623	2.9204765 *	1.9398958 *
2 C	3.7724586	4.2845694	3.8348645	5.0592183
3 C	4.9486815	5.1758434	4.3827519	5.3295504
4 C	5.1691111	4.9949655	3.8868224	4.4916299
5 C	4.3583619	3.8796430	2.6211257 *	3.0944626
6 C	2.9096049 *	2.4985735 *	1.4641900 *	2.5341238 *
7 C	2.4747738 *	2.8445264 *	2.4974423 *	3.8433665
8 C	1.4025445 *	2.4463444 *	2.8639067 *	4.3192745
9 C	0.0000000	1.4305431 *	2.4849101 *	3.8027670
10 C	1.4305431 *	0.0000000	1.4150271 *	2.4748284 *
11 C	2.4849101 *	1.4150271 *	0.0000000	1.4569459 *
12 N	3.8027670	2.4748284 *	1.4569459 *	0.0000000
13 C	4.3272749	2.9142040 *	2.4399669 *	1.3333831 *
14 C	5.7501058	4.3266411	3.8388806	2.5176067 *
15 C	6.7810260	5.3581530	4.6241144	3.1764618
16 C	8.1088316	6.6795329	6.0187544	4.5768506
17 C	8.5518597	7.1355766	6.7017161	5.3278403
18 C	7.7953592	6.4296870	6.2208524	4.9920741
19 C	6.4074836	5.0484414	4.8800384	3.7443567
20 O	6.6921010	5.3466180	4.3447573	2.9706290 *
21 N	5.3841823	4.5659712	3.1562555	2.9040668 *
22 H	4.0638297	4.8773204	4.6867896	6.0037330
23 H	5.9250656	6.2490619	5.4867778	6.4103627
24 H	6.2552736	5.9930250	4.7910116	5.1658724
25 H	2.1851186 *	3.4572727	3.9685352	5.4242065
26 H	1.1037558 *	2.1978328 *	3.4755041	4.6721973
27 H	2.1831612 *	1.1035566 *	2.1854836 *	2.6904745 *
28 H	3.9301375	2.6212344 *	2.6378703 *	2.0940551 *
29 H	8.9359296	7.5184441	6.7472774	5.3002748
30 H	9.6372479	8.2244649	7.8012379	6.4200955
31 H	8.4165865	7.1118722	7.0565393	5.9204809
32 H	5.9845425	4.7341736	4.8341248	3.9632042
33 H	7.5969251	6.2721184	5.2589074	3.9273524
34 H	5.5396198	4.6959486	3.3414455	3.0242229
35 H	6.2960722	5.5533571	4.1509516	3.8934861

	C	C	C	C
--	---	---	---	---

1 CO	2.8533698 *	3.2634425	3.0192634	4.2968463
2 C	6.2255839	7.5655897	8.0946788	9.4928739
3 C	6.5875801	7.7930712	8.1020735	9.4589007

4 C	5.7651506	6.8221796	6.9751373	8.2882458
5 C	4.3596661	5.4312694	5.6685949	7.0164886
6 C	3.7289681	5.0370788	5.5952621	6.9996600
7 C	4.9224963	6.3148809	6.9815175	8.3879629
8 C	5.1388416	6.5888638	7.4686014	8.8521903
9 C	4.3272749	5.7501058	6.7810260	8.1088316
10 C	2.9142040 *	4.3266411	5.3581530	6.6795329
11 C	2.4399669 *	3.8388806	4.6241144	6.0187544
12 N	1.3333831 *	2.5176067 *	3.1764618	4.5768506
13 C	0.0000000	1.4671945 *	2.6123632 *	3.8898955
14 C	1.4671945 *	0.0000000	1.4377058 *	2.5024146 *
15 C	2.6123632 *	1.4377058 *	0.0000000	1.4068128 *
16 C	3.8898955	2.5024146 *	1.4068128 *	0.0000000
17 C	4.3454577	2.8839646 *	2.4406764 *	1.4280207 *
18 C	3.7897990	2.4983881 *	2.8229182 *	2.4715048 *
19 C	2.4652151 *	1.4436511 *	2.4444999 *	2.8454583 *
20 O	3.0546804	2.4998416 *	1.4646564 *	2.4593698 *
21 N	4.0068090	4.7430058	4.7084046	5.9575981
22 H	7.1117095	8.4948155	9.0956697	10.4988636
23 H	7.6778649	8.8564165	9.1022984	10.4374498
24 H	6.4134724	7.3176615	7.2852260	8.5161106
25 H	6.2208670	7.6741804	8.5715771	9.9527474
26 H	4.9832962	6.3402824	7.4656001	8.7313111
27 H	2.6414593 *	3.8901759	5.0468476	6.2606853
28 H	1.1077967 *	2.1704966 *	3.5318299	4.6701728
29 H	4.8040644	3.5055857	2.1964103 *	1.1072565 *
30 H	5.4498946	3.9888210	3.4390520	2.1912221 *
31 H	4.6523575	3.4943532	3.9270047	3.4727539
32 H	2.6334693 *	2.1988318 *	3.4501567	3.9515966
33 H	4.0277147	3.3283880	2.0435559 *	2.5028576 *
34 H	3.8975962	4.6071180	4.6981111	5.9088055
35 H	4.9735716	5.5722548	5.3338082	6.4738353

C C C O

1 CO	5.4584327	5.6237094	4.7045330	1.9563929 *
2 C	10.3717482	10.0088508	8.6821740	7.3624956
3 C	10.4718805	10.2794441	9.0299673	7.1816513
4 C	9.3684227	9.2975218	8.1294743	5.9768505
5 C	8.0365270	7.9108633	6.7267976	4.7907575
6 C	7.8422835	7.4938463	6.1916623	4.9975463
7 C	9.1655054	8.7104492	7.3575255	6.4233501
8 C	9.4528969	8.8146200	7.4221884	7.1388771
9 C	8.5518597	7.7953592	6.4074836	6.6921010
10 C	7.1355766	6.4296870	5.0484414	5.3466180
11 C	6.7017161	6.2208524	4.8800384	4.3447573

12 N	5.3278403	4.9920741	3.7443567	2.9706290 *
13 C	4.3454577	3.7897990	2.4652151 *	3.0546804
14 C	2.8839646 *	2.4983881 *	1.4436511 *	2.4998416 *
15 C	2.4406764 *	2.8229182 *	2.4444999 *	1.4646564 *
16 C	1.4280207 *	2.4715048 *	2.8454583 *	2.4593698 *
17 C	0.0000000	1.4226541 *	2.4558095 *	3.7687236
18 C	1.4226541 *	0.0000000	1.4155986 *	4.2864669
19 C	2.4558095 *	1.4155986 *	0.0000000	3.7917905
20 O	3.7687236	4.2864669	3.7917905	0.0000000
21 N	7.0654933	7.1242613	6.0967177	3.7359176
22 H	11.3315432	10.9006236	9.5464563	8.4075577
23 H	11.4927102	11.3448983	10.1121584	8.1120277
24 H	9.6790772	9.7451919	8.6678025	6.1687483
25 H	10.5338004	9.8588670	8.4609735	8.2311241
26 H	9.0355270	8.1632779	6.8022935	7.5176421
27 H	6.5397802	5.7204887	4.3727810	5.2971445
28 H	4.8429822	3.9810066	2.5655197 *	4.1458720
29 H	2.1996521 *	3.4724594	3.9526835	2.6892768 *
30 H	1.1049623 *	2.2005645 *	3.4608665	4.6475866
31 H	2.1959404 *	1.1041822 *	2.1877946 *	5.3902211
32 H	3.4568524	2.1852800 *	1.1061766 *	4.6896001
33 H	3.9208598	4.7213567	4.4820044	0.9920547 *
34 H	6.9037364	6.8777435	5.8474094	3.9643269
35 H	7.6728742	7.8758810	6.9451935	4.2035530

N H H H

1 CO	1.9827562 *	6.5081565	6.1687696	4.3497775
2 C	4.3350729	1.1051207 *	2.1886908 *	3.4342131
3 C	3.8139600	2.1830775 *	1.1057353 *	2.1946355 *
4 C	2.4731116 *	3.4496280	2.2042955 *	1.1070168 *
5 C	1.5091209 *	3.9397732	3.4699815	2.1775227 *
6 C	2.5900759 *	3.5168429	4.0305040	3.5004274
7 C	3.8788591	2.1910059 *	3.4878480	3.9444424
8 C	5.1034205	2.6667526 *	4.6688239	5.3868914
9 C	5.3841823	4.0638297	5.9250656	6.2552736
10 C	4.5659712	4.8773204	6.2490619	5.9930250
11 C	3.1562555	4.6867896	5.4867778	4.7910116
12 N	2.9040668 *	6.0037330	6.4103627	5.1658724
13 C	4.0068090	7.1117095	7.6778649	6.4134724
14 C	4.7430058	8.4948155	8.8564165	7.3176615
15 C	4.7084046	9.0956697	9.1022984	7.2852260
16 C	5.9575981	10.4988636	10.4374498	8.5161106
17 C	7.0654933	11.3315432	11.4927102	9.6790772
18 C	7.1242613	10.9006236	11.3448983	9.7451919
19 C	6.0967177	9.5464563	10.1121584	8.6678025

20	O	3.7359176	8.4075577	8.1120277	6.1687483
21	N	0.0000000	5.4385059	4.6760057	2.6452518 *
22	H	5.4385059	0.0000000	2.5400405 *	4.3613283
23	H	4.6760057	2.5400405 *	0.0000000	2.5239981 *
24	H	2.6452518 *	4.3613283	2.5239981 *	0.0000000
25	H	6.0424854	2.3851056 *	4.7775747	5.9640935
26	H	6.4676633	4.7602696	6.8437121	7.3356764
27	H	5.2602039	5.9475356	7.3307351	6.9456605
28	H	4.7624293	7.1433335	8.0231786	7.0186329
29	H	6.2709736	11.0550677	10.7755859	8.7204160
30	H	8.0502341	12.4221748	12.5289742	10.6494978
31	H	8.1436578	11.7159885	12.2883367	10.7584086
32	H	6.4992809	9.3865569	10.2017987	8.9763403
33	H	4.3320002	9.1303347	8.6509558	6.5977240
34	H	1.0427176 *	5.8012175	5.1573614	3.2017028
35	H	1.0403606 *	5.8084401	4.5750692	2.1928010 *

H H H H

1	CO	6.5769967	6.3232644	4.5234915	3.8712445
2	C	2.6765372 *	4.6616170	5.3803976	6.3656061
3	C	4.0747082	5.9218726	6.2531207	6.9199573
4	C	4.8798538	6.2419826	5.9914759	6.2676300
5	C	4.6630043	5.4619690	4.7928730	4.8933629
6	C	3.5158330	4.0131820	3.4970248	4.0184399
7	C	2.1958449 *	3.4803533	3.9438505	4.9834518
8	C	1.1049891 *	2.1844950 *	3.4330192	4.9214845
9	C	2.1851186 *	1.1037558 *	2.1831612 *	3.9301375
10	C	3.4572727	2.1978328 *	1.1035566 *	2.6212344 *
11	C	3.9685352	3.4755041	2.1854836 *	2.6378703 *
12	N	5.4242065	4.6721973	2.6904745 *	2.0940551 *
13	C	6.2208670	4.9832962	2.6414593 *	1.1077967 *
14	C	7.6741804	6.3402824	3.8901759	2.1704966 *
15	C	8.5715771	7.4656001	5.0468476	3.5318299
16	C	9.9527474	8.7313111	6.2606853	4.6701728
17	C	10.5338004	9.0355270	6.5397802	4.8429822
18	C	9.8588670	8.1632779	5.7204887	3.9810066
19	C	8.4609735	6.8022935	4.3727810	2.5655197 *
20	O	8.2311241	7.5176421	5.2971445	4.1458720
21	N	6.0424854	6.4676633	5.2602039	4.7624293
22	H	2.3851056 *	4.7602696	5.9475356	7.1433335
23	H	4.7775747	6.8437121	7.3307351	8.0231786
24	H	5.9640935	7.3356764	6.9456605	7.0186329
25	H	0.0000000	2.5339386 *	4.3546932	5.9396638
26	H	2.5339386 *	0.0000000	2.5037479 *	4.4129041
27	H	4.3546932	2.5037479 *	0.0000000	2.1408737 *

28 H	5.9396638	4.4129041	2.1408737 *	0.0000000
29 H	10.6899192	9.6114063	7.1732922	5.6706723
30 H	11.6314871	10.0952163	7.5992816	5.9218553
31 H	10.5248393	8.6702647	6.3122304	4.6371205
32 H	8.0796519	6.2426000	3.9581756	2.2449116 *
33 H	9.0793887	8.4252430	6.2174527	5.1095732
34 H	6.2680602	6.5910845	5.3439461	4.5436064
35 H	6.7443054	7.3921406	6.2706640	5.7750080

H H H H

1 CO	4.6361411	6.4404747	6.6910022	5.2863506
2 C	10.0196144	11.4550680	10.8657890	8.6052536
3 C	9.8543376	11.5220036	11.2105578	9.1032831
4 C	8.6162743	10.3883308	10.2759475	8.3362519
5 C	7.4353859	9.0773024	8.8799344	6.9362028
6 C	7.5920799	8.9285744	8.3794202	6.2116930
7 C	9.0105056	10.2609268	9.5293341	7.2259033
8 C	9.5879836	10.5518662	9.5169457	7.1003219
9 C	8.9359296	9.6372479	8.4165865	5.9845425
10 C	7.5184441	8.2244649	7.1118722	4.7341736
11 C	6.7472774	7.8012379	7.0565393	4.8341248
12 N	5.3002748	6.4200955	5.9204809	3.9632042
13 C	4.8040644	5.4498946	4.6523575	2.6334693 *
14 C	3.5055857	3.9888210	3.4943532	2.1988318 *
15 C	2.1964103 *	3.4390520	3.9270047	3.4501567
16 C	1.1072565 *	2.1912221 *	3.4727539	3.9515966
17 C	2.1996521 *	1.1049623 *	2.1959404 *	3.4568524
18 C	3.4724594	2.2005645 *	1.1041822 *	2.1852800 *
19 C	3.9526835	3.4608665	2.1877946 *	1.1061766 *
20 O	2.6892768 *	4.6475866	5.3902211	4.6896001
21 N	6.2709736	8.0502341	8.1436578	6.4992809
22 H	11.0550677	12.4221748	11.7159885	9.3865569
23 H	10.7755859	12.5289742	12.2883367	10.2017987
24 H	8.7204160	10.6494978	10.7584086	8.9763403
25 H	10.6899192	11.6314871	10.5248393	8.0796519
26 H	9.6114063	10.0952163	8.6702647	6.2426000
27 H	7.1732922	7.5992816	6.3122304	3.9581756
28 H	5.6706723	5.9218553	4.6371205	2.2449116 *
29 H	0.0000000	2.5185317 *	4.3845447	5.0588150
30 H	2.5185317 *	0.0000000	2.5390872 *	4.3739055
31 H	4.3845447	2.5390872 *	0.0000000	2.5145095 *
32 H	5.0588150	4.3739055	2.5145095 *	0.0000000
33 H	2.3036231 *	4.6203373	5.8056117	5.4621848
34 H	6.2983520	7.8869963	7.8475614	6.1925135
35 H	6.6290295	8.5964159	8.9195586	7.4244373

	H	H	H
1 CO	2.6594316 *	2.4975939 *	2.6301303 *
2 C	8.0761804	4.7294971	4.7241875
3 C	7.7847571	4.2965612	3.9069398
4 C	6.5348817	3.0397896	2.4752928 *
5 C	5.4633674	2.0963520 *	2.0831270 *
6 C	5.8108880	2.9415534 *	3.4186436
7 C	7.2255479	4.2024989	4.5516182
8 C	7.9995940	5.3309691	5.8791595
9 C	7.5969251	5.5396198	6.2960722
10 C	6.2721184	4.6959486	5.5533571
11 C	5.2589074	3.3414455	4.1509516
12 N	3.9273524	3.0242229	3.8934861
13 C	4.0277147	3.8975962	4.9735716
14 C	3.3283880	4.6071180	5.5722548
15 C	2.0435559 *	4.6981111	5.3338082
16 C	2.5028576 *	5.9088055	6.4738353
17 C	3.9208598	6.9037364	7.6728742
18 C	4.7213567	6.8777435	7.8758810
19 C	4.4820044	5.8474094	6.9451935
20 O	0.9920547 *	3.9643269	4.2035530
21 N	4.3320002	1.0427176 *	1.0403606 *
22 H	9.1303347	5.8012175	5.8084401
23 H	8.6509558	5.1573614	4.5750692
24 H	6.5977240	3.2017028	2.1928010 *
25 H	9.0793887	6.2680602	6.7443054
26 H	8.4252430	6.5910845	7.3921406
27 H	6.2174527	5.3439461	6.2706640
28 H	5.1095732	4.5436064	5.7750080
29 H	2.3036231 *	6.2983520	6.6290295
30 H	4.6203373	7.8869963	8.5964159
31 H	5.8056117	7.8475614	8.9195586
32 H	5.4621848	6.1925135	7.4244373
33 H	0.0000000	4.6287356	4.6035800
34 H	4.6287356	0.0000000	1.6635095 *
35 H	4.6035800	1.6635095 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.77 , TOTAL = 5581.4 SECONDS (93.0 MIN)

WALL CLOCK TIME: STEP = 0.78 , TOTAL = 5160.7 SECONDS (86.0 MIN)

CPU UTILIZATION: STEP = 99.35%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.38 , TOTAL = 5582.8 SECONDS (93.0 MIN)

WALL CLOCK TIME: STEP = 1.37 , TOTAL = 5162.0 SECONDS (86.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.635171195 -284.635171195 0.019751464 0.002167262 197179259
11388467

2 1 -284.635686207 -0.000515013 0.003589027 0.000203104 162624844
14361347

3 2 -284.635687140 -0.000000933 0.001813703 0.000321614 148882799
15486138

4 3 -284.635694017 -0.000006877 0.001065840 0.000251987 142145527
15995049

5 4 -284.635693116 0.000000902 0.000787701 0.000364077 139337126
16276857

6 5 -284.635695123 -0.000002008 0.000456939 0.000053015 133792593
16678626

7 6 -284.635695142 -0.000000019 0.000443779 0.000062485 131168144
16834505

8 7 -284.635695367 -0.000000225 0.000340254 0.000036580 123658295
17409898

9 8 -284.635695470 -0.000000103 0.000383960 0.000035136 124286461
17417679

10 9 -284.635695574 -0.000000104 0.000538494 0.000038759 143307998
16087209

11 10 -284.635695655 -0.000000081 0.000309192 0.000040557 166991767
14085901

12 11 -284.635695721 -0.000000066 0.000494775 0.000035096 161655802
14526665

-----DISABLING FDIFF OPTION-----

13 12 -284.635695777 -0.000000056 0.000573971 0.000020844 197160381
11390208

14 13 -284.635695831 -0.000000054 0.000244384 0.000016133 197159945
11390216

15 14	-284.635695847	-0.000000016	0.000110441	0.000008828	197160125
11390206					
16 15	-284.635695856	-0.000000009	0.000076710	0.000007115	197159965
11390210					
17 16	-284.635695860	-0.000000004	0.000081462	0.000006422	197159995
11390211					
18 17	-284.635695864	-0.000000003	0.000096099	0.000005174	197160005
11390219					
19 18	-284.635695866	-0.000000003	0.000048300	0.000003209	197159945
11390213					
20 19	-284.635695867	-0.000000001	0.000030346	0.000003566	197160038
11390209					
21 20	-284.635695868	-0.000000001	0.000050091	0.000003194	197159938
11390212					
22 21	-284.635695869	-0.000000001	0.000047012	0.000003020	197159951
11390213					
23 22	-284.635695869	-0.000000001	0.000036610	0.000003189	197159954
11390212					
24 23	-284.635695870	0.000000000	0.000106170	0.000003160	197159933
11390215					
25 24	-284.635695871	-0.000000001	0.000060389	0.000002387	197159975
11390217					
26 25	-284.635695871	-0.000000001	0.000052205	0.000001909	197159979
11390215					
27 26	-284.635695872	0.000000000	0.000023349	0.000001210	197159921
11390217					
28 27	-284.635695872	0.000000000	0.000006551	0.000000628	197159927
11390215					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 95.2 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 30.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.9 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6356958717 AFTER 28 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6018531218
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999650704

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 99.38 , TOTAL = 5682.1 SECONDS (94.7 MIN)
WALL CLOCK TIME: STEP = 90.83 , TOTAL = 5252.9 SECONDS (87.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.75 , TOTAL = 5685.9 SECONDS (94.8 MIN)
WALL CLOCK TIME: STEP = 3.71 , TOTAL = 5256.6 SECONDS (87.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.88 , TOTAL = 5688.8 SECONDS (94.8 MIN)
WALL CLOCK TIME: STEP = 2.69 , TOTAL = 5259.3 SECONDS (87.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 57 ENERGY= -284.6356959

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0012741	-0.0003318	0.0008568
2 C	6.0	-0.0002635	-0.0013637	-0.0003255
3 C	6.0	-0.0008081	0.0007811	-0.0000890
4 C	6.0	-0.0000074	0.0011625	-0.0000895
5 C	6.0	-0.0000795	0.0000184	0.0003148
6 C	6.0	-0.0003131	0.0001966	0.0000664
7 C	6.0	0.0002544	-0.0002240	-0.0003164
8 C	6.0	0.0012805	0.0002968	-0.0005839
9 C	6.0	-0.0002221	0.0003845	0.0003935

10 C	6.0	0.0002548	0.0000125	0.0008102
11 C	6.0	0.0000664	-0.0001198	0.0000840
12 N	7.0	0.0004104	0.0001929	-0.0004108
13 C	6.0	0.0003865	-0.0003475	-0.0003936
14 C	6.0	0.0003807	-0.0003411	-0.0008580
15 C	6.0	-0.0003534	-0.0007531	-0.0015498
16 C	6.0	-0.0002813	-0.0000813	-0.0010221
17 C	6.0	-0.0002097	0.0001970	-0.0001031
18 C	6.0	0.0004120	-0.0002903	0.0005175
19 C	6.0	-0.0000393	0.0000448	0.0002386
20 O	8.0	-0.0008015	0.0004133	0.0005033
21 N	7.0	-0.0008852	0.0006359	-0.0003766
22 H	1.0	-0.0005344	0.0006779	0.0001873
23 H	1.0	0.0010644	-0.0005259	0.0007847
24 H	1.0	-0.0006193	0.0005536	0.0003407
25 H	1.0	0.0001929	-0.0000973	-0.0014393
26 H	1.0	0.0001586	-0.0004031	-0.0000523
27 H	1.0	0.0002481	-0.0007929	0.0003570
28 H	1.0	-0.0000595	-0.0001979	-0.0001557
29 H	1.0	-0.0003459	-0.0002570	-0.0000741
30 H	1.0	0.0001462	0.0001767	0.0007313
31 H	1.0	-0.0001351	-0.0001015	0.0002358
32 H	1.0	0.0000041	0.0003820	0.0006263
33 H	1.0	-0.0002412	-0.0000642	0.0002908
34 H	1.0	0.0012101	0.0002022	0.0011062
35 H	1.0	0.0010034	-0.0000363	-0.0006052

MAXIMUM GRADIENT = 0.0015498 RMS GRADIENT = 0.0005547
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000930911
 PREDICTED ENERGY CHANGE WAS -0.0000544112 RATIO= 1.711
 GDIIS STEP HAS LENGTH = 0.166856
 RADIUS OF STEP TAKEN= 0.16686 CURRENT TRUST RADIUS= 0.17261

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 5688.8 SECONDS (94.8 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5259.3 SECONDS (87.7
 MIN)
 CPU UTILIZATION: STEP = 92.39% , TOTAL = 100.00%

1NSERCH= 58

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z

CO	27.0	0.1400408295	-1.7667263643	0.8999573489
C	6.0	4.9849564614	0.6629678389	0.5048263231
C	6.0	5.2019311937	-0.6963653811	0.2437086665
C	6.0	4.0713058194	-1.5411571130	0.0054112075
C	6.0	2.7599821983	-1.0369475933	0.0705693651
C	6.0	2.4754609249	0.3416610731	0.4428963069
C	6.0	3.6501805129	1.2034528685	0.6123473752
C	6.0	3.4939637151	2.6061808434	0.9156342273
C	6.0	2.2247697982	3.1545293721	1.1493753177
C	6.0	1.0704211307	2.3121834853	1.0665885576
C	6.0	1.1672509678	0.9563671949	0.6746684935
N	7.0	-0.0434252962	0.1470892660	0.6325009792
C	6.0	-1.2370973529	0.6763886487	0.3630026243
C	6.0	-2.5501000857	0.0290381074	0.4505324829
C	6.0	-2.8445025484	-1.3260120532	0.8291482416
C	6.0	-4.1530148989	-1.8366839581	0.9134476892
C	6.0	-5.2510699712	-0.9642841584	0.6426598691
C	6.0	-5.0164831839	0.3919803711	0.2779938538
C	6.0	-3.6887737575	0.8730349560	0.1741189160
O	8.0	-1.7401536333	-2.2200972957	1.1816590622
N	7.0	1.6682824553	-1.9952550099	-0.3383702958
H	1.0	5.8367268078	1.3507471373	0.6553619375
H	1.0	6.2231590519	-1.1161817084	0.1959999821
H	1.0	4.2346933714	-2.6021252735	-0.2688626855
H	1.0	4.4024439276	3.2336327551	0.9811119217
H	1.0	2.1101355126	4.2157994122	1.4335031156
H	1.0	0.0919846446	2.7323189875	1.3583451973
H	1.0	-1.2747876735	1.7323687618	0.0289188621
H	1.0	-4.3423982128	-2.8890558284	1.1998077700
H	1.0	-6.2828263288	-1.3501242044	0.7280572258
H	1.0	-5.8674847798	1.0663764006	0.0782659824
H	1.0	-3.5103938647	1.9284293901	-0.1065947332
H	1.0	-2.0821101962	-3.0628226184	1.5781271832
H	1.0	1.3280200817	-1.7445292523	-1.2930881997
H	1.0	2.0849093792	-2.9450740579	-0.4187431712

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4344043	5.2152727	4.0380613
2 C	5.4344043	0.0000000	1.4010879 *	2.4376915 *
3 C	5.2152727	1.4010879 *	0.0000000	1.4313534 *
4 C	4.0380613	2.4376915 *	1.4313534 *	0.0000000
5 C	2.8433351 *	2.8335141 *	2.4716570 *	1.4064290 *

6 C	3.1793693	2.5307393 *	2.9241776 *	2.5066149 *
7 C	4.6071428	1.4440608 *	2.4805512 *	2.8422882 *
8 C	5.5110219	2.4835256 *	3.7782864	4.2851187
9 C	5.3504264	3.7738512	4.9510718	5.1737627
10 C	4.1869893	4.2847492	5.1766662	4.9979636
11 C	2.9191016 *	3.8327281	4.3813121	3.8883245
12 N	1.9411036 *	5.0563875	5.3269447	4.4915954
13 C	2.8554581 *	6.2236844	6.5848138	5.7640719
14 C	3.2655185	7.5618709	7.7886440	6.8195793
15 C	3.0177379	8.0846555	8.0922364	6.9680152
16 C	4.2936469	9.4824971	9.4479571	8.2795723
17 C	5.4565732	10.3654804	10.4640420	9.3619207
18 C	5.6246416	10.0076812	10.2762670	9.2951187
19 C	4.7069101	8.6825740	9.0284270	8.1286912
20 O	1.9544903 *	7.3482837	7.1689645	5.9680466
21 N	1.9802028 *	4.3332962	3.8095411	2.4695975 *
22 H	6.4985151	1.1050855 *	2.1824513 *	3.4499648
23 H	6.1581728	2.1894959 *	1.1051824 *	2.2016813 *
24 H	4.3393791	3.4383604	2.1977714 *	1.1079599 *
25 H	6.5710165	2.6785233 *	4.0777235	4.8846968
26 H	6.3211201	4.6636518	5.9248776	6.2472541
27 H	4.5225919	5.3806953	6.2537864	5.9939991
28 H	3.8735145	6.3682417	6.9204604	6.2687511
29 H	4.6305284	10.0049696	9.8395244	8.6042914
30 H	6.4386590	11.4483755	11.5135420	10.3810772
31 H	6.6926835	10.8683105	11.2101115	10.2754123
32 H	5.2908408	8.6108191	9.1058700	8.3386297
33 H	2.6604013 *	8.0608263	7.7741914	6.5309594
34 H	2.4942406 *	4.7330458	4.2973922	3.0418872
35 H	2.6286856 *	4.7202987	3.9001741	2.4691417 *

C C C C

1 CO	2.8433351 *	3.1793693	4.6071428	5.5110219
2 C	2.8335141 *	2.5307393 *	1.4440608 *	2.4835256 *
3 C	2.4716570 *	2.9241776 *	2.4805512 *	3.7782864
4 C	1.4064290 *	2.5066149 *	2.8422882 *	4.2851187
5 C	0.0000000	1.4560706 *	2.4709048 *	3.8112004
6 C	1.4560706 *	0.0000000	1.4667532 *	2.5276232 *
7 C	2.4709048 *	1.4667532 *	0.0000000	1.4436178 *
8 C	3.8112004	2.5276232 *	1.4436178 *	0.0000000
9 C	4.3610496	2.9110456 *	2.4752564 *	1.4022033 *
10 C	3.8811532	2.4992174 *	2.8444291 *	2.4459723 *
11 C	2.6220283 *	1.4638973 *	2.4959716 *	2.8624363 *
12 N	3.0946412	2.5334948 *	3.8417488	4.3174549
13 C	4.3586332	3.7284735	4.9219360	5.1393033

14 C	5.4293343	5.0352810	6.3125996	6.5870093
15 C	5.6629718	5.5885898	6.9732420	7.4596096
16 C	7.0099608	6.9930893	8.3799136	8.8439434
17 C	8.0317821	7.8386656	9.1614553	9.4497804
18 C	7.9093789	7.4939276	8.7109896	8.8168575
19 C	6.7264559	6.1929305	7.3594477	7.4259920
20 O	4.7838882	4.9879638	6.4109682	7.1245852
21 N	1.5091034 *	2.5928925 *	3.8811746	5.1067457
22 H	3.9382008	3.5158932	2.1919239 *	2.6706543 *
23 H	3.4663532	4.0288342	3.4891644	4.6714413
24 H	2.1771009 *	3.5024817	3.9497609	5.3924175
25 H	4.6652572	3.5165949	2.1962509 *	1.1060378 *
26 H	5.4654588	4.0154343	3.4814174	2.1849578 *
27 H	4.7941577	3.4977494	3.9439450	3.4329820
28 H	4.8938958	4.0211702	4.9875297	4.9285699
29 H	7.4262569	7.5824567	8.9986139	9.5753302
30 H	9.0720866	8.9247437	10.2566451	10.5486093
31 H	8.8801586	8.3822975	9.5336239	9.5241221
32 H	6.9384770	6.2169310	7.2330004	7.1109299
33 H	5.4610218	5.8009234	7.2106168	7.9792918
34 H	2.1001784 *	2.9466002 *	4.2087661	5.3383935
35 H	2.0823296 *	3.4201726	4.5523068	5.8806826

C C C N

1 CO	5.3504264	4.1869893	2.9191016 *	1.9411036 *
2 C	3.7738512	4.2847492	3.8327281	5.0563875
3 C	4.9510718	5.1766662	4.3813121	5.3269447
4 C	5.1737627	4.9979636	3.8883245	4.4915954
5 C	4.3610496	3.8811532	2.6220283 *	3.0946412
6 C	2.9110456 *	2.4992174 *	1.4638973 *	2.5334948 *
7 C	2.4752564 *	2.8444291 *	2.4959716 *	3.8417488
8 C	1.4022033 *	2.4459723 *	2.8624363 *	4.3174549
9 C	0.0000000	1.4314053 *	2.4850774 *	3.8021789
10 C	1.4314053 *	0.0000000	1.4146431 *	2.4732001 *
11 C	2.4850774 *	1.4146431 *	0.0000000	1.4568617 *
12 N	3.8021789	2.4732001 *	1.4568617 *	0.0000000
13 C	4.3294443	2.9147040 *	2.4405767 *	1.3332817 *
14 C	5.7494747	4.3244019	3.8378217	2.5160420 *
15 C	6.7731321	5.3497170	4.6181474	3.1709196
16 C	8.1020991	6.6723937	6.0135995	4.5719814
17 C	8.5504132	7.1327558	6.6996097	5.3249241
18 C	7.7991491	6.4311325	6.2220938	4.9916883
19 C	6.4129821	5.0514935	4.8824656	3.7450870
20 O	6.6789424	5.3342423	4.3358929	2.9637871 *
21 N	5.3891877	4.5700519	3.1605939	2.9089815 *

22 H	4.0674209	4.8796657	4.6861405	6.0021249
23 H	5.9274796	6.2499856	5.4851426	6.4075320
24 H	6.2602128	5.9955383	4.7919018	5.1645848
25 H	2.1855971 *	3.4581427	3.9681632	5.4234706
26 H	1.1046102 *	2.1998604 *	3.4768894	4.6726685
27 H	2.1841938 *	1.1040714 *	2.1857759 *	2.6886053 *
28 H	3.9401607	2.6292485 *	2.6424844 *	2.0961097 *
29 H	8.9249740	7.5079459	6.7393830	5.2935038
30 H	9.6357981	8.2217607	7.7991285	6.4172350
31 H	8.4256894	7.1178196	7.0608289	5.9221562
32 H	5.9977399	4.7442062	4.8410369	3.9672794
33 H	7.5755204	6.2522649	5.2467583	3.9184154
34 H	5.5471221	4.7001436	3.3455575	3.0277016
35 H	6.2995015	5.5564515	4.1543820	3.8982556

C C C C

1 CO	2.8554581 *	3.2655185	3.0177379	4.2936469
2 C	6.2236844	7.5618709	8.0846555	9.4824971
3 C	6.5848138	7.7886440	8.0922364	9.4479571
4 C	5.7640719	6.8195793	6.9680152	8.2795723
5 C	4.3586332	5.4293343	5.6629718	7.0099608
6 C	3.7284735	5.0352810	5.5885898	6.9930893
7 C	4.9219360	6.3125996	6.9732420	8.3799136
8 C	5.1393033	6.5870093	7.4596096	8.8439434
9 C	4.3294443	5.7494747	6.7731321	8.1020991
10 C	2.9147040 *	4.3244019	5.3497170	6.6723937
11 C	2.4405767 *	3.8378217	4.6181474	6.0135995
12 N	1.3332817 *	2.5160420 *	3.1709196	4.5719814
13 C	0.0000000	1.4665266 *	2.6097225 *	3.8885857
14 C	1.4665266 *	0.0000000	1.4374226 *	2.5029074 *
15 C	2.6097225 *	1.4374226 *	0.0000000	1.4071591 *
16 C	3.8885857	2.5029074 *	1.4071591 *	0.0000000
17 C	4.3453414	2.8842400 *	2.4407359 *	1.4283320 *
18 C	3.7910252	2.4989082 *	2.8236092 *	2.4731202 *
19 C	2.4667923 *	1.4440612 *	2.4449264 *	2.8468761 *
20 O	3.0517036	2.4998339 *	1.4639805 *	2.4578126 *
21 N	4.0088447	4.7449849	4.7091628	5.9564835
22 H	7.1119070	8.4928049	9.0861975	10.4891022
23 H	7.6744136	8.8513497	9.0921610	10.4258736
24 H	6.4100235	7.3125900	7.2766138	8.5051401
25 H	6.2230204	7.6739045	8.5633923	9.9452786
26 H	4.9877217	6.3413719	7.4582409	8.7252545
27 H	2.6427288 *	3.8874752	5.0371676	6.2524989
28 H	1.1082087 *	2.1692199 *	3.5295984	4.6695525
29 H	4.8016175	3.5055696	2.1964029 *	1.1069574 *

30 H	5.4497156	3.9890292	3.4398941	2.1925343 *
31 H	4.6554971	3.4956679	3.9275652	3.4734270
32 H	2.6374239 *	2.2000550 *	3.4511469	3.9534196
33 H	4.0214768	3.3241671	2.0392946 *	2.4967701 *
34 H	3.8965764	4.6071217	4.6998925	5.9092332
35 H	4.9761277	5.5753292	5.3364498	6.4741764

C C C O

1 CO	5.4565732	5.6246416	4.7069101	1.9544903 *
2 C	10.3654804	10.0076812	8.6825740	7.3482837
3 C	10.4640420	10.2762670	9.0284270	7.1689645
4 C	9.3619207	9.2951187	8.1286912	5.9680466
5 C	8.0317821	7.9093789	6.7264559	4.7838882
6 C	7.8386656	7.4939276	6.1929305	4.9879638
7 C	9.1614553	8.7109896	7.3594477	6.4109682
8 C	9.4497804	8.8168575	7.4259920	7.1245852
9 C	8.5504132	7.7991491	6.4129821	6.6789424
10 C	7.1327558	6.4311325	5.0514935	5.3342423
11 C	6.6996097	6.2220938	4.8824656	4.3358929
12 N	5.3249241	4.9916883	3.7450870	2.9637871 *
13 C	4.3453414	3.7910252	2.4667923 *	3.0517036
14 C	2.8842400 *	2.4989082 *	1.4440612 *	2.4998339 *
15 C	2.4407359 *	2.8236092 *	2.4449264 *	1.4639805 *
16 C	1.4283320 *	2.4731202 *	2.8468761 *	2.4578126 *
17 C	0.0000000	1.4238911 *	2.4568357 *	3.7675085
18 C	1.4238911 *	0.0000000	1.4159858 *	4.2864783
19 C	2.4568357 *	1.4159858 *	0.0000000	3.7920607
20 O	3.7675085	4.2864783	3.7920607	0.0000000
21 N	7.0641885	7.1249484	6.0981787	3.7387805
22 H	11.3269046	10.9020093	9.5496055	8.3926775
23 H	11.4839240	11.3406716	10.1095932	8.0996606
24 H	9.6691832	9.7389932	8.6633886	6.1602561
25 H	10.5322071	9.8633438	8.4670812	8.2167448
26 H	9.0358201	8.1697912	6.8108349	7.5039269
27 H	6.5364603	5.7219566	4.3764670	5.2834057
28 H	4.8434942	3.9823316	2.5664891 *	4.1433517
29 H	2.2001918 *	3.4740941	3.9538070	2.6869149 *
30 H	1.1048468 *	2.2002523 *	3.4609815	4.6474168
31 H	2.1959258 *	1.1040403 *	2.1893722 *	5.3901065
32 H	3.4581971	2.1856095 *	1.1065609 *	4.6908018
33 H	3.9142392	4.7155652	4.4770059	0.9921226 *
34 H	6.9021974	6.8764594	5.8457300	3.9704192
35 H	7.6724636	7.8772553	6.9472915	4.2092738

N H H H

1	CO	1.9802028 *	6.4985151	6.1581728	4.3393791
2	C	4.3332962	1.1050855 *	2.1894959 *	3.4383604
3	C	3.8095411	2.1824513 *	1.1051824 *	2.1977714 *
4	C	2.4695975 *	3.4499648	2.2016813 *	1.1079599 *
5	C	1.5091034 *	3.9382008	3.4663532	2.1771009 *
6	C	2.5928925 *	3.5158932	4.0288342	3.5024817
7	C	3.8811746	2.1919239 *	3.4891644	3.9497609
8	C	5.1067457	2.6706543 *	4.6714413	5.3924175
9	C	5.3891877	4.0674209	5.9274796	6.2602128
10	C	4.5700519	4.8796657	6.2499856	5.9955383
11	C	3.1605939	4.6861405	5.4851426	4.7919018
12	N	2.9089815 *	6.0021249	6.4075320	5.1645848
13	C	4.0088447	7.1119070	7.6744136	6.4100235
14	C	4.7449849	8.4928049	8.8513497	7.3125900
15	C	4.7091628	9.0861975	9.0921610	7.2766138
16	C	5.9564835	10.4891022	10.4258736	8.5051401
17	C	7.0641885	11.3269046	11.4839240	9.6691832
18	C	7.1249484	10.9020093	11.3406716	9.7389932
19	C	6.0981787	9.5496055	10.1095932	8.6633886
20	O	3.7387805	8.3926775	8.0996606	6.1602561
21	N	0.0000000	5.4368339	4.6696062	2.6381031 *
22	H	5.4368339	0.0000000	2.5389134 *	4.3641612
23	H	4.6696062	2.5389134 *	0.0000000	2.5254943 *
24	H	2.6381031 *	4.3641612	2.5254943 *	0.0000000
25	H	6.0463162	2.3892548 *	4.7804069	5.9704814
26	H	6.4739452	4.7646103	6.8467802	7.3413822
27	H	5.2643627	5.9502091	7.3316645	6.9473834
28	H	4.7635850	7.1492450	8.0225533	7.0164730
29	H	6.2684251	11.0402417	10.7601911	8.7066539
30	H	8.0482043	12.4170672	12.5194842	10.6385890
31	H	8.1446277	11.7218802	12.2866224	10.7532510
32	H	6.5013620	9.3959012	10.2031011	8.9743319
33	H	4.3448945	9.1125777	8.6415961	6.5973950
34	H	1.0440920 *	5.8056550	5.1550548	3.1989465
35	H	1.0402855 *	5.8037846	4.5659464	2.1821204 *

H H H H

1	CO	6.5710165	6.3211201	4.5225919	3.8735145
2	C	2.6785233 *	4.6636518	5.3806953	6.3682417
3	C	4.0777235	5.9248776	6.2537864	6.9204604
4	C	4.8846968	6.2472541	5.9939991	6.2687511
5	C	4.6652572	5.4654588	4.7941577	4.8938958
6	C	3.5165949	4.0154343	3.4977494	4.0211702
7	C	2.1962509 *	3.4814174	3.9439450	4.9875297

8 C	1.1060378 *	2.1849578 *	3.4329820	4.9285699
9 C	2.1855971 *	1.1046102 *	2.1841938 *	3.9401607
10 C	3.4581427	2.1998604 *	1.1040714 *	2.6292485 *
11 C	3.9681632	3.4768894	2.1857759 *	2.6424844 *
12 N	5.4234706	4.6726685	2.6886053 *	2.0961097 *
13 C	6.2230204	4.9877217	2.6427288 *	1.1082087 *
14 C	7.6739045	6.3413719	3.8874752	2.1692199 *
15 C	8.5633923	7.4582409	5.0371676	3.5295984
16 C	9.9452786	8.7252545	6.2524989	4.6695525
17 C	10.5322071	9.0358201	6.5364603	4.8434942
18 C	9.8633438	8.1697912	5.7219566	3.9823316
19 C	8.4670812	6.8108349	4.3764670	2.5664891 *
20 O	8.2167448	7.5039269	5.2834057	4.1433517
21 N	6.0463162	6.4739452	5.2643627	4.7635850
22 H	2.3892548 *	4.7646103	5.9502091	7.1492450
23 H	4.7804069	6.8467802	7.3316645	8.0225533
24 H	5.9704814	7.3413822	6.9473834	7.0164730
25 H	0.0000000	2.5345585 *	4.3558787	5.9490692
26 H	2.5345585 *	0.0000000	2.5058523 *	4.4269617
27 H	4.3558787	2.5058523 *	0.0000000	2.1529843 *
28 H	5.9490692	4.4269617	2.1529843 *	0.0000000
29 H	10.6774251	9.6004569	7.1616158	5.6691076
30 H	11.6296975	10.0954925	7.5961714	5.9220781
31 H	10.5348738	8.6831998	6.3189590	4.6409964
32 H	8.0931862	6.2605362	3.9710727	2.2482746 *
33 H	9.0582128	8.4008439	6.1934367	5.1034965
34 H	6.2774330	6.6008729	5.3479017	4.5399483
35 H	6.7458860	7.3965912	6.2739608	5.7763688

H H H H

1 CO	4.6305284	6.4386590	6.6926835	5.2908408
2 C	10.0049696	11.4483755	10.8683105	8.6108191
3 C	9.8395244	11.5135420	11.2101115	9.1058700
4 C	8.6042914	10.3810772	10.2754123	8.3386297
5 C	7.4262569	9.0720866	8.8801586	6.9384770
6 C	7.5824567	8.9247437	8.3822975	6.2169310
7 C	8.9986139	10.2566451	9.5336239	7.2330004
8 C	9.5753302	10.5486093	9.5241221	7.1109299
9 C	8.9249740	9.6357981	8.4256894	5.9977399
10 C	7.5079459	8.2217607	7.1178196	4.7442062
11 C	6.7393830	7.7991285	7.0608289	4.8410369
12 N	5.2935038	6.4172350	5.9221562	3.9672794
13 C	4.8016175	5.4497156	4.6554971	2.6374239 *
14 C	3.5055696	3.9890292	3.4956679	2.2000550 *
15 C	2.1964029 *	3.4398941	3.9275652	3.4511469

16 C	1.1069574 *	2.1925343 *	3.4734270	3.9534196
17 C	2.2001918 *	1.1048468 *	2.1959258 *	3.4581971
18 C	3.4740941	2.2002523 *	1.1040403 *	2.1856095 *
19 C	3.9538070	3.4609815	2.1893722 *	1.1065609 *
20 O	2.6869149 *	4.6474168	5.3901065	4.6908018
21 N	6.2684251	8.0482043	8.1446277	6.5013620
22 H	11.0402417	12.4170672	11.7218802	9.3959012
23 H	10.7601911	12.5194842	12.2866224	10.2031011
24 H	8.7066539	10.6385890	10.7532510	8.9743319
25 H	10.6774251	11.6296975	10.5348738	8.0931862
26 H	9.6004569	10.0954925	8.6831998	6.2605362
27 H	7.1616158	7.5961714	6.3189590	3.9710727
28 H	5.6691076	5.9220781	4.6409964	2.2482746 *
29 H	0.0000000	2.5211347 *	4.3851099	5.0603441
30 H	2.5211347 *	0.0000000	2.5365749 *	4.3740072
31 H	4.3851099	2.5365749 *	0.0000000	2.5165823 *
32 H	5.0603441	4.3740072	2.5165823 *	0.0000000
33 H	2.2983086 *	4.6154058	5.7990455	5.4581021
34 H	6.2990567	7.8845144	7.8458328	6.1893975
35 H	6.6282070	8.5952322	8.9207245	7.4267012

H H H

1 CO	2.6604013 *	2.4942406 *	2.6286856 *
2 C	8.0608263	4.7330458	4.7202987
3 C	7.7741914	4.2973922	3.9001741
4 C	6.5309594	3.0418872	2.4691417 *
5 C	5.4610218	2.1001784 *	2.0823296 *
6 C	5.8009234	2.9466002 *	3.4201726
7 C	7.2106168	4.2087661	4.5523068
8 C	7.9792918	5.3383935	5.8806826
9 C	7.5755204	5.5471221	6.2995015
10 C	6.2522649	4.7001436	5.5564515
11 C	5.2467583	3.3455575	4.1543820
12 N	3.9184154	3.0277016	3.8982556
13 C	4.0214768	3.8965764	4.9761277
14 C	3.3241671	4.6071217	5.5753292
15 C	2.0392946 *	4.6998925	5.3364498
16 C	2.4967701 *	5.9092332	6.4741764
17 C	3.9142392	6.9021974	7.6724636
18 C	4.7155652	6.8764594	7.8772553
19 C	4.4770059	5.8457300	6.9472915
20 O	0.9921226 *	3.9704192	4.2092738
21 N	4.3448945	1.0440920 *	1.0402855 *
22 H	9.1125777	5.8056550	5.8037846
23 H	8.6415961	5.1550548	4.5659464

24 H	6.5973950	3.1989465	2.1821204 *
25 H	9.0582128	6.2774330	6.7458860
26 H	8.4008439	6.6008729	7.3965912
27 H	6.1934367	5.3479017	6.2739608
28 H	5.1034965	4.5399483	5.7763688
29 H	2.2983086 *	6.2990567	6.6282070
30 H	4.6154058	7.8845144	8.5952322
31 H	5.7990455	7.8458328	8.9207245
32 H	5.4581021	6.1893975	7.4267012
33 H	0.0000000	4.6487379	4.6222730
34 H	4.6487379	0.0000000	1.6669339 *
35 H	4.6222730	1.6669339 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.72 , TOTAL = 5689.5 SECONDS (94.8 MIN)
WALL CLOCK TIME: STEP = 0.73 , TOTAL = 5260.0 SECONDS (87.7 MIN)

CPU UTILIZATION: STEP = 98.52%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.12 , TOTAL = 5690.6 SECONDS (94.8 MIN)
WALL CLOCK TIME: STEP = 1.11 , TOTAL = 5261.1 SECONDS (87.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.635323912	-284.635323912	0.015645337	0.001884720	197289482
11382250						
2	1	-284.635823070	-0.000499158	0.004489818	0.000167580	163054319
14339684						
3	2	-284.635825377	-0.000002307	0.003690390	0.000326334	149323589
15434903						
4	3	-284.635830489	-0.000005112	0.001155859	0.000071576	142888859
15907083						
5	4	-284.635830897	-0.000000408	0.000427855	0.000085065	137512610
16394953						

6 5	-284.635831216	-0.000000318	0.000466322	0.000091472	130067998
16959222					
7 6	-284.635831371	-0.000000155	0.000361229	0.000062016	152135055
15249787					
8 7	-284.635831549	-0.000000178	0.000356795	0.000034272	149327697
15449686					
9 8	-284.635831661	-0.000000112	0.000543689	0.000037061	147444690
15655971					
10 9	-284.635831750	-0.000000090	0.000511641	0.000038967	167612399
14065881					
11 10	-284.635831847	-0.000000096	0.000499711	0.000035842	165771952
14220636					
12 11	-284.635831935	-0.000000088	0.000606192	0.000031728	165855802
14219595					

-----DISABLING FDIFF OPTION-----

13 12	-284.635832017	-0.000000082	0.000554188	0.000025367	197280887
11383117					
14 13	-284.635832060	-0.000000042	0.000185070	0.000016962	197280730
11383125					
15 14	-284.635832086	-0.000000026	0.000149471	0.000013504	197280668
11383128					
16 15	-284.635832100	-0.000000014	0.000164252	0.000011979	197280496
11383134					
17 16	-284.635832113	-0.000000013	0.000301243	0.000008965	197280439
11383137					
18 17	-284.635832122	-0.000000009	0.000052325	0.000006706	197280226
11383140					
19 18	-284.635832126	-0.000000004	0.000048845	0.000005865	197280221
11383139					
20 19	-284.635832128	-0.000000002	0.000056319	0.000004653	197280134
11383142					
21 20	-284.635832130	-0.000000003	0.000120708	0.000004406	197280166
11383145					
22 21	-284.635832133	-0.000000002	0.000072876	0.000004938	197280164
11383145					
23 22	-284.635832134	-0.000000001	0.000072429	0.000004948	197280251
11383146					
24 23	-284.635832136	-0.000000002	0.000199010	0.000003948	197280242
11383147					
25 24	-284.635832138	-0.000000002	0.000048855	0.000002969	197280342
11383145					
26 25	-284.635832138	-0.000000001	0.000022894	0.000002454	197280247
11383145					
27 26	-284.635832139	0.000000000	0.000015842	0.000000938	197280328
11383144					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 91.7 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 29.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 3.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6358321388 AFTER 27 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6001454399
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999600464

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 96.12 , TOTAL = 5786.8 SECONDS (96.4 MIN)
WALL CLOCK TIME: STEP = 88.24 , TOTAL = 5349.4 SECONDS (89.2
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.74 , TOTAL = 5790.5 SECONDS (96.5 MIN)
WALL CLOCK TIME: STEP = 3.72 , TOTAL = 5353.1 SECONDS (89.2
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.83 , TOTAL = 5793.3 SECONDS (96.6 MIN)
WALL CLOCK TIME: STEP = 2.68 , TOTAL = 5355.8 SECONDS (89.3
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 58 ENERGY= -284.6358321

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0009491	-0.0004345	0.0003176
2 C	6.0	-0.0005096	-0.0007599	-0.0002944
3 C	6.0	-0.0009458	0.0002910	-0.0000046
4 C	6.0	0.0002775	0.0007886	0.0002963
5 C	6.0	0.0003429	-0.0001348	0.0004591
6 C	6.0	-0.0003137	0.0007240	0.0002342
7 C	6.0	-0.0000432	0.0004662	-0.0003295
8 C	6.0	0.0001727	-0.0001145	-0.0006006
9 C	6.0	0.0003560	0.0003459	0.0001209
10 C	6.0	-0.0001095	-0.0006997	0.0001918
11 C	6.0	0.0007000	0.0001279	0.0001604
12 N	7.0	0.0001118	0.0004187	0.0000679
13 C	6.0	0.0003231	-0.0008634	-0.0003028
14 C	6.0	0.0009302	-0.0001001	-0.0008127
15 C	6.0	0.0003059	-0.0008717	-0.0014065
16 C	6.0	-0.0001142	-0.0008523	-0.0008339
17 C	6.0	-0.0005586	-0.0005704	0.0000537
18 C	6.0	-0.0000033	0.0008822	0.0005381
19 C	6.0	0.0001063	0.0000245	0.0003730
20 O	8.0	-0.0003526	0.0006509	-0.0000253
21 N	7.0	0.0000439	-0.0000775	0.0002025
22 H	1.0	-0.0004767	0.0005016	0.0003389
23 H	1.0	0.0005853	-0.0005854	0.0004041
24 H	1.0	-0.0009168	-0.0001474	0.0000403
25 H	1.0	0.0007773	0.0002812	-0.0013182
26 H	1.0	0.0001694	0.0001156	0.0003575
27 H	1.0	0.0000313	-0.0006394	0.0006398
28 H	1.0	-0.0004473	-0.0000973	-0.0004098
29 H	1.0	-0.0002425	-0.0000367	-0.0000229
30 H	1.0	0.0001620	0.0003420	0.0004957
31 H	1.0	-0.0001888	-0.0003048	0.0002603
32 H	1.0	-0.0000621	0.0005748	0.0003691
33 H	1.0	-0.0007760	0.0002658	0.0004550
34 H	1.0	0.0004061	0.0005673	0.0002729
35 H	1.0	0.0012079	-0.0000783	-0.0002881

MAXIMUM GRADIENT = 0.0014065 RMS GRADIENT = 0.0005029
HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0001362671
PREDICTED ENERGY CHANGE WAS -0.0000901959 RATIO= 1.511
GDIIS STEP HAS LENGTH = 0.110389
RADIUS OF STEP TAKEN= 0.11039 CURRENT TRUST RADIUS= 0.16686

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 5793.3 SECONDS (96.6 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5355.8 SECONDS (89.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

INSERCH= 59

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1452299731	-1.7674377071	0.8907600980
C	6.0	4.9832134062	0.6606883534	0.5091444017
C	6.0	5.1986432199	-0.6984481617	0.2429513833
C	6.0	4.0691282348	-1.5448488504	0.0039635874
C	6.0	2.7588682763	-1.0371923723	0.0669239510
C	6.0	2.4750084464	0.3415820118	0.4418037935
C	6.0	3.6489687549	1.2032362335	0.6170613501
C	6.0	3.4917781898	2.6052585046	0.9252354765
C	6.0	2.2219180553	3.1544664308	1.1529331070
C	6.0	1.0674307218	2.3136142620	1.0629240286
C	6.0	1.1657672243	0.9570117663	0.6716219544
N	7.0	-0.0439358166	0.1478297700	0.6315066394
C	6.0	-1.2368951784	0.6777189597	0.3597345735
C	6.0	-2.5506149691	0.0321440468	0.4518158563
C	6.0	-2.8409106568	-1.3212920942	0.8390396361
C	6.0	-4.1479053142	-1.8339838139	0.9258930321
C	6.0	-5.2471527269	-0.9652603227	0.6454815649
C	6.0	-5.0160488798	0.3895650479	0.2730853378
C	6.0	-3.6892269295	0.8727273171	0.1680162503
O	8.0	-1.7347943796	-2.2144069594	1.1886475903
N	7.0	1.6692764700	-1.9947307928	-0.3482890054
H	1.0	5.8380958465	1.3435541751	0.6615299497
H	1.0	6.2184319497	-1.1172730607	0.1854136896
H	1.0	4.2321954260	-2.6056009461	-0.2744678379
H	1.0	4.3998591872	3.2318772357	1.0009406935
H	1.0	2.1081253875	4.2145848367	1.4429458434
H	1.0	0.0891762446	2.7342138893	1.3549548852
H	1.0	-1.2749691462	1.7311656218	0.0188060184
H	1.0	-4.3356963772	-2.8863416577	1.2192140791

H	1.0	-6.2793172537	-1.3534749915	0.7265400315
H	1.0	-5.8690609818	1.0610265077	0.0672461465
H	1.0	-3.5129886500	1.9260855913	-0.1218492791
H	1.0	-2.0774600042	-3.0483085334	1.5923250551
H	1.0	1.3243386785	-1.7429776145	-1.3030436088
H	1.0	2.0875205712	-2.9456676832	-0.4279232728

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4265560	5.2057065	4.0290112
2 C	5.4265560	0.0000000	1.4016136 *	2.4403184 *
3 C	5.2057065	1.4016136 *	0.0000000	1.4315423 *
4 C	4.0290112	2.4403184 *	1.4315423 *	0.0000000
5 C	2.8360306 *	2.8330318 *	2.4694605 *	1.4065775 *
6 C	3.1744911	2.5293192 *	2.9222237 *	2.5082949 *
7 C	4.6017388	1.4443729 *	2.4815021 *	2.8468218 *
8 C	5.5064549	2.4857321 *	3.7806583	4.2901592
9 C	5.3485053	3.7759959	4.9531717	5.1784052
10 C	4.1874909	4.2862793	5.1780104	5.0019319
11 C	2.9175577 *	3.8323755	4.3804560	3.8903187
12 N	1.9419695 *	5.0547231	5.3246405	4.4918000
13 C	2.8585047 *	6.2219261	6.5820687	5.7637024
14 C	3.2708938	7.5602199	7.7864236	6.8197125
15 C	3.0197279	8.0779945	8.0856467	6.9639046
16 C	4.2937947	9.4749352	9.4400117	8.2736445
17 C	5.4572375	10.3596664	10.4569533	9.3563112
18 C	5.6278755	10.0057223	10.2725175	9.2927298
19 C	4.7112514	8.6817366	9.0259871	8.1279556
20 O	1.9552519 *	7.3389050	7.1599601	5.9613171
21 N	1.9772765 *	4.3322766	3.8060929	2.4669342 *
22 H	6.4914974	1.1046950 *	2.1803397 *	3.4502916
23 H	6.1484966	2.1889982 *	1.1039447 *	2.1989206 *
24 H	4.3316926	3.4419067	2.1997672 *	1.1087425 *
25 H	6.5656043	2.6820101 *	4.0816739	4.8908546
26 H	6.3200048	4.6656507	5.9269875	6.2519820
27 H	4.5258685	5.3820538	6.2551078	5.9979641
28 H	3.8752412	6.3679826	6.9181588	6.2683226
29 H	4.6301759	9.9963844	9.8307476	8.5975295
30 H	6.4399643	11.4432824	11.5068021	10.3754067
31 H	6.6970203	10.8686432	11.2080640	10.2743465
32 H	5.2962303	8.6130617	9.1057008	8.3397669
33 H	2.6595440 *	8.0487917	7.7642985	6.5240961
34 H	2.4907168 *	4.7380375	4.3001602	3.0465378

35 H 2.6267174 * 4.7189974 3.8960432 2.4648709 *

C C C C

1 CO 2.8360306 * 3.1744911 4.6017388 5.5064549
2 C 2.8330318 * 2.5293192 * 1.4443729 * 2.4857321 *
3 C 2.4694605 * 2.9222237 * 2.4815021 * 3.7806583
4 C 1.4065775 * 2.5082949 * 2.8468218 * 4.2901592
5 C 0.0000000 1.4567533 * 2.4727415 * 3.8133062
6 C 1.4567533 * 0.0000000 1.4667467 * 2.5281927 *
7 C 2.4727415 * 1.4667467 * 0.0000000 1.4440729 *
8 C 3.8133062 2.5281927 * 1.4440729 * 0.0000000
9 C 4.3632253 2.9124008 * 2.4760718 * 1.4021485 *
10 C 3.8834112 2.5011950 * 2.8453596 * 2.4457054 *
11 C 2.6230671 * 1.4648149 * 2.4959754 * 2.8620559 *
12 N 3.0949543 2.5334970 * 3.8407858 4.3158436
13 C 4.3580712 3.7279957 4.9207776 5.1376601
14 C 5.4297546 5.0351507 6.3113866 6.5844938
15 C 5.6598939 5.5840794 6.9671409 7.4517231
16 C 7.0054426 6.9878763 8.3732507 8.8358156
17 C 8.0272209 7.8346088 9.1566458 9.4443518
18 C 7.9074317 7.4931107 8.7099317 8.8157654
19 C 6.7257672 6.1931311 7.3593474 7.4257579
20 O 4.7788181 4.9812945 6.4024918 7.1144657
21 N 1.5088048 * 2.5945728 * 3.8830498 5.1091368
22 H 3.9374043 3.5160467 2.1940702 * 2.6770590 *
23 H 3.4625184 4.0258184 3.4890148 4.6732449
24 H 2.1787948 * 3.5052302 3.9550244 5.3981999
25 H 4.6679968 3.5173130 2.1969488 * 1.1058903 *
26 H 5.4679124 4.0170934 3.4820258 2.1845939 *
27 H 4.7968515 3.5001039 3.9446802 3.4320531
28 H 4.8926440 4.0214676 4.9881643 4.9302670
29 H 7.4215883 7.5769095 8.9912242 9.5662665
30 H 9.0677409 8.9214635 10.2527860 10.5444467
31 H 8.8793967 8.3833996 9.5349573 9.5260752
32 H 6.9392248 6.2196837 7.2361685 7.1150840
33 H 5.4554109 5.7913751 7.1985247 7.9639339
34 H 2.1054261 * 2.9519353 * 4.2155526 5.3451080
35 H 2.0827529 * 3.4223651 4.5545051 5.8835159

C C C N

1 CO 5.3485053 4.1874909 2.9175577 * 1.9419695 *
2 C 3.7759959 4.2862793 3.8323755 5.0547231
3 C 4.9531717 5.1780104 4.3804560 5.3246405
4 C 5.1784052 5.0019319 3.8903187 4.4918000

5 C	4.3632253	3.8834112	2.6230671 *	3.0949543
6 C	2.9124008 *	2.5011950 *	1.4648149 *	2.5334970 *
7 C	2.4760718 *	2.8453596 *	2.4959754 *	3.8407858
8 C	1.4021485 *	2.4457054 *	2.8620559 *	4.3158436
9 C	0.0000000	1.4310748 *	2.4851402 *	3.8007688
10 C	1.4310748 *	0.0000000	1.4153295 *	2.4722215 *
11 C	2.4851402 *	1.4153295 *	0.0000000	1.4559417 *
12 N	3.8007688	2.4722215 *	1.4559417 *	0.0000000
13 C	4.3274509	2.9121378 *	2.4388655 *	1.3333397 *
14 C	5.7460886	4.3207423	3.8360385	2.5157727 *
15 C	6.7648487	5.3420783	4.6121757	3.1661423
16 C	8.0938763	6.6649139	6.0074475	4.5669261
17 C	8.5449795	7.1273586	6.6948753	5.3209615
18 C	7.7978829	6.4291939	6.2205850	4.9908727
19 C	6.4123342	5.0500304	4.8817713	3.7454569
20 O	6.6694565	5.3264668	4.3287954	2.9579674 *
21 N	5.3919674	4.5733552	3.1633090	2.9130159 *
22 H	4.0740179	4.8848111	4.6883016	6.0024124
23 H	5.9292475	6.2509060	5.4834731	6.4044308
24 H	6.2655458	6.0002526	4.7948177	5.1659916
25 H	2.1846102 *	3.4571850	3.9677216	5.4217289
26 H	1.1049467 *	2.2002616 *	3.4777524	4.6720764
27 H	2.1831199 *	1.1041594 *	2.1873361 *	2.6889550 *
28 H	3.9421123	2.6298795 *	2.6424755 *	2.0970926 *
29 H	8.9161686	7.5005167	6.7332997	5.2887432
30 H	9.6319442	8.2179927	7.7955531	6.4142754
31 H	8.4276419	7.1186563	7.0615081	5.9232087
32 H	6.0019284	4.7470104	4.8434964	3.9703988
33 H	7.5599031	6.2386552	5.2353422	3.9081572
34 H	5.5517951	4.7031630	3.3487896	3.0314703
35 H	6.3030791	5.5608682	4.1580688	3.9032326

C C C C

1 CO	2.8585047 *	3.2708938	3.0197279	4.2937947
2 C	6.2219261	7.5602199	8.0779945	9.4749352
3 C	6.5820687	7.7864236	8.0856467	9.4400117
4 C	5.7637024	6.8197125	6.9639046	8.2736445
5 C	4.3580712	5.4297546	5.6598939	7.0054426
6 C	3.7279957	5.0351507	5.5840794	6.9878763
7 C	4.9207776	6.3113866	6.9671409	8.3732507
8 C	5.1376601	6.5844938	7.4517231	8.8358156
9 C	4.3274509	5.7460886	6.7648487	8.0938763
10 C	2.9121378 *	4.3207423	5.3420783	6.6649139
11 C	2.4388655 *	3.8360385	4.6121757	6.0074475
12 N	1.3333397 *	2.5157727 *	3.1661423	4.5669261

13 C	0.0000000	1.4666648 *	2.6074210 *	3.8862792
14 C	1.4666648 *	0.0000000	1.4373598 *	2.5017032 *
15 C	2.6074210 *	1.4373598 *	0.0000000	1.4066383 *
16 C	3.8862792	2.5017032 *	1.4066383 *	0.0000000
17 C	4.3431783	2.8816033 *	2.4401279 *	1.4288653 *
18 C	3.7911138	2.4976106 *	2.8246350 *	2.4746718 *
19 C	2.4675322 *	1.4434541 *	2.4461468 *	2.8479902 *
20 O	3.0494906	2.5010949 *	1.4640263 *	2.4570035 *
21 N	4.0111244	4.7493024	4.7122242	5.9572631
22 H	7.1126588	8.4931882	9.0806426	10.4826931
23 H	7.6703511	8.8480684	9.0851824	10.4174341
24 H	6.4104098	7.3138023	7.2744881	8.5007263
25 H	6.2215649	7.6713051	8.5548998	9.9364409
26 H	4.9871765	6.3386916	7.4500734	8.7172499
27 H	2.6416094 *	3.8839850	5.0297820	6.2454291
28 H	1.1078952 *	2.1682814 *	3.5273863	4.6676396
29 H	4.8003960	3.5061338	2.1973386 *	1.1084944 *
30 H	5.4485150	3.9873091	3.4403970	2.1939798 *
31 H	4.6571917	3.4955081	3.9294785	3.4757353
32 H	2.6402545 *	2.2005157 *	3.4526017	3.9546182
33 H	4.0136155	3.3187083	2.0329490 *	2.4910761 *
34 H	3.8967322	4.6093226	4.7027270	5.9094750
35 H	4.9800678	5.5815414	5.3416501	6.4768199

C C C O

1 CO	5.4572375	5.6278755	4.7112514	1.9552519 *
2 C	10.3596664	10.0057223	8.6817366	7.3389050
3 C	10.4569533	10.2725175	9.0259871	7.1599601
4 C	9.3563112	9.2927298	8.1279556	5.9613171
5 C	8.0272209	7.9074317	6.7257672	4.7788181
6 C	7.8346088	7.4931107	6.1931311	4.9812945
7 C	9.1566458	8.7099317	7.3593474	6.4024918
8 C	9.4443518	8.8157654	7.4257579	7.1144657
9 C	8.5449795	7.7978829	6.4123342	6.6694565
10 C	7.1273586	6.4291939	5.0500304	5.3264668
11 C	6.6948753	6.2205850	4.8817713	4.3287954
12 N	5.3209615	4.9908727	3.7454569	2.9579674 *
13 C	4.3431783	3.7911138	2.4675322 *	3.0494906
14 C	2.8816033 *	2.4976106 *	1.4434541 *	2.5010949 *
15 C	2.4401279 *	2.8246350 *	2.4461468 *	1.4640263 *
16 C	1.4288653 *	2.4746718 *	2.8479902 *	2.4570035 *
17 C	0.0000000	1.4239521 *	2.4562786 *	3.7672348
18 C	1.4239521 *	0.0000000	1.4159597 *	4.2878381
19 C	2.4562786 *	1.4159597 *	0.0000000	3.7936648
20 O	3.7672348	4.2878381	3.7936648	0.0000000

21 N	7.0628877	7.1249244	6.0993808	3.7414075
22 H	11.3231452	10.9029098	9.5517073	8.3836512
23 H	11.4758182	11.3354227	10.1055484	8.0909820
24 H	9.6641123	9.7365731	8.6627647	6.1561926
25 H	10.5264977	9.8624458	8.4671522	8.2055603
26 H	9.0314374	8.1702637	6.8119565	7.4943069
27 H	6.5319116	5.7211138	4.3761040	5.2766822
28 H	4.8416606	3.9824901	2.5666750 *	4.1409554
29 H	2.2023794 *	3.4770108	3.9564554	2.6864701 *
30 H	1.1057327 *	2.1999220 *	3.4607071	4.6483799
31 H	2.1970354 *	1.1049253 *	2.1902711 *	5.3924174
32 H	3.4577453	2.1854196 *	1.1066371 *	4.6928728
33 H	3.9092908	4.7111222	4.4722444	0.9878092 *
34 H	6.8982675	6.8725858	5.8430959	3.9735457
35 H	7.6727859	7.8788254	6.9502587	4.2140402

N H H H

1 CO	1.9772765 *	6.4914974	6.1484966	4.3316926
2 C	4.3322766	1.1046950 *	2.1889982 *	3.4419067
3 C	3.8060929	2.1803397 *	1.1039447 *	2.1997672 *
4 C	2.4669342 *	3.4502916	2.1989206 *	1.1087425 *
5 C	1.5088048 *	3.9374043	3.4625184	2.1787948 *
6 C	2.5945728 *	3.5160467	4.0258184	3.5052302
7 C	3.8830498	2.1940702 *	3.4890148	3.9550244
8 C	5.1091368	2.6770590 *	4.6732449	5.3981999
9 C	5.3919674	4.0740179	5.9292475	6.2655458
10 C	4.5733552	4.8848111	6.2509060	6.0002526
11 C	3.1633090	4.6883016	5.4834731	4.7948177
12 N	2.9130159 *	6.0024124	6.4044308	5.1659916
13 C	4.0111244	7.1126588	7.6703511	6.4104098
14 C	4.7493024	8.4931882	8.8480684	7.3138023
15 C	4.7122242	9.0806426	9.0851824	7.2744881
16 C	5.9572631	10.4826931	10.4174341	8.5007263
17 C	7.0628877	11.3231452	11.4758182	9.6641123
18 C	7.1249244	10.9029098	11.3354227	9.7365731
19 C	6.0993808	9.5517073	10.1055484	8.6627647
20 O	3.7414075	8.3836512	8.0909820	6.1561926
21 N	0.0000000	5.4353414	4.6636452	2.6357476 *
22 H	5.4353414	0.0000000	2.5351554 *	4.3647261
23 H	4.6636452	2.5351554 *	0.0000000	2.5242319 *
24 H	2.6357476 *	4.3647261	2.5242319 *	0.0000000
25 H	6.0492920	2.3978091 *	4.7840777	5.9775354
26 H	6.4774000	4.7713842	6.8487018	7.3468440
27 H	5.2688399	5.9552371	7.3327726	6.9522118
28 H	4.7629450	7.1525541	8.0182555	7.0158688

29 H	6.2699071	11.0321838	10.7511847	8.7016476
30 H	8.0465277	12.4141006	12.5116883	10.6330492
31 H	8.1447439	11.7256350	12.2827700	10.7515723
32 H	6.5023033	9.4019044	10.2008328	8.9748176
33 H	4.3490278	9.1000474	8.6330829	6.5948963
34 H	1.0459054 *	5.8103555	5.1535580	3.2027672
35 H	1.0418977 *	5.8009609	4.5589075	2.1768841 *

H H H H

1 CO	6.5656043	6.3200048	4.5258685	3.8752412
2 C	2.6820101 *	4.6656507	5.3820538	6.3679826
3 C	4.0816739	5.9269875	6.2551078	6.9181588
4 C	4.8908546	6.2519820	5.9979641	6.2683226
5 C	4.6679968	5.4679124	4.7968515	4.8926440
6 C	3.5173130	4.0170934	3.5001039	4.0214676
7 C	2.1969488 *	3.4820258	3.9446802	4.9881643
8 C	1.1058903 *	2.1845939 *	3.4320531	4.9302670
9 C	2.1846102 *	1.1049467 *	2.1831199 *	3.9421123
10 C	3.4571850	2.2002616 *	1.1041594 *	2.6298795 *
11 C	3.9677216	3.4777524	2.1873361 *	2.6424755 *
12 N	5.4217289	4.6720764	2.6889550 *	2.0970926 *
13 C	6.2215649	4.9871765	2.6416094 *	1.1078952 *
14 C	7.6713051	6.3386916	3.8839850	2.1682814 *
15 C	8.5548998	7.4500734	5.0297820	3.5273863
16 C	9.9364409	8.7172499	6.2454291	4.6676396
17 C	10.5264977	9.0314374	6.5319116	4.8416606
18 C	9.8624458	8.1702637	5.7211138	3.9824901
19 C	8.4671522	6.8119565	4.3761040	2.5666750 *
20 O	8.2055603	7.4943069	5.2766822	4.1409554
21 N	6.0492920	6.4774000	5.2688399	4.7629450
22 H	2.3978091 *	4.7713842	5.9552371	7.1525541
23 H	4.7840777	6.8487018	7.3327726	8.0182555
24 H	5.9775354	7.3468440	6.9522118	7.0158688
25 H	0.0000000	2.5324152 *	4.3537320	5.9515041
26 H	2.5324152 *	0.0000000	2.5050741 *	4.4318026
27 H	4.3537320	2.5050741 *	0.0000000	2.1569173 *
28 H	5.9515041	4.4318026	2.1569173 *	0.0000000
29 H	10.6672479	9.5914572	7.1546186	5.6683687
30 H	11.6252123	10.0928550	7.5935377	5.9210975
31 H	10.5373194	8.6875188	6.3212610	4.6429638
32 H	8.0980806	6.2675941	3.9761305	2.2508907 *
33 H	9.0413568	8.3839763	6.1796620	5.0954222
34 H	6.2862032	6.6066126	5.3512453	4.5357865
35 H	6.7491202	7.4006616	6.2795772	5.7774280

	H	H	H	H
1 CO	4.6301759	6.4399643	6.6970203	5.2962303
2 C	9.9963844	11.4432824	10.8686432	8.6130617
3 C	9.8307476	11.5068021	11.2080640	9.1057008
4 C	8.5975295	10.3754067	10.2743465	8.3397669
5 C	7.4215883	9.0677409	8.8793967	6.9392248
6 C	7.5769095	8.9214635	8.3833996	6.2196837
7 C	8.9912242	10.2527860	9.5349573	7.2361685
8 C	9.5662665	10.5444467	9.5260752	7.1150840
9 C	8.9161686	9.6319442	8.4276419	6.0019284
10 C	7.5005167	8.2179927	7.1186563	4.7470104
11 C	6.7332997	7.7955531	7.0615081	4.8434964
12 N	5.2887432	6.4142754	5.9232087	3.9703988
13 C	4.8003960	5.4485150	4.6571917	2.6402545 *
14 C	3.5061338	3.9873091	3.4955081	2.2005157 *
15 C	2.1973386 *	3.4403970	3.9294785	3.4526017
16 C	1.1084944 *	2.1939798 *	3.4757353	3.9546182
17 C	2.2023794 *	1.1057327 *	2.1970354 *	3.4577453
18 C	3.4770108	2.1999220 *	1.1049253 *	2.1854196 *
19 C	3.9564554	3.4607071	2.1902711 *	1.1066371 *
20 O	2.6864701 *	4.6483799	5.3924174	4.6928728
21 N	6.2699071	8.0465277	8.1447439	6.5023033
22 H	11.0321838	12.4141006	11.7256350	9.4019044
23 H	10.7511847	12.5116883	12.2827700	10.2008328
24 H	8.7016476	10.6330492	10.7515723	8.9748176
25 H	10.6672479	11.6252123	10.5373194	8.0980806
26 H	9.5914572	10.0928550	8.6875188	6.2675941
27 H	7.1546186	7.5935377	6.3212610	3.9761305
28 H	5.6683687	5.9210975	4.6429638	2.2508907 *
29 H	0.0000000	2.5238998 *	4.3886162	5.0630776
30 H	2.5238998 *	0.0000000	2.5362957 *	4.3735404
31 H	4.3886162	2.5362957 *	0.0000000	2.5169746 *
32 H	5.0630776	4.3735404	2.5169746 *	0.0000000
33 H	2.2945755 *	4.6127702	5.7955792	5.4537815
34 H	6.3011953	7.8794991	7.8412456	6.1852228
35 H	6.6313119	8.5948728	8.9222184	7.4292237

	H	H	H
1 CO	2.6595440 *	2.4907168 *	2.6267174 *
2 C	8.0487917	4.7380375	4.7189974
3 C	7.7642985	4.3001602	3.8960432
4 C	6.5240961	3.0465378	2.4648709 *
5 C	5.4554109	2.1054261 *	2.0827529 *
6 C	5.7913751	2.9519353 *	3.4223651

7 C	7.1985247	4.2155526	4.5545051
8 C	7.9639339	5.3451080	5.8835159
9 C	7.5599031	5.5517951	6.3030791
10 C	6.2386552	4.7031630	5.5608682
11 C	5.2353422	3.3487896	4.1580688
12 N	3.9081572	3.0314703	3.9032326
13 C	4.0136155	3.8967322	4.9800678
14 C	3.3187083	4.6093226	5.5815414
15 C	2.0329490 *	4.7027270	5.3416501
16 C	2.4910761 *	5.9094750	6.4768199
17 C	3.9092908	6.8982675	7.6727859
18 C	4.7111222	6.8725858	7.8788254
19 C	4.4722444	5.8430959	6.9502587
20 O	0.9878092 *	3.9735457	4.2140402
21 N	4.3490278	1.0459054 *	1.0418977 *
22 H	9.1000474	5.8103555	5.8009609
23 H	8.6330829	5.1535580	4.5589075
24 H	6.5948963	3.2027672	2.1768841 *
25 H	9.0413568	6.2862032	6.7491202
26 H	8.3839763	6.6066126	7.4006616
27 H	6.1796620	5.3512453	6.2795772
28 H	5.0954222	4.5357865	5.7774280
29 H	2.2945755 *	6.3011953	6.6313119
30 H	4.6127702	7.8794991	8.5948728
31 H	5.7955792	7.8412456	8.9222184
32 H	5.4537815	6.1852228	7.4292237
33 H	0.0000000	4.6539535	4.6302270
34 H	4.6539535	0.0000000	1.6717493 *
35 H	4.6302270	1.6717493 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.71 , TOTAL = 5794.1 SECONDS (96.6 MIN)
WALL CLOCK TIME: STEP = 0.72 , TOTAL = 5356.5 SECONDS (89.3 MIN)

CPU UTILIZATION: STEP = 98.25% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.11 , TOTAL = 5795.2 SECONDS (96.6 MIN)
WALL CLOCK TIME: STEP = 1.10 , TOTAL = 5357.6 SECONDS (89.3 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

		NONZERO BLOCKS				
ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD	
INTEGRALS SKIPPED						
-----START SECOND ORDER SCF-----						
1	0	-284.635669280	-284.635669280	0.017604321	0.001765367	197374794 11377194
2	1	-284.635931395	-0.000262115	0.003532321	0.000200485	162124400 14395700
3	2	-284.635930662	0.000000733	0.001479038	0.000410329	147598736 15563146
4	3	-284.635936334	-0.000005672	0.000812908	0.000109536	140067841 16154958
5	4	-284.635936041	0.000000293	0.000381975	0.000230067	135600426 16552388
6	5	-284.635936815	-0.000000774	0.000353499	0.000048682	126972857 17244170
7	6	-284.635936833	-0.000000018	0.000276773	0.000040741	128266145 17078017
8	7	-284.635937018	-0.000000185	0.000381168	0.000040905	120775069 17691770
9	8	-284.635937098	-0.000000080	0.000456752	0.000041635	147311611 15671248
10	9	-284.635937181	-0.000000082	0.000343473	0.000038745	164822071 14322974
11	10	-284.635937240	-0.000000059	0.000353174	0.000032221	165181874 14232096
-----DISABLING FDIFF OPTION-----						
12	11	-284.635937320	-0.000000080	0.000447744	0.000031554	197370462 11377584
13	12	-284.635937376	-0.000000056	0.000317682	0.000022732	197370437 11377585
14	13	-284.635937398	-0.000000022	0.000142290	0.000013086	197370197 11377600
15	14	-284.635937413	-0.000000015	0.000113108	0.000011955	197370240 11377593
16	15	-284.635937422	-0.000000009	0.000130184	0.000009722	197370227 11377594
17	16	-284.635937431	-0.000000009	0.000174212	0.000005805	197370170 11377594
18	17	-284.635937434	-0.000000003	0.000066087	0.000004482	197370233 11377593
19	18	-284.635937435	-0.000000001	0.000029409	0.000002280	197370202 11377595

20 19 -284.635937436 0.000000000 0.000011016 0.000001015 197370213
11377592
21 20 -284.635937436 0.000000000 0.000011776 0.000000968 197370260
11377592

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 70.8 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 22.7 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.9 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6359374358 AFTER 21 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5992912972
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999568127

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 73.82 , TOTAL = 5869.0 SECONDS (97.8 MIN)
WALL CLOCK TIME: STEP = 67.74 , TOTAL = 5425.4 SECONDS (90.4
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.90 , TOTAL = 5872.9 SECONDS (97.9 MIN)
WALL CLOCK TIME: STEP = 3.86 , TOTAL = 5429.2 SECONDS (90.5
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84, TOTAL = 5875.7 SECONDS (97.9 MIN)
WALL CLOCK TIME: STEP = 2.67, TOTAL = 5431.9 SECONDS (90.5 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 59 ENERGY= -284.6359374

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000431	-0.0005591	-0.0003982
2 C	6.0	-0.0003370	-0.0001541	-0.0002102
3 C	6.0	-0.0003401	0.0002792	0.0002877
4 C	6.0	0.0001311	-0.0001690	0.0005964
5 C	6.0	0.0003811	0.0001104	0.0006229
6 C	6.0	0.0003580	0.0004815	0.0001747
7 C	6.0	-0.0003259	0.0007229	-0.0003228
8 C	6.0	-0.0000293	0.0001732	-0.0005434
9 C	6.0	0.0000757	0.0001738	-0.0001497
10 C	6.0	-0.0002775	-0.0001263	-0.0000527
11 C	6.0	0.0001585	-0.0003038	0.0001269
12 N	7.0	0.0001829	0.0004562	0.0005816
13 C	6.0	0.0008016	-0.0004731	-0.0003038
14 C	6.0	-0.0000982	0.0002299	-0.0006771
15 C	6.0	0.0002652	-0.0011013	-0.0009255
16 C	6.0	0.0006644	-0.0001234	-0.0008649
17 C	6.0	0.0001769	-0.0001903	-0.0000877
18 C	6.0	0.0002856	0.0007793	0.0006103
19 C	6.0	0.0003477	-0.0001114	0.0003664
20 O	8.0	-0.0012459	-0.0027319	0.0012163
21 N	7.0	0.0005942	0.0006903	0.0010815
22 H	1.0	-0.0004538	0.0000300	0.0003289
23 H	1.0	-0.0003166	-0.0003844	-0.0000576
24 H	1.0	-0.0008950	-0.0007171	-0.0001576
25 H	1.0	0.0006156	0.0003190	-0.0011422
26 H	1.0	0.0002228	0.0002924	0.0006056
27 H	1.0	0.0000870	-0.0004534	0.0008020
28 H	1.0	-0.0006935	-0.0003615	-0.0005130
29 H	1.0	-0.0003069	-0.0010077	0.0003254
30 H	1.0	-0.0004312	0.0001993	0.0002724
31 H	1.0	-0.0006352	0.0001329	0.0002084
32 H	1.0	-0.0001896	0.0006067	0.0001976
33 H	1.0	0.0000903	0.0037227	-0.0011422

34 H 1.0 -0.0006483 0.0008809 -0.0008432
35 H 1.0 0.0018286 -0.0013128 -0.0000130

MAXIMUM GRADIENT = 0.0037227 RMS GRADIENT = 0.0007132
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0001052970
PREDICTED ENERGY CHANGE WAS -0.0000878604 RATIO= 1.198
GDIIS STEP HAS LENGTH = 0.148006
RADIUS OF STEP TAKEN= 0.14801 CURRENT TRUST RADIUS= 0.15611

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 5875.8 SECONDS (97.9 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5431.9 SECONDS (90.5
MIN)
CPU UTILIZATION: STEP = 92.51% , TOTAL = 100.00%

INSERCH= 60

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1497461545	-1.7642942562	0.8787075093
C	6.0	4.9815045337	0.6583002471	0.5146885157
C	6.0	5.1955662618	-0.7014652104	0.2433502159
C	6.0	4.0668161767	-1.5477699723	-0.0009292171
C	6.0	2.7572302063	-1.0368693303	0.0591872923
C	6.0	2.4739953634	0.3414773104	0.4379430737
C	6.0	3.6481763648	1.2019903701	0.6209932245
C	6.0	3.4896373699	2.6030639981	0.9361906173
C	6.0	2.2205957942	3.1536967791	1.1610466904
C	6.0	1.0656268864	2.3142276876	1.0621844545
C	6.0	1.1642035359	0.9586056621	0.6664888995
N	7.0	-0.0451553934	0.1507658471	0.6245568502
C	6.0	-1.2374893782	0.6805541891	0.3504353340
C	6.0	-2.5504236678	0.0345246955	0.4477450805
C	6.0	-2.8365399755	-1.3155887518	0.8474862344
C	6.0	-4.1422201006	-1.8308640243	0.9390791490
C	6.0	-5.2436912753	-0.9675516151	0.6515906922
C	6.0	-5.0162276363	0.3849949155	0.2675581915
C	6.0	-3.6903777198	0.8699734143	0.1558451578
O	8.0	-1.7276704571	-2.2071864895	1.1950035230
N	7.0	1.6678650524	-1.9925175618	-0.3617036195
H	1.0	5.8394860298	1.3364597773	0.6711846045
H	1.0	6.2143778946	-1.1194974512	0.1819359078
H	1.0	4.2298499160	-2.6077776270	-0.2845975874

H	1.0	4.3982178239	3.2280532517	1.0217464087
H	1.0	2.1077065956	4.2122141723	1.4594001137
H	1.0	0.0868954667	2.7345970333	1.3560320849
H	1.0	-1.2753492973	1.7319881265	0.0035176975
H	1.0	-4.3261376034	-2.8827977089	1.2369014428
H	1.0	-6.2753394119	-1.3577667008	0.7324440298
H	1.0	-5.8706236318	1.0539652930	0.0582305587
H	1.0	-3.5153882998	1.9198815398	-0.1463620967
H	1.0	-2.0712087026	-3.0327200625	1.6284703124
H	1.0	1.3202310168	-1.7397307495	-1.3143195662
H	1.0	2.0821111073	-2.9438317984	-0.4391447796

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4173206	5.1955351	4.0204578
2 C	5.4173206	0.0000000	1.4030000 *	2.4432074 *
3 C	5.1955351	1.4030000 *	0.0000000	1.4317755 *
4 C	4.0204578	2.4432074 *	1.4317755 *	0.0000000
5 C	2.8283800 *	2.8334568 *	2.4681764 *	1.4070000 *
6 C	3.1671251	2.5286101 *	2.9210518 *	2.5097694 *
7 C	4.5939389	1.4438364 *	2.4819696 *	2.8501278 *
8 C	5.4983630	2.4870540 *	3.7828738	4.2942696
9 C	5.3436663	3.7772212	4.9552891	5.1829053
10 C	4.1841179	4.2867173	5.1789277	5.0052346
11 C	2.9134764 *	3.8321030	4.3802702	3.8926246
12 N	1.9416576 *	5.0534119	5.3232302	4.4927238
13 C	2.8602059 *	6.2212024	6.5807028	5.7640735
14 C	3.2729796	7.5580103	7.7835608	6.8185650
15 C	3.0199696	8.0702424	8.0781717	6.9591697
16 C	4.2929070	9.4666994	9.4315341	8.2675289
17 C	5.4566976	10.3545529	10.4506249	9.3513627
18 C	5.6285196	10.0045199	10.2694555	9.2902826
19 C	4.7125840	8.6818844	9.0242494	8.1267533
20 O	1.9547097 *	7.3271326	7.1487095	5.9532479
21 N	1.9736744 *	4.3330249	3.8049418	2.4663587 *
22 H	6.4831228	1.1047731 *	2.1796360 *	3.4515035
23 H	6.1384861	2.1888960 *	1.1029505 *	2.1974709 *
24 H	4.3257357	3.4454474	2.2012187 *	1.1093530 *
25 H	6.5569433	2.6834608 *	4.0844560	4.8953223
26 H	6.3158108	4.6670653	5.9294097	6.2568434
27 H	4.5245786	5.3829421	6.2564448	6.0016481
28 H	3.8756735	6.3688556	6.9175113	6.2686175
29 H	4.6274062	9.9846466	9.8187677	8.5881428

30 H	6.4395949	11.4380278	11.5000705	10.3698659
31 H	6.6978072	10.8689277	11.2060860	10.2725477
32 H	5.2968981	8.6154375	9.1051669	8.3387998
33 H	2.6652746 *	8.0377176	7.7562443	6.5219145
34 H	2.4859618 *	4.7434952	4.3037837	3.0505038
35 H	2.6195568 *	4.7214019	3.8971285	2.4657810 *

C C C C

1 CO	2.8283800 *	3.1671251	4.5939389	5.4983630
2 C	2.8334568 *	2.5286101 *	1.4438364 *	2.4870540 *
3 C	2.4681764 *	2.9210518 *	2.4819696 *	3.7828738
4 C	1.4070000 *	2.5097694 *	2.8501278 *	4.2942696
5 C	0.0000000	1.4572294 *	2.4742481 *	3.8150583
6 C	1.4572294 *	0.0000000	1.4672052 *	2.5287455 *
7 C	2.4742481 *	1.4672052 *	0.0000000	1.4448153 *
8 C	3.8150583	2.5287455 *	1.4448153 *	0.0000000
9 C	4.3661098	2.9147330 *	2.4776606 *	1.4015075 *
10 C	3.8855342	2.5029828 *	2.8462753 *	2.4444074 *
11 C	2.6245894 *	1.4658224 *	2.4962826 *	2.8608783 *
12 N	3.0957204	2.5332422 *	3.8400241	4.3134258
13 C	4.3579988	3.7279686	4.9208563	5.1366215
14 C	5.4286326	5.0337960	6.3099630	6.5816647
15 C	5.6559141	5.5781161	6.9599605	7.4420580
16 C	7.0005037	6.9817270	8.3659824	8.8263795
17 C	8.0231223	7.8308294	9.1527678	9.4393497
18 C	7.9051732	7.4922871	8.7100112	8.8157041
19 C	6.7243617	6.1934145	7.3607727	7.4273251
20 O	4.7722170	4.9722051	6.3915338	7.1011122
21 N	1.5090160 *	2.5955371 *	3.8848690	5.1110423
22 H	3.9379605	3.5172317	2.1960053 *	2.6825926 *
23 H	3.4603128	4.0237356	3.4881897	4.6744598
24 H	2.1804930 *	3.5075910	3.9588851	5.4028797
25 H	4.6700027	3.5179226	2.1972929 *	1.1060967 *
26 H	5.4713211	4.0199684	3.4838801	2.1846842 *
27 H	4.7996305	3.5025927	3.9461230	3.4310669
28 H	4.8919698	4.0224161	4.9903185	4.9329251
29 H	7.4140786	7.5680970	8.9807861	9.5536090
30 H	9.0633086	8.9176802	10.2489484	10.5396615
31 H	8.8775814	8.3835844	9.5365700	9.5281166
32 H	6.9376054	6.2213736	7.2402252	7.1210282
33 H	5.4552627	5.7845867	7.1874299	7.9475985
34 H	2.1084359 *	2.9551689 *	4.2211951	5.3507930
35 H	2.0834170 *	3.4228807	4.5567855	5.8856377

C C C N

1	CO	5.3436663	4.1841179	2.9134764 *	1.9416576 *
2	C	3.7772212	4.2867173	3.8321030	5.0534119
3	C	4.9552891	5.1789277	4.3802702	5.3232302
4	C	5.1829053	5.0052346	3.8926246	4.4927238
5	C	4.3661098	3.8855342	2.6245894 *	3.0957204
6	C	2.9147330 *	2.5029828 *	1.4658224 *	2.5332422 *
7	C	2.4776606 *	2.8462753 *	2.4962826 *	3.8400241
8	C	1.4015075 *	2.4444074 *	2.8608783 *	4.3134258
9	C	0.0000000	1.4312356 *	2.4857548 *	3.7998742
10	C	1.4312356 *	0.0000000	1.4156283 *	2.4710165 *
11	C	2.4857548 *	1.4156283 *	0.0000000	1.4549613 *
12	N	3.7998742	2.4710165 *	1.4549613 *	0.0000000
13	C	4.3280340	2.9120131 *	2.4383050 *	1.3332211 *
14	C	5.7446201	4.3186112	3.8340879	2.5141884 *
15	C	6.7562901	5.3337200	4.6055042	3.1609684
16	C	8.0858235	6.6572224	6.0011314	4.5619865
17	C	8.5416518	7.1236338	6.6911449	5.3175314
18	C	7.7997208	6.4297997	6.2197994	4.9893758
19	C	6.4160292	5.0524154	4.8821688	3.7449427
20	O	6.6580049	5.3163274	4.3202434	2.9523221 *
21	N	5.3951647	4.5758281	3.1654357	2.9156153 *
22	H	4.0790540	4.8886237	4.6905290	6.0030866
23	H	5.9303577	6.2509953	5.4824780	6.4024401
24	H	6.2706919	6.0043539	4.7981083	5.1683454
25	H	2.1833395 *	3.4558465	3.9667932	5.4195039
26	H	1.1055396 *	2.2013775 *	3.4792060	4.6719525
27	H	2.1831951 *	1.1049760 *	2.1886543 *	2.6886199 *
28	H	3.9475006	2.6343780 *	2.6436848 *	2.0974581 *
29	H	8.9053208	7.4907091	6.7249979	5.2824504
30	H	9.6290144	8.2147464	7.7920941	6.4111234
31	H	8.4316610	7.1209379	7.0617183	5.9222103
32	H	6.0110840	4.7541344	4.8459630	3.9707182
33	H	7.5438600	6.2249713	5.2272346	3.9047813
34	H	5.5573130	4.7060784	3.3509650	3.0327379
35	H	6.3055250	5.5618719	4.1586053	3.9029807

C C C C

1	CO	2.8602059 *	3.2729796	3.0199696	4.2929070
2	C	6.2212024	7.5580103	8.0702424	9.4666994
3	C	6.5807028	7.7835608	8.0781717	9.4315341
4	C	5.7640735	6.8185650	6.9591697	8.2675289
5	C	4.3579988	5.4286326	5.6559141	7.0005037
6	C	3.7279686	5.0337960	5.5781161	6.9817270
7	C	4.9208563	6.3099630	6.9599605	8.3659824

8 C	5.1366215	6.5816647	7.4420580	8.8263795
9 C	4.3280340	5.7446201	6.7562901	8.0858235
10 C	2.9120131 *	4.3186112	5.3337200	6.6572224
11 C	2.4383050 *	3.8340879	4.6055042	6.0011314
12 N	1.3332211 *	2.5141884 *	3.1609684	4.5619865
13 C	0.0000000	1.4664991 *	2.6054959 *	3.8847373
14 C	1.4664991 *	0.0000000	1.4368235 *	2.5009798 *
15 C	2.6054959 *	1.4368235 *	0.0000000	1.4066622 *
16 C	3.8847373	2.5009798 *	1.4066622 *	0.0000000
17 C	4.3424188	2.8808680 *	2.4400578 *	1.4287045 *
18 C	3.7911854	2.4970955 *	2.8247725 *	2.4748455 *
19 C	2.4678748 *	1.4431477 *	2.4462396 *	2.8481819 *
20 O	3.0483798	2.5021165 *	1.4646865 *	2.4570645 *
21 N	4.0116753	4.7495334	4.7127526	5.9561109
22 H	7.1145396	8.4932647	9.0740218	10.4755985
23 H	7.6680443	8.8444428	9.0774734	10.4085748
24 H	6.4115670	7.3136993	7.2722233	8.4966191
25 H	6.2210615	7.6688800	8.5449851	9.9266589
26 H	4.9892646	6.3383525	7.4415467	8.7092544
27 H	2.6427849 *	3.8821164	5.0208663	6.2372031
28 H	1.1078351 *	2.1689939 *	3.5266590	4.6677767
29 H	4.7982337	3.5052386	2.1969727 *	1.1086425 *
30 H	5.4479919	3.9867940	3.4409817	2.1947021 *
31 H	4.6573332	3.4949547	3.9298059	3.4764225
32 H	2.6403718 *	2.1997024 *	3.4520773	3.9546420
33 H	4.0145818	3.3214078	2.0357328 *	2.4917476 *
34 H	3.8950124	4.6081256	4.7044708	5.9096940
35 H	4.9778869	5.5783115	5.3385132	6.4715143

C C C O

1 CO	5.4566976	5.6285196	4.7125840	1.9547097 *
2 C	10.3545529	10.0045199	8.6818844	7.3271326
3 C	10.4506249	10.2694555	9.0242494	7.1487095
4 C	9.3513627	9.2902826	8.1267533	5.9532479
5 C	8.0231223	7.9051732	6.7243617	4.7722170
6 C	7.8308294	7.4922871	6.1934145	4.9722051
7 C	9.1527678	8.7100112	7.3607727	6.3915338
8 C	9.4393497	8.8157041	7.4273251	7.1011122
9 C	8.5416518	7.7997208	6.4160292	6.6580049
10 C	7.1236338	6.4297997	5.0524154	5.3163274
11 C	6.6911449	6.2197994	4.8821688	4.3202434
12 N	5.3175314	4.9893758	3.7449427	2.9523221 *
13 C	4.3424188	3.7911854	2.4678748 *	3.0483798
14 C	2.8808680 *	2.4970955 *	1.4431477 *	2.5021165 *
15 C	2.4400578 *	2.8247725 *	2.4462396 *	1.4646865 *

16 C	1.4287045 *	2.4748455 *	2.8481819 *	2.4570645 *
17 C	0.0000000	1.4242903 *	2.4566328 *	3.7675449
18 C	1.4242903 *	0.0000000	1.4161786 *	4.2888422
19 C	2.4566328 *	1.4161786 *	0.0000000	3.7948627
20 O	3.7675449	4.2888422	3.7948627	0.0000000
21 N	7.0602359	7.1221929	6.0969236	3.7415346
22 H	11.3201445	10.9048026	9.5551812	8.3721964
23 H	11.4686971	11.3312545	10.1026164	8.0799446
24 H	9.6599572	9.7340389	8.6613364	6.1515642
25 H	10.5217169	9.8632431	8.4696932	8.1913586
26 H	9.0291517	8.1742604	6.8181823	7.4825616
27 H	6.5281925	5.7225231	4.3800756	5.2668590
28 H	4.8430622	3.9847558	2.5687809 *	4.1402089
29 H	2.2028756 *	3.4776888	3.9567871	2.6851885 *
30 H	1.1059399 *	2.1997044 *	3.4608264	4.6493836
31 H	2.1981017 *	1.1051389 *	2.1901721 *	5.3936467
32 H	3.4584722	2.1862584 *	1.1064617 *	4.6933876
33 H	3.9094578	4.7123236	4.4745223	0.9936889 *
34 H	6.8953709	6.8678603	5.8376485	3.9755403
35 H	7.6656877	7.8719076	6.9441162	4.2104065

N H H H

1 CO	1.9736744 *	6.4831228	6.1384861	4.3257357
2 C	4.3330249	1.1047731 *	2.1888960 *	3.4454474
3 C	3.8049418	2.1796360 *	1.1029505 *	2.2012187 *
4 C	2.4663587 *	3.4515035	2.1974709 *	1.1093530 *
5 C	1.5090160 *	3.9379605	3.4603128	2.1804930 *
6 C	2.5955371 *	3.5172317	4.0237356	3.5075910
7 C	3.8848690	2.1960053 *	3.4881897	3.9588851
8 C	5.1110423	2.6825926 *	4.6744598	5.4028797
9 C	5.3951647	4.0790540	5.9303577	6.2706919
10 C	4.5758281	4.8886237	6.2509953	6.0043539
11 C	3.1654357	4.6905290	5.4824780	4.7981083
12 N	2.9156153 *	6.0030866	6.4024401	5.1683454
13 C	4.0116753	7.1145396	7.6680443	6.4115670
14 C	4.7495334	8.4932647	8.8444428	7.3136993
15 C	4.7127526	9.0740218	9.0774734	7.2722233
16 C	5.9561109	10.4755985	10.4085748	8.4966191
17 C	7.0602359	11.3201445	11.4686971	9.6599572
18 C	7.1221929	10.9048026	11.3312545	9.7340389
19 C	6.0969236	9.5551812	10.1026164	8.6613364
20 O	3.7415346	8.3721964	8.0799446	6.1515642
21 N	0.0000000	5.4361172	4.6613825	2.6359546 *
22 H	5.4361172	0.0000000	2.5321205 *	4.3659428
23 H	4.6613825	2.5321205 *	0.0000000	2.5240806 *

24 H	2.6359546 *	4.3659428	2.5240806 *	0.0000000
25 H	6.0517039	2.4038040 *	4.7859081	5.9826252
26 H	6.4814023	4.7767588	6.8500958	7.3523675
27 H	5.2721621	5.9595387	7.3333885	6.9567740
28 H	4.7610755	7.1570318	8.0161597	7.0159672
29 H	6.2670731	11.0209833	10.7389314	8.6945683
30 H	8.0432932	12.4109470	12.5041141	10.6280715
31 H	8.1416346	11.7295432	12.2795157	10.7492073
32 H	6.4976422	9.4086363	10.1987232	8.9725984
33 H	4.3615921	9.0876410	8.6257653	6.5987684
34 H	1.0450970 *	5.8162566	5.1552055	3.2061994
35 H	1.0404786 *	5.8027229	4.5595576	2.1793575 *

H H H H

1 CO	6.5569433	6.3158108	4.5245786	3.8756735
2 C	2.6834608 *	4.6670653	5.3829421	6.3688556
3 C	4.0844560	5.9294097	6.2564448	6.9175113
4 C	4.8953223	6.2568434	6.0016481	6.2686175
5 C	4.6700027	5.4713211	4.7996305	4.8919698
6 C	3.5179226	4.0199684	3.5025927	4.0224161
7 C	2.1972929 *	3.4838801	3.9461230	4.9903185
8 C	1.1060967 *	2.1846842 *	3.4310669	4.9329251
9 C	2.1833395 *	1.1055396 *	2.1831951 *	3.9475006
10 C	3.4558465	2.2013775 *	1.1049760 *	2.6343780 *
11 C	3.9667932	3.4792060	2.1886543 *	2.6436848 *
12 N	5.4195039	4.6719525	2.6886199 *	2.0974581 *
13 C	6.2210615	4.9892646	2.6427849 *	1.1078351 *
14 C	7.6688800	6.3383525	3.8821164	2.1689939 *
15 C	8.5449851	7.4415467	5.0208663	3.5266590
16 C	9.9266589	8.7092544	6.2372031	4.6677767
17 C	10.5217169	9.0291517	6.5281925	4.8430622
18 C	9.8632431	8.1742604	5.7225231	3.9847558
19 C	8.4696932	6.8181823	4.3800756	2.5687809 *
20 O	8.1913586	7.4825616	5.2668590	4.1402089
21 N	6.0517039	6.4814023	5.2721621	4.7610755
22 H	2.4038040 *	4.7767588	5.9595387	7.1570318
23 H	4.7859081	6.8500958	7.3333885	8.0161597
24 H	5.9826252	7.3523675	6.9567740	7.0159672
25 H	0.0000000	2.5311174 *	4.3523266	5.9551964
26 H	2.5311174 *	0.0000000	2.5055369 *	4.4402908
27 H	4.3523266	2.5055369 *	0.0000000	2.1656940 *
28 H	5.9551964	4.4402908	2.1656940 *	0.0000000
29 H	10.6537866	9.5803471	7.1445207	5.6678738
30 H	11.6205966	10.0910164	7.5904108	5.9226531
31 H	10.5405942	8.6943410	6.3246222	4.6453476

32 H	8.1056124	6.2811191	3.9871541	2.2528965 *
33 H	9.0232409	8.3654641	6.1638935	5.0966957
34 H	6.2936543	6.6135684	5.3545778	4.5306251
35 H	6.7520899	7.4036560	6.2807722	5.7733684

H H H H

1 CO	4.6274062	6.4395949	6.6978072	5.2968981
2 C	9.9846466	11.4380278	10.8689277	8.6154375
3 C	9.8187677	11.5000705	11.2060860	9.1051669
4 C	8.5881428	10.3698659	10.2725477	8.3387998
5 C	7.4140786	9.0633086	8.8775814	6.9376054
6 C	7.5680970	8.9176802	8.3835844	6.2213736
7 C	8.9807861	10.2489484	9.5365700	7.2402252
8 C	9.5536090	10.5396615	9.5281166	7.1210282
9 C	8.9053208	9.6290144	8.4316610	6.0110840
10 C	7.4907091	8.2147464	7.1209379	4.7541344
11 C	6.7249979	7.7920941	7.0617183	4.8459630
12 N	5.2824504	6.4111234	5.9222103	3.9707182
13 C	4.7982337	5.4479919	4.6573332	2.6403718 *
14 C	3.5052386	3.9867940	3.4949547	2.1997024 *
15 C	2.1969727 *	3.4409817	3.9298059	3.4520773
16 C	1.1086425 *	2.1947021 *	3.4764225	3.9546420
17 C	2.2028756 *	1.1059399 *	2.1981017 *	3.4584722
18 C	3.4776888	2.1997044 *	1.1051389 *	2.1862584 *
19 C	3.9567871	3.4608264	2.1901721 *	1.1064617 *
20 O	2.6851885 *	4.6493836	5.3936467	4.6933876
21 N	6.2670731	8.0432932	8.1416346	6.4976422
22 H	11.0209833	12.4109470	11.7295432	9.4086363
23 H	10.7389314	12.5041141	12.2795157	10.1987232
24 H	8.6945683	10.6280715	10.7492073	8.9725984
25 H	10.6537866	11.6205966	10.5405942	8.1056124
26 H	9.5803471	10.0910164	8.6943410	6.2811191
27 H	7.1445207	7.5904108	6.3246222	3.9871541
28 H	5.6678738	5.9226531	4.6453476	2.2528965 *
29 H	0.0000000	2.5257839 *	4.3900803	5.0632460
30 H	2.5257839 *	0.0000000	2.5366927 *	4.3740837
31 H	4.3900803	2.5366927 *	0.0000000	2.5176979 *
32 H	5.0632460	4.3740837	2.5176979 *	0.0000000
33 H	2.2935796 *	4.6133553	5.7967408	5.4556345
34 H	6.3005404	7.8757747	7.8356252	6.1757672
35 H	6.6240854	8.5869204	8.9149175	7.4211474

H H H

1 CO	2.6652746 *	2.4859618 *	2.6195568 *
------	-------------	-------------	-------------

2 C	8.0377176	4.7434952	4.7214019
3 C	7.7562443	4.3037837	3.8971285
4 C	6.5219145	3.0505038	2.4657810 *
5 C	5.4552627	2.1084359 *	2.0834170 *
6 C	5.7845867	2.9551689 *	3.4228807
7 C	7.1874299	4.2211951	4.5567855
8 C	7.9475985	5.3507930	5.8856377
9 C	7.5438600	5.5573130	6.3055250
10 C	6.2249713	4.7060784	5.5618719
11 C	5.2272346	3.3509650	4.1586053
12 N	3.9047813	3.0327379	3.9029807
13 C	4.0145818	3.8950124	4.9778869
14 C	3.3214078	4.6081256	5.5783115
15 C	2.0357328 *	4.7044708	5.3385132
16 C	2.4917476 *	5.9096940	6.4715143
17 C	3.9094578	6.8953709	7.6656877
18 C	4.7123236	6.8678603	7.8719076
19 C	4.4745223	5.8376485	6.9441162
20 O	0.9936889 *	3.9755403	4.2104065
21 N	4.3615921	1.0450970 *	1.0404786 *
22 H	9.0876410	5.8162566	5.8027229
23 H	8.6257653	5.1552055	4.5595576
24 H	6.5987684	3.2061994	2.1793575 *
25 H	9.0232409	6.2936543	6.7520899
26 H	8.3654641	6.6135684	7.4036560
27 H	6.1638935	5.3545778	6.2807722
28 H	5.0966957	4.5306251	5.7733684
29 H	2.2935796 *	6.3005404	6.6240854
30 H	4.6133553	7.8757747	8.5869204
31 H	5.7967408	7.8356252	8.9149175
32 H	5.4556345	6.1757672	7.4211474
33 H	0.0000000	4.6726542	4.6403662
34 H	4.6726542	0.0000000	1.6721996 *
35 H	4.6403662	1.6721996 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.61 , TOTAL = 5876.4 SECONDS (97.9 MIN)
WALL CLOCK TIME: STEP = 0.60 , TOTAL = 5432.5 SECONDS (90.5 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.95 , TOTAL = 5877.3 SECONDS (98.0 MIN)
 WALL CLOCK TIME: STEP = 0.95 , TOTAL = 5433.5 SECONDS (90.6 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
 INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.635543115	-284.635543115	0.020262134	0.002323373	197493200
11369938						
2	1	-284.635988870	-0.000445755	0.004079198	0.000421510	162662916
14381012						
3	2	-284.635977263	0.000011607	0.003467408	0.000646190	150286444
15379739						
4	3	-284.636001435	-0.000024173	0.000939499	0.000109223	144530304
15823196						
5	4	-284.636000413	0.000001023	0.000516784	0.000314530	137014721
16463286						
6	5	-284.636002042	-0.000001630	0.000517085	0.000073042	130769236
16966430						
7	6	-284.636002091	-0.000000048	0.000395984	0.000057526	149699923
15444745						
8	7	-284.636002323	-0.000000232	0.000569780	0.000035536	145018176
15859142						
9	8	-284.636002429	-0.000000106	0.000466048	0.000039455	168113742
14020088						
10	9	-284.636002510	-0.000000081	0.000188635	0.000039898	165744549
14225406						
11	10	-284.636002569	-0.000000059	0.000326855	0.000033426	162253552
14432235						

-----DISABLING FDIFF OPTION-----

12	11	-284.636002630	-0.000000061	0.000460399	0.000027345	197482294
11371243						
13	12	-284.636002697	-0.000000067	0.000512674	0.000024586	197482423
11371240						
14	13	-284.636002731	-0.000000035	0.000177578	0.000023972	197482367
11371248						
15	14	-284.636002753	-0.000000022	0.000196065	0.000020981	197482353
11371247						
16	15	-284.636002774	-0.000000021	0.000285588	0.000017100	197482311
11371240						

17 16	-284.636002795	-0.000000021	0.000288262	0.000010785	197482320
11371238					
18 17	-284.636002802	-0.000000007	0.000089255	0.000007783	197482227
11371251					
19 18	-284.636002806	-0.000000004	0.000050883	0.000005171	197482218
11371250					
20 19	-284.636002807	-0.000000001	0.000030432	0.000003839	197482230
11371251					
21 20	-284.636002808	-0.000000001	0.000077603	0.000003727	197482215
11371251					
22 21	-284.636002810	-0.000000002	0.000074518	0.000004174	197482196
11371252					
23 22	-284.636002811	-0.000000001	0.000059211	0.000004617	197482125
11371256					
24 23	-284.636002813	-0.000000001	0.000127567	0.000004272	197482122
11371255					
25 24	-284.636002814	-0.000000002	0.000093376	0.000002865	197482140
11371253					
26 25	-284.636002815	-0.000000001	0.000024360	0.000002890	197482152
11371252					
27 26	-284.636002815	0.000000000	0.000019672	0.000001101	197482131
11371254					

 DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 91.6 SECONDS (3.4 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 29.2 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
 TIME TO SOLVE SCF EQUATIONS= 3.5 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6360028154 AFTER 27 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.5969343008
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999494252

 SPIN SZ = 1.500
 S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
 PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 96.11 , TOTAL = 5973.4 SECONDS (99.6 MIN)
WALL CLOCK TIME: STEP = 87.87 , TOTAL = 5521.3 SECONDS (92.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.92 , TOTAL = 5977.3 SECONDS (99.6 MIN)
WALL CLOCK TIME: STEP = 3.89 , TOTAL = 5525.2 SECONDS (92.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.95 , TOTAL = 5980.3 SECONDS (99.7 MIN)
WALL CLOCK TIME: STEP = 2.76 , TOTAL = 5528.0 SECONDS (92.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 60 ENERGY= -284.6360028

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0008254	-0.0003963	-0.0010732
2 C	6.0	-0.0007623	0.0011862	0.0000265
3 C	6.0	0.0003810	-0.0004688	0.0004066
4 C	6.0	0.0000403	-0.0009152	0.0007730
5 C	6.0	0.0004726	0.0003837	0.0007450
6 C	6.0	0.0005330	0.0001197	0.0001055
7 C	6.0	0.0002741	0.0005679	-0.0004174
8 C	6.0	-0.0010899	0.0003564	-0.0004903
9 C	6.0	0.0004738	0.0001310	-0.0003670
10 C	6.0	0.0000441	-0.0002130	-0.0003911
11 C	6.0	-0.0003600	-0.0005174	0.0001699
12 N	7.0	0.0001088	0.0004722	0.0008210
13 C	6.0	0.0008150	-0.0002878	-0.0002804
14 C	6.0	-0.0004959	0.0001390	-0.0004508
15 C	6.0	0.0003703	-0.0004812	-0.0005512

16 C	6.0	0.0006240	0.0001038	-0.0006468
17 C	6.0	0.0004490	-0.0005053	0.0000244
18 C	6.0	0.0001217	0.0006828	0.0005609
19 C	6.0	0.0005880	0.0000403	0.0001528
20 O	8.0	0.0009585	0.0010493	-0.0015731
21 N	7.0	0.0009810	-0.0001100	0.0003005
22 H	1.0	-0.0002041	-0.0001996	0.0003215
23 H	1.0	-0.0010065	-0.0001417	-0.0002880
24 H	1.0	-0.0008263	-0.0011499	-0.0003562
25 H	1.0	0.0006521	0.0004376	-0.0009966
26 H	1.0	0.0002077	0.0006571	0.0008865
27 H	1.0	-0.0002608	-0.0001275	0.0010928
28 H	1.0	-0.0007313	-0.0004782	-0.0006090
29 H	1.0	-0.0002151	-0.0011374	0.0002451
30 H	1.0	-0.0005951	0.0001965	0.0000679
31 H	1.0	-0.0006769	0.0003570	0.0003333
32 H	1.0	-0.0000941	0.0004411	0.0000735
33 H	1.0	-0.0018687	-0.0003626	0.0012271
34 H	1.0	-0.0009411	0.0007155	-0.0002412
35 H	1.0	0.0012076	-0.0005450	0.0003982

MAXIMUM GRADIENT = 0.0018687 RMS GRADIENT = 0.0006257
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000653796
 PREDICTED ENERGY CHANGE WAS -0.0000404881 RATIO= 1.615
 GDIIS STEP HAS LENGTH = 0.052441
 RADIUS OF STEP TAKEN= 0.05244 CURRENT TRUST RADIUS= 0.14801

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 5980.3 SECONDS (99.7 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5528.0 SECONDS (92.1
 MIN)
 CPU UTILIZATION: STEP = 92.12% , TOTAL = 100.00%

INSERCH= 61

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1510897049	-1.7641957130	0.8799147737
C	6.0	4.9820494215	0.6579758973	0.5151493782
C	6.0	5.1951718265	-0.7016440262	0.2416404991
C	6.0	4.0667396416	-1.5476877320	-0.0009570579
C	6.0	2.7567837710	-1.0379594277	0.0587591984
C	6.0	2.4732915018	0.3404745569	0.4387230636

C	6.0	3.6479959238	1.2007153014	0.6233448910
C	6.0	3.4885852304	2.6013065807	0.9389512170
C	6.0	2.2195394949	3.1528351402	1.1586250030
C	6.0	1.0644835716	2.3144571160	1.0587810896
C	6.0	1.1640638289	0.9585297421	0.6663124385
N	7.0	-0.0462047406	0.1496156041	0.6265733345
C	6.0	-1.2388574060	0.6809379151	0.3556997938
C	6.0	-2.5506412613	0.0362378900	0.4550133089
C	6.0	-2.8367335038	-1.3126048847	0.8549083400
C	6.0	-4.1430237608	-1.8289506305	0.9446179459
C	6.0	-5.2434979314	-0.9674247307	0.6509206267
C	6.0	-5.0163651755	0.3850676958	0.2653083725
C	6.0	-3.6916716901	0.8705433796	0.1582543299
O	8.0	-1.7270431735	-2.2065670438	1.1941793700
N	7.0	1.6675802645	-1.9933189034	-0.3615480101
H	1.0	5.8417299988	1.3349848271	0.6687163256
H	1.0	6.2145457396	-1.1171102076	0.1757632550
H	1.0	4.2334541365	-2.6072016363	-0.2829115726
H	1.0	4.3953434374	3.2276610509	1.0300362431
H	1.0	2.1057067907	4.2116659597	1.4542940269
H	1.0	0.0864274598	2.7378340054	1.3491306826
H	1.0	-1.2734459648	1.7321601025	0.0071269446
H	1.0	-4.3254867984	-2.8798680305	1.2392842841
H	1.0	-6.2739832247	-1.3587423741	0.7249326743
H	1.0	-5.8691368079	1.0535942904	0.0542665985
H	1.0	-3.5158488238	1.9194932022	-0.1451277820
H	1.0	-2.0678415967	-3.0349185203	1.6169064133
H	1.0	1.3204276492	-1.7428170101	-1.3148924946
H	1.0	2.0807694657	-2.9439743863	-0.4378105051

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4164694	5.1941481	4.0193439
2 C	5.4164694	0.0000000	1.4031374 *	2.4431762 *
3 C	5.1941481	1.4031374 *	0.0000000	1.4310845 *
4 C	4.0193439	2.4431762 *	1.4310845 *	0.0000000
5 C	2.8268989 *	2.8348361 *	2.4682565 *	1.4069020 *
6 C	3.1649500	2.5299238 *	2.9212130 *	2.5094925 *
7 C	4.5918274	1.4442891 *	2.4816169 *	2.8493540 *
8 C	5.4954501	2.4872831 *	3.7826132	4.2932323
9 C	5.3416623	3.7775448	4.9550235	5.1818620
10 C	4.1835022	4.2879818	5.1794952	5.0052721
11 C	2.9128983 *	3.8327793	4.3802232	3.8925443

12 N	1.9405620 *	5.0551148	5.3239877	4.4934335
13 C	2.8610195 *	6.2229923	6.5818899	5.7657035
14 C	3.2743629	7.5585451	7.7838049	6.8195645
15 C	3.0218615	8.0704393	8.0784203	6.9602953
16 C	4.2950891	9.4676400	9.4322264	8.2688231
17 C	5.4579170	10.3548143	10.4500706	9.3510520
18 C	5.6302455	10.0052583	10.2692254	9.2902763
19 C	4.7148127	8.6836626	9.0252265	8.1281078
20 O	1.9549521 *	7.3265689	7.1476698	5.9523434
21 N	1.9731880 *	4.3340129	3.8047553	2.4666939 *
22 H	6.4832794	1.1049772 *	2.1790567 *	3.4509208
23 H	6.1384076	2.1875010 *	1.1027580 *	2.1976574 *
24 H	4.3276464	3.4436435	2.1980004 *	1.1089913 *
25 H	6.5539957	2.6856311 *	4.0866529	4.8964154
26 H	6.3135855	4.6673389	5.9292443	6.2556823
27 H	4.5268771	5.3840922	6.2574606	6.0026093
28 H	3.8749922	6.3673527	6.9153030	6.2669809
29 H	4.6274840	9.9835335	9.8174790	8.5873376
30 H	6.4397185	11.4371951	11.4981245	10.3678911
31 H	6.6981164	10.8681723	11.2042356	10.2708986
32 H	5.2978028	8.6163604	9.1050443	8.3389314
33 H	2.6611180 *	8.0344447	7.7515734	6.5163199
34 H	2.4869635 *	4.7455594	4.3035426	3.0506936
35 H	2.6176214 *	4.7222456	3.8973326	2.4666850 *

C C C C

1 CO	2.8268989 *	3.1649500	4.5918274	5.4954501
2 C	2.8348361 *	2.5299238 *	1.4442891 *	2.4872831 *
3 C	2.4682565 *	2.9212130 *	2.4816169 *	3.7826132
4 C	1.4069020 *	2.5094925 *	2.8493540 *	4.2932323
5 C	0.0000000	1.4576765 *	2.4748092 *	3.8150398
6 C	1.4576765 *	0.0000000	1.4676613 *	2.5283218 *
7 C	2.4748092 *	1.4676613 *	0.0000000	1.4445328 *
8 C	3.8150398	2.5283218 *	1.4445328 *	0.0000000
9 C	4.3659014	2.9141072 *	2.4774552 *	1.4010415 *
10 C	3.8862090	2.5031618 *	2.8468512 *	2.4439539 *
11 C	2.6252327 *	1.4655600 *	2.4960807 *	2.8594488 *
12 N	3.0966905	2.5336883 *	3.8408254	4.3131321
13 C	4.3598085	3.7286536	4.9217007	5.1358263
14 C	5.4295191	5.0331626	6.3093142	6.5792120
15 C	5.6565642	5.5769389	6.9586001	7.4387783
16 C	7.0012682	6.9812580	8.3655293	8.8243225
17 C	8.0224770	7.8297169	9.1520629	9.4375887
18 C	7.9050309	7.4917967	8.7100301	8.8147428
19 C	6.7256866	6.1940622	7.3617962	7.4270531

20	O	4.7706946	4.9700047	6.3895595	7.0981385
21	N	1.5085537 *	2.5954183 *	3.8850888	5.1105715
22	H	3.9395184	3.5197053	2.1983075 *	2.6858682 *
23	H	3.4606463	4.0237650	3.4870937	4.6733222
24	H	2.1817001 *	3.5082366	3.9578142	5.4015124
25	H	4.6715923	3.5184913	2.1982801 *	1.1058150 *
26	H	5.4708304	4.0190329	3.4835264	2.1843050 *
27	H	4.8012996	3.5033262	3.9464248	3.4295137
28	H	4.8907034	4.0200877	4.9882611	4.9295693
29	H	7.4124775	7.5653745	8.9781384	9.5495129
30	H	9.0609846	8.9153839	10.2472832	10.5373400
31	H	8.8758731	8.3816739	9.5352667	9.5260192
32	H	6.9378682	6.2212526	7.2407088	7.1205473
33	H	5.4490989	5.7795574	7.1832136	7.9435846
34	H	2.1087584 *	2.9570875 *	4.2235910	5.3527683
35	H	2.0824192 *	3.4219862	4.5563914	5.8845186

C C C N

1	CO	5.3416623	4.1835022	2.9128983 *	1.9405620 *
2	C	3.7775448	4.2879818	3.8327793	5.0551148
3	C	4.9550235	5.1794952	4.3802232	5.3239877
4	C	5.1818620	5.0052721	3.8925443	4.4934335
5	C	4.3659014	3.8862090	2.6252327 *	3.0966905
6	C	2.9141072 *	2.5031618 *	1.4655600 *	2.5336883 *
7	C	2.4774552 *	2.8468512 *	2.4960807 *	3.8408254
8	C	1.4010415 *	2.4439539 *	2.8594488 *	4.3131321
9	C	0.0000000	1.4307343 *	2.4842256 *	3.7994741
10	C	1.4307343 *	0.0000000	1.4150925 *	2.4712286 *
11	C	2.4842256 *	1.4150925 *	0.0000000	1.4562525 *
12	N	3.7994741	2.4712286 *	1.4562525 *	0.0000000
13	C	4.3261385	2.9099979 *	2.4387636 *	1.3334528 *
14	C	5.7413302	4.3155470	3.8333149	2.5128648 *
15	C	6.7526510	5.3307258	4.6043458	3.1586827
16	C	8.0836996	6.6557489	6.0010565	4.5606801
17	C	8.5399785	7.1223402	6.6907687	5.3160350
18	C	7.7985170	6.4287529	6.2199169	4.9888320
19	C	6.4149836	5.0514204	4.8830351	3.7454624
20	O	6.6558223	5.3151306	4.3191412	2.9494052 *
21	N	5.3943013	4.5758054	3.1659811	2.9164381 *
22	H	4.0822609	4.8921979	4.6927907	6.0062178
23	H	5.9294625	6.2512811	5.4823615	6.4035007
24	H	6.2699205	6.0054341	4.7996483	5.1713329
25	H	2.1808844 *	3.4538956	3.9651507	5.4189018
26	H	1.1052153 *	2.1999949 *	3.4771399	4.6707706
27	H	2.1814411 *	1.1046016 *	2.1893982 *	2.6904563 *

28 H	3.9427418	2.6288706 *	2.6409247 *	2.0962543 *
29 H	8.9015382	7.4876816	6.7228536	5.2787727
30 H	9.6271672	8.2132177	7.7908748	6.4085914
31 H	8.4293003	7.1185614	7.0604213	5.9204096
32 H	6.0096242	4.7523508	4.8459745	3.9706951
33 H	7.5418800	6.2240489	5.2246024	3.8998760
34 H	5.5582462	4.7075797	3.3536394	3.0361612
35 H	6.3038837	5.5609105	4.1580013	3.9022085

C C C C

1 CO	2.8610195 *	3.2743629	3.0218615	4.2950891
2 C	6.2229923	7.5585451	8.0704393	9.4676400
3 C	6.5818899	7.7838049	8.0784203	9.4322264
4 C	5.7657035	6.8195645	6.9602953	8.2688231
5 C	4.3598085	5.4295191	5.6565642	7.0012682
6 C	3.7286536	5.0331626	5.5769389	6.9812580
7 C	4.9217007	6.3093142	6.9586001	8.3655293
8 C	5.1358263	6.5792120	7.4387783	8.8243225
9 C	4.3261385	5.7413302	6.7526510	8.0836996
10 C	2.9099979 *	4.3155470	5.3307258	6.6557489
11 C	2.4387636 *	3.8333149	4.6043458	6.0010565
12 N	1.3334528 *	2.5128648 *	3.1586827	4.5606801
13 C	0.0000000	1.4650181 *	2.6031961 *	3.8833680
14 C	1.4650181 *	0.0000000	1.4356677 *	2.5008644 *
15 C	2.6031961 *	1.4356677 *	0.0000000	1.4074995 *
16 C	3.8833680	2.5008644 *	1.4074995 *	0.0000000
17 C	4.3406682	2.8804853 *	2.4399335 *	1.4281206 *
18 C	3.7901550	2.4974917 *	2.8249804 *	2.4750887 *
19 C	2.4680423 *	1.4443275 *	2.4458909 *	2.8476928 *
20 O	3.0461547	2.5009707 *	1.4648160 *	2.4580149 *
21 N	4.0141592	4.7517645	4.7150801	5.9578692
22 H	7.1176172	8.4949578	9.0752481	10.4776866
23 H	7.6693267	8.8451510	9.0788277	10.4104323
24 H	6.4160642	7.3182140	7.2772363	8.5016402
25 H	6.2197064	7.6656726	8.5409380	9.9237257
26 H	4.9858860	6.3335881	7.4367027	8.7060584
27 H	2.6408534 *	3.8797163	5.0194801	6.2375805
28 H	1.1080467 *	2.1697885 *	3.5260736	4.6684982
29 H	4.7945116	3.5026892	2.1955512 *	1.1065931 *
30 H	5.4451006	3.9852355	3.4400157	2.1932500 *
31 H	4.6550212	3.4939984	3.9287906	3.4758103
32 H	2.6399881 *	2.1996467 *	3.4507576	3.9536977
33 H	4.0106665	3.3188993	2.0342566 *	2.4925311 *
34 H	3.9006931	4.6133261	4.7090452	5.9128764
35 H	4.9789126	5.5793158	5.3398805	6.4722476

	C	C	C	O
1 CO	5.4579170	5.6302455	4.7148127	1.9549521 *
2 C	10.3548143	10.0052583	8.6836626	7.3265689
3 C	10.4500706	10.2692254	9.0252265	7.1476698
4 C	9.3510520	9.2902763	8.1281078	5.9523434
5 C	8.0224770	7.9050309	6.7256866	4.7706946
6 C	7.8297169	7.4917967	6.1940622	4.9700047
7 C	9.1520629	8.7100301	7.3617962	6.3895595
8 C	9.4375887	8.8147428	7.4270531	7.0981385
9 C	8.5399785	7.7985170	6.4149836	6.6558223
10 C	7.1223402	6.4287529	5.0514204	5.3151306
11 C	6.6907687	6.2199169	4.8830351	4.3191412
12 N	5.3160350	4.9888320	3.7454624	2.9494052 *
13 C	4.3406682	3.7901550	2.4680423 *	3.0461547
14 C	2.8804853 *	2.4974917 *	1.4443275 *	2.5009707 *
15 C	2.4399335 *	2.8249804 *	2.4458909 *	1.4648160 *
16 C	1.4281206 *	2.4750887 *	2.8476928 *	2.4580149 *
17 C	0.0000000	1.4246129 *	2.4554046 *	3.7677656
18 C	1.4246129 *	0.0000000	1.4149064 *	4.2894069
19 C	2.4554046 *	1.4149064 *	0.0000000	3.7949327
20 O	3.7677656	4.2894069	3.7949327	0.0000000
21 N	7.0597842	7.1221344	6.0986460	3.7402180
22 H	11.3218234	10.9070304	9.5583484	8.3728746
23 H	11.4688685	11.3312805	10.1036734	8.0804036
24 H	9.6629981	9.7372161	8.6658501	6.1538471
25 H	10.5190178	9.8613085	8.4685194	8.1878810
26 H	9.0265829	8.1719306	6.8156009	7.4800633
27 H	6.5287475	5.7226456	4.3793828	5.2687558
28 H	4.8439180	3.9863216	2.5715829 *	4.1386490
29 H	2.2014440 *	3.4764561	3.9542298	2.6846374 *
30 H	1.1047657 *	2.1985748 *	3.4582036	4.6490497
31 H	2.1981669 *	1.1039411 *	2.1876187 *	5.3930504
32 H	3.4572763	2.1850558 *	1.1060064 *	4.6923280
33 H	3.9105565	4.7134822	4.4740499	0.9904584 *
34 H	6.8957069	6.8687605	5.8413144	3.9746175
35 H	7.6640053	7.8705919	6.9445602	4.2079208

	N	H	H	H
1 CO	1.9731880 *	6.4832794	6.1384076	4.3276464
2 C	4.3340129	1.1049772 *	2.1875010 *	3.4436435
3 C	3.8047553	2.1790567 *	1.1027580 *	2.1980004 *
4 C	2.4666939 *	3.4509208	2.1976574 *	1.1089913 *
5 C	1.5085537 *	3.9395184	3.4606463	2.1817001 *

6 C	2.5954183 *	3.5197053	4.0237650	3.5082366
7 C	3.8850888	2.1983075 *	3.4870937	3.9578142
8 C	5.1105715	2.6858682 *	4.6733222	5.4015124
9 C	5.3943013	4.0822609	5.9294625	6.2699205
10 C	4.5758054	4.8921979	6.2512811	6.0054341
11 C	3.1659811	4.6927907	5.4823615	4.7996483
12 N	2.9164381 *	6.0062178	6.4035007	5.1713329
13 C	4.0141592	7.1176172	7.6693267	6.4160642
14 C	4.7517645	8.4949578	8.8451510	7.3182140
15 C	4.7150801	9.0752481	9.0788277	7.2772363
16 C	5.9578692	10.4776866	10.4104323	8.5016402
17 C	7.0597842	11.3218234	11.4688685	9.6629981
18 C	7.1221344	10.9070304	11.3312805	9.7372161
19 C	6.0986460	9.5583484	10.1036734	8.6658501
20 O	3.7402180	8.3728746	8.0804036	6.1538471
21 N	0.0000000	5.4371478	4.6616885	2.6394591 *
22 H	5.4371478	0.0000000	2.5287871 *	4.3626805
23 H	4.6616885	2.5287871 *	0.0000000	2.5210075 *
24 H	2.6394591 *	4.3626805	2.5210075 *	0.0000000
25 H	6.0527539	2.4093172 *	4.7870990	5.9829477
26 H	6.4800520	4.7801983	6.8493105	7.3513364
27 H	5.2735447	5.9627558	7.3342498	6.9592240
28 H	4.7607510	7.1568972	8.0135385	7.0171313
29 H	6.2662179	11.0210176	10.7392122	8.6975225
30 H	8.0406193	12.4116813	12.5029328	10.6292352
31 H	8.1399439	11.7303508	12.2777076	10.7506958
32 H	6.4980669	9.4110719	10.1982601	8.9756140
33 H	4.3534570	9.0860576	8.6228083	6.5953452
34 H	1.0450511 *	5.8180532	5.1542172	3.2090292
35 H	1.0393686 *	5.8033368	4.5609222	2.1843674 *

H H H H

1 CO	6.5539957	6.3135855	4.5268771	3.8749922
2 C	2.6856311 *	4.6673389	5.3840922	6.3673527
3 C	4.0866529	5.9292443	6.2574606	6.9153030
4 C	4.8964154	6.2556823	6.0026093	6.2669809
5 C	4.6715923	5.4708304	4.8012996	4.8907034
6 C	3.5184913	4.0190329	3.5033262	4.0200877
7 C	2.1982801 *	3.4835264	3.9464248	4.9882611
8 C	1.1058150 *	2.1843050 *	3.4295137	4.9295693
9 C	2.1808844 *	1.1052153 *	2.1814411 *	3.9427418
10 C	3.4538956	2.1999949 *	1.1046016 *	2.6288706 *
11 C	3.9651507	3.4771399	2.1893982 *	2.6409247 *
12 N	5.4189018	4.6707706	2.6904563 *	2.0962543 *
13 C	6.2197064	4.9858860	2.6408534 *	1.1080467 *

14 C	7.6656726	6.3335881	3.8797163	2.1697885 *
15 C	8.5409380	7.4367027	5.0194801	3.5260736
16 C	9.9237257	8.7060584	6.2375805	4.6684982
17 C	10.5190178	9.0265829	6.5287475	4.8439180
18 C	9.8613085	8.1719306	5.7226456	3.9863216
19 C	8.4685194	6.8156009	4.3793828	2.5715829 *
20 O	8.1878810	7.4800633	5.2687558	4.1386490
21 N	6.0527539	6.4800520	5.2735447	4.7607510
22 H	2.4093172 *	4.7801983	5.9627558	7.1568972
23 H	4.7870990	6.8493105	7.3342498	8.0135385
24 H	5.9829477	7.3513364	6.9592240	7.0171313
25 H	0.0000000	2.5279827 *	4.3483915	5.9513057
26 H	2.5279827 *	0.0000000	2.5021449 *	4.4340631
27 H	4.3483915	2.5021449 *	0.0000000	2.1590761 *
28 H	5.9513057	4.4340631	2.1590761 *	0.0000000
29 H	10.6488768	9.5758203	7.1439226	5.6660364
30 H	11.6173455	10.0886383	7.5912045	5.9223556
31 H	10.5374687	8.6908932	6.3231386	4.6457559
32 H	8.1042752	6.2780645	3.9848318	2.2553593 *
33 H	9.0187072	8.3640861	6.1674347	5.0938682
34 H	6.2975749	6.6136922	5.3568656	4.5333632
35 H	6.7528446	7.4016127	6.2812025	5.7719117

H H H H

1 CO	4.6274840	6.4397185	6.6981164	5.2978028
2 C	9.9835335	11.4371951	10.8681723	8.6163604
3 C	9.8174790	11.4981245	11.2042356	9.1050443
4 C	8.5873376	10.3678911	10.2708986	8.3389314
5 C	7.4124775	9.0609846	8.8758731	6.9378682
6 C	7.5653745	8.9153839	8.3816739	6.2212526
7 C	8.9781384	10.2472832	9.5352667	7.2407088
8 C	9.5495129	10.5373400	9.5260192	7.1205473
9 C	8.9015382	9.6271672	8.4293003	6.0096242
10 C	7.4876816	8.2132177	7.1185614	4.7523508
11 C	6.7228536	7.7908748	7.0604213	4.8459745
12 N	5.2787727	6.4085914	5.9204096	3.9706951
13 C	4.7945116	5.4451006	4.6550212	2.6399881 *
14 C	3.5026892	3.9852355	3.4939984	2.1996467 *
15 C	2.1955512 *	3.4400157	3.9287906	3.4507576
16 C	1.1065931 *	2.1932500 *	3.4758103	3.9536977
17 C	2.2014440 *	1.1047657 *	2.1981669 *	3.4572763
18 C	3.4764561	2.1985748 *	1.1039411 *	2.1850558 *
19 C	3.9542298	3.4582036	2.1876187 *	1.1060064 *
20 O	2.6846374 *	4.6490497	5.3930504	4.6923280
21 N	6.2662179	8.0406193	8.1399439	6.4980669

22 H	11.0210176	12.4116813	11.7303508	9.4110719
23 H	10.7392122	12.5029328	12.2777076	10.1982601
24 H	8.6975225	10.6292352	10.7506958	8.9756140
25 H	10.6488768	11.6173455	10.5374687	8.1042752
26 H	9.5758203	10.0886383	8.6908932	6.2780645
27 H	7.1439226	7.5912045	6.3231386	3.9848318
28 H	5.6660364	5.9223556	4.6457559	2.2553593 *
29 H	0.0000000	2.5248800 *	4.3885360	5.0602350
30 H	2.5248800 *	0.0000000	2.5363481 *	4.3716289
31 H	4.3885360	2.5363481 *	0.0000000	2.5154529 *
32 H	5.0602350	4.3716289	2.5154529 *	0.0000000
33 H	2.2942539 *	4.6148468	5.7972084	5.4541438
34 H	6.3002424	7.8729586	7.8348165	6.1782227
35 H	6.6224524	8.5829380	8.9119978	7.4203178

H H H

1 CO	2.6611180 *	2.4869635 *	2.6176214 *
2 C	8.0344447	4.7455594	4.7222456
3 C	7.7515734	4.3035426	3.8973326
4 C	6.5163199	3.0506936	2.4666850 *
5 C	5.4490989	2.1087584 *	2.0824192 *
6 C	5.7795574	2.9570875 *	3.4219862
7 C	7.1832136	4.2235910	4.5563914
8 C	7.9435846	5.3527683	5.8845186
9 C	7.5418800	5.5582462	6.3038837
10 C	6.2240489	4.7075797	5.5609105
11 C	5.2246024	3.3536394	4.1580013
12 N	3.8998760	3.0361612	3.9022085
13 C	4.0106665	3.9006931	4.9789126
14 C	3.3188993	4.6133261	5.5793158
15 C	2.0342566 *	4.7090452	5.3398805
16 C	2.4925311 *	5.9128764	6.4722476
17 C	3.9105565	6.8957069	7.6640053
18 C	4.7134822	6.8687605	7.8705919
19 C	4.4740499	5.8413144	6.9445602
20 O	0.9904584 *	3.9746175	4.2079208
21 N	4.3534570	1.0450511 *	1.0393686 *
22 H	9.0860576	5.8180532	5.8033368
23 H	8.6228083	5.1542172	4.5609222
24 H	6.5953452	3.2090292	2.1843674 *
25 H	9.0187072	6.2975749	6.7528446
26 H	8.3640861	6.6136922	7.4016127
27 H	6.1674347	5.3568656	6.2812025
28 H	5.0938682	4.5333632	5.7719117
29 H	2.2942539 *	6.3002424	6.6224524

30 H	4.6148468	7.8729586	8.5829380
31 H	5.7972084	7.8348165	8.9119978
32 H	5.4541438	6.1782227	7.4203178
33 H	0.0000000	4.6631899	4.6304542
34 H	4.6631899	0.0000000	1.6703807 *
35 H	4.6304542	1.6703807 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.81 , TOTAL = 5981.1 SECONDS (99.7 MIN)
WALL CLOCK TIME: STEP = 0.80 , TOTAL = 5528.8 SECONDS (92.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80 , TOTAL = 5981.9 SECONDS (99.7 MIN)
WALL CLOCK TIME: STEP = 0.97 , TOTAL = 5529.8 SECONDS (92.2 MIN)
CPU UTILIZATION: STEP = 82.55% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636006348	-284.636006348	0.017294352	0.000980673	197501270
11369498					
2 1	-284.636105520	-0.000099172	0.001747190	0.000145082	159088042
14615354					
3 2	-284.636102681	0.000002839	0.001372536	0.000236381	144766977
15740592					
4 3	-284.636108372	-0.000005690	0.000681405	0.000065892	140158564
16107235					
5 4	-284.636108062	0.000000309	0.000385068	0.000149523	131592980
16849376					
6 5	-284.636108501	-0.000000439	0.000226540	0.000029430	126377594
17273100					
7 6	-284.636108503	-0.000000002	0.000132688	0.000030573	120952327
17613474					
8 7	-284.636108576	-0.000000072	0.000124769	0.000018485	115197480
18057768					

9 8	-284.636108579	-0.000000003	0.000177767	0.000015039	112076208
18284929					
10 9	-284.636108600	-0.000000021	0.000302470	0.000016113	133724385
16821176					
11 10	-284.636108620	-0.000000020	0.000204704	0.000015582	160545203
14627003					
12 11	-284.636108636	-0.000000016	0.000227009	0.000017148	157851121
14860812					

-----DISABLING FDIFF OPTION-----

13 12	-284.636108646	-0.000000010	0.000471145	0.000013900	197516204
11368055					
14 13	-284.636108672	-0.000000025	0.000325775	0.000009270	197515814
11368056					
15 14	-284.636108676	-0.000000004	0.000072251	0.000013226	197515657
11368058					
16 15	-284.636108681	-0.000000005	0.000035047	0.000004773	197515632
11368059					
17 16	-284.636108681	0.000000000	0.000024265	0.000004022	197515556
11368062					
18 17	-284.636108682	-0.000000001	0.000077571	0.000003197	197515573
11368061					
19 18	-284.636108683	-0.000000001	0.000055721	0.000003127	197515601
11368058					
20 19	-284.636108684	-0.000000001	0.000034700	0.000003723	197515640
11368057					
21 20	-284.636108684	-0.000000001	0.000087247	0.000003694	197515604
11368057					
22 21	-284.636108685	-0.000000001	0.000021812	0.000002541	197515498
11368065					
23 22	-284.636108686	0.000000000	0.000011829	0.000001697	197515528
11368062					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 77.0 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 25.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6361086856 AFTER 23 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6009579894
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999505199

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 80.22 , TOTAL = 6062.1 SECONDS (101.0 MIN)
WALL CLOCK TIME: STEP = 73.50 , TOTAL = 5603.3 SECONDS (93.4 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.74 , TOTAL = 6065.9 SECONDS (101.1 MIN)
WALL CLOCK TIME: STEP = 3.72 , TOTAL = 5607.0 SECONDS (93.4 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.88 , TOTAL = 6068.8 SECONDS (101.1 MIN)
WALL CLOCK TIME: STEP = 2.72 , TOTAL = 5609.7 SECONDS (93.5 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 61 ENERGY= -284.6361087

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0009894	-0.0003894	-0.0011228
2 C	6.0	-0.0004164	0.0013634	0.0001580
3 C	6.0	0.0000902	-0.0012951	0.0002877
4 C	6.0	0.0000000	-0.0005708	0.0008635
5 C	6.0	0.0004811	-0.0000636	0.0004142
6 C	6.0	0.0000180	0.0001816	0.0001539

7 C	6.0	0.0000098	0.0005916	-0.0002815
8 C	6.0	-0.0012691	0.0001460	-0.0005921
9 C	6.0	0.0006743	-0.0000300	-0.0004651
10 C	6.0	-0.0001483	-0.0003594	-0.0003550
11 C	6.0	0.0004758	0.0002630	0.0003155
12 N	7.0	-0.0003610	-0.0001127	0.0006780
13 C	6.0	-0.0002220	-0.0005968	0.0000035
14 C	6.0	0.0006755	-0.0004294	0.0000964
15 C	6.0	0.0007449	0.0004693	-0.0003328
16 C	6.0	-0.0004526	-0.0010930	0.0000512
17 C	6.0	0.0001280	-0.0009238	0.0001502
18 C	6.0	-0.0000280	0.0013748	-0.0000364
19 C	6.0	-0.0007210	0.0001549	-0.0000830
20 O	8.0	0.0001658	-0.0011877	-0.0006476
21 N	7.0	0.0012432	-0.0005281	0.0004149
22 H	1.0	0.0000988	-0.0002976	0.0002006
23 H	1.0	-0.0010404	0.0001449	-0.0003864
24 H	1.0	-0.0004729	-0.0008733	-0.0001588
25 H	1.0	0.0003204	0.0005457	-0.0007855
26 H	1.0	0.0001149	0.0004511	0.0007776
27 H	1.0	-0.0000090	-0.0000074	0.0009987
28 H	1.0	-0.0003899	-0.0003093	-0.0007244
29 H	1.0	0.0001114	0.0000849	-0.0002230
30 H	1.0	0.0001617	0.0004712	-0.0001816
31 H	1.0	0.0000401	0.0000404	0.0006549
32 H	1.0	-0.0001271	0.0001239	0.0001084
33 H	1.0	-0.0007812	0.0018728	-0.0000662
34 H	1.0	-0.0008885	0.0005173	-0.0002731
35 H	1.0	0.0007840	0.0002705	0.0003881

MAXIMUM GRADIENT = 0.0018728 RMS GRADIENT = 0.0005821
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001058702
 PREDICTED ENERGY CHANGE WAS -0.0000762159 RATIO= 1.389
 GDIIS STEP HAS LENGTH = 0.095516
 RADIUS OF STEP TAKEN= 0.05244 CURRENT TRUST RADIUS= 0.05244

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 6068.8 SECONDS (101.1 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5609.7 SECONDS (93.5 MIN)
 CPU UTILIZATION: STEP = 90.68%, TOTAL = 100.00%

1NSERCH= 62

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1515233474	-1.7645937484	0.8795936168
C	6.0	4.9832562347	0.6570851877	0.5167860247
C	6.0	5.1955350786	-0.7013207983	0.2405885050
C	6.0	4.0667233805	-1.5468865993	-0.0029170280
C	6.0	2.7562943524	-1.0381958099	0.0562590744
C	6.0	2.4730325278	0.3396855371	0.4389963664
C	6.0	3.6480668478	1.1989973140	0.6264603314
C	6.0	3.4881244146	2.5991001649	0.9434842874
C	6.0	2.2185919408	3.1509340400	1.1600420360
C	6.0	1.0635451314	2.3136238402	1.0585576217
C	6.0	1.1636201761	0.9577728898	0.6658488883
N	7.0	-0.0466941241	0.1481936880	0.6257589271
C	6.0	-1.2393327725	0.6807412416	0.3562241002
C	6.0	-2.5514295497	0.0374728655	0.4578449203
C	6.0	-2.8375877241	-1.3104411217	0.8626434259
C	6.0	-4.1434296062	-1.8262713353	0.9528532690
C	6.0	-5.2438752094	-0.9664397569	0.6515931744
C	6.0	-5.0166316050	0.3834714350	0.2602766929
C	6.0	-3.6917581445	0.8695804803	0.1556292661
O	8.0	-1.7270565535	-2.2049394962	1.1991841887
N	7.0	1.6663251851	-1.9919778991	-0.3655237115
H	1.0	5.8435060988	1.3336109372	0.6688025993
H	1.0	6.2155094985	-1.1156489223	0.1725761508
H	1.0	4.2370420918	-2.6054773224	-0.2835396984
H	1.0	4.3929416497	3.2268317588	1.0383087122
H	1.0	2.1040306665	4.2097040738	1.4537025018
H	1.0	0.0857972978	2.7388653341	1.3457898552
H	1.0	-1.2706025982	1.7313151111	0.0051927310
H	1.0	-4.3258213171	-2.8761823590	1.2497540720
H	1.0	-6.2733699493	-1.3594060168	0.7232406517
H	1.0	-5.8678947880	1.0523061993	0.0457627243
H	1.0	-3.5161214684	1.9178250941	-0.1500913242
H	1.0	-2.0644966464	-3.0358683767	1.6169418002
H	1.0	1.3202345443	-1.7400843533	-1.3187708677
H	1.0	2.0783985920	-2.9422782772	-0.4449668851

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4168073	5.1943172	4.0193299
2 C	5.4168073	0.0000000	1.4023602 *	2.4428703 *

3 C	5.1943172	1.4023602 *	0.0000000	1.4312555 *
4 C	4.0193299	2.4428703 *	1.4312555 *	0.0000000
5 C	2.8267235 *	2.8364453 *	2.4692828 *	1.4069443 *
6 C	3.1640989	2.5314061 *	2.9214859 *	2.5088428 *
7 C	4.5905081	1.4451394 *	2.4808797 *	2.8480287 *
8 C	5.4935247	2.4877525 *	3.7818107	4.2918130
9 C	5.3398350	3.7784162	4.9545386	5.1805002
10 C	4.1827826	4.2897287	5.1799909	5.0049325
11 C	2.9122683 *	3.8343516	4.3806137	3.8921171
12 N	1.9397108 *	5.0568020	5.3245655	4.4931875
13 C	2.8614786 *	6.2247051	6.5826280	5.7658946
14 C	3.2758618	7.5603494	7.7851447	6.8207364
15 C	3.0234627	8.0719500	8.0801635	6.9623712
16 C	4.2960205	9.4685590	9.4334032	8.2703183
17 C	5.4588790	10.3560718	10.4508612	9.3516067
18 C	5.6309469	10.0069185	10.2696402	9.2899349
19 C	4.7152742	8.6851288	9.0254601	8.1276372
20 O	1.9557876 *	7.3270151	7.1485698	5.9536516
21 N	1.9739922 *	4.3356703	3.8063749	2.4680967 *
22 H	6.4839782	1.1049099 *	2.1781141 *	3.4504246
23 H	6.1394569	2.1862101 *	1.1030146 *	2.1986463 *
24 H	4.3302919	3.4411729	2.1952748 *	1.1083194 *
25 H	6.5520339	2.6877602 *	4.0878963	4.8968313
26 H	6.3114278	4.6678532	5.9285083	6.2539779
27 H	4.5280020	5.3857367	6.2582562	6.0028703
28 H	3.8740674	6.3660386	6.9126019	6.2636827
29 H	4.6280950	9.9839945	9.8185878	8.5890057
30 H	6.4395557	11.4376787	11.4979047	10.3672554
31 H	6.6980291	10.8685575	11.2032426	10.2691193
32 H	5.2983090	8.6182140	9.1052466	8.3381907
33 H	2.6590536 *	8.0323763	7.7493562	6.5140516
34 H	2.4898379 *	4.7469378	4.3044844	3.0515566
35 H	2.6180622 *	4.7242549	3.8997970	2.4690001 *

C C C C

1 CO	2.8267235 *	3.1640989	4.5905081	5.4935247
2 C	2.8364453 *	2.5314061 *	1.4451394 *	2.4877525 *
3 C	2.4692828 *	2.9214859 *	2.4808797 *	3.7818107
4 C	1.4069443 *	2.5088428 *	2.8480287 *	4.2918130
5 C	0.0000000	1.4578347 *	2.4749587 *	3.8147956
6 C	1.4578347 *	0.0000000	1.4677415 *	2.5278200 *
7 C	2.4749587 *	1.4677415 *	0.0000000	1.4444285 *
8 C	3.8147956	2.5278200 *	1.4444285 *	0.0000000
9 C	4.3653487	2.9133769 *	2.4775320 *	1.4011176 *
10 C	3.8864762	2.5033864 *	2.8476048 *	2.4440383 *

11 C	2.6252813 *	1.4656244 *	2.4964407 *	2.8590832 *
12 N	3.0965456	2.5338847 *	3.8412820	4.3131003
13 C	4.3600183	3.7289176	4.9222243	5.1355454
14 C	5.4304942	5.0335779	6.3096217	6.5782971
15 C	5.6582586	5.5771930	6.9582166	7.4367790
16 C	7.0022236	6.9809018	8.3645801	8.8218262
17 C	8.0226108	7.8295482	9.1518513	9.4364237
18 C	7.9045012	7.4919241	8.7106930	8.8151380
19 C	6.7250923	6.1940076	7.3622842	7.4271574
20 O	4.7715830	4.9692807	6.3880161	7.0952302
21 N	1.5085204 *	2.5951269 *	3.8850554	5.1098388
22 H	3.9410092	3.5214756	2.1999698 *	2.6878869 *
23 H	3.4620367	4.0243151	3.4864538	4.6725036
24 H	2.1827616 *	3.5082435	3.9558841	5.3994530
25 H	4.6726327	3.5186417	2.1992203 *	1.1053202 *
26 H	5.4698034	4.0178146	3.4832072	2.1840520 *
27 H	4.8021490	3.5038879	3.9469473	3.4288794
28 H	4.8876065	4.0174149	4.9862456	4.9273649
29 H	7.4134329	7.5646248	8.9765515	9.5462175
30 H	9.0599601	8.9144413	10.2464483	10.5358934
31 H	8.8739477	8.3805447	9.5347918	9.5254171
32 H	6.9371349	6.2215363	7.2419155	7.1217627
33 H	5.4466918	5.7767716	7.1797300	7.9396484
34 H	2.1084645 *	2.9570478 *	4.2238524	5.3522021
35 H	2.0823785 *	3.4217559	4.5565314	5.8840461

C C C N

1 CO	5.3398350	4.1827826	2.9122683 *	1.9397108 *
2 C	3.7784162	4.2897287	3.8343516	5.0568020
3 C	4.9545386	5.1799909	4.3806137	5.3245655
4 C	5.1805002	5.0049325	3.8921171	4.4931875
5 C	4.3653487	3.8864762	2.6252813 *	3.0965456
6 C	2.9133769 *	2.5033864 *	1.4656244 *	2.5338847 *
7 C	2.4775320 *	2.8476048 *	2.4964407 *	3.8412820
8 C	1.4011176 *	2.4440383 *	2.8590832 *	4.3131003
9 C	0.0000000	1.4302170 *	2.4833743 *	3.7991353
10 C	1.4302170 *	0.0000000	1.4151208 *	2.4716459 *
11 C	2.4833743 *	1.4151208 *	0.0000000	1.4566696 *
12 N	3.7991353	2.4716459 *	1.4566696 *	0.0000000
13 C	4.3249531	2.9090934 *	2.4386055 *	1.3336577 *
14 C	5.7393228	4.3139032	3.8329900	2.5127980 *
15 C	6.7496124	5.3283268	4.6036059	3.1579767
16 C	8.0802734	6.6530062	5.9998376	4.5594676
17 C	8.5381323	7.1209542	6.6902014	5.3154272
18 C	7.7985182	6.4289416	6.2201144	4.9889088

19	C	6.4144881	5.0510841	4.8829090	3.7453855
20	O	6.6524473	5.3126875	4.3177781	2.9478247 *
21	N	5.3927630	4.5748834	3.1650389	2.9150319 *
22	H	4.0846031	4.8949322	4.6949542	6.0084545
23	H	5.9290951	6.2520086	5.4830632	6.4045193
24	H	6.2685198	6.0058192	4.8004180	5.1729995
25	H	2.1790769 *	3.4524252	3.9643249	5.4183554
26	H	1.1046967 *	2.1986063 *	3.4756498	4.6697938
27	H	2.1801642 *	1.1042298 *	2.1900484 *	2.6921326 *
28	H	3.9399839	2.6261962 *	2.6382332 *	2.0950723 *
29	H	8.8973887	7.4843781	6.7211700	5.2770399
30	H	9.6253509	8.2118152	7.7898289	6.4073279
31	H	8.4283524	7.1176917	7.0594367	5.9194757
32	H	6.0103199	4.7529817	4.8463843	3.9712045
33	H	7.5385761	6.2220178	5.2224981	3.8977201
34	H	5.5564035	4.7063925	3.3528611	3.0356686
35	H	6.3026141	5.5601277	4.1570579	3.9004474

C C C C

1	CO	2.8614786 *	3.2758618	3.0234627	4.2960205
2	C	6.2247051	7.5603494	8.0719500	9.4685590
3	C	6.5826280	7.7851447	8.0801635	9.4334032
4	C	5.7658946	6.8207364	6.9623712	8.2703183
5	C	4.3600183	5.4304942	5.6582586	7.0022236
6	C	3.7289176	5.0335779	5.5771930	6.9809018
7	C	4.9222243	6.3096217	6.9582166	8.3645801
8	C	5.1355454	6.5782971	7.4367790	8.8218262
9	C	4.3249531	5.7393228	6.7496124	8.0802734
10	C	2.9090934 *	4.3139032	5.3283268	6.6530062
11	C	2.4386055 *	3.8329900	4.6036059	5.9998376
12	N	1.3336577 *	2.5127980 *	3.1579767	4.5594676
13	C	0.0000000	1.4648273 *	2.6030149 *	3.8826353
14	C	1.4648273 *	0.0000000	1.4361826 *	2.5006079 *
15	C	2.6030149 *	1.4361826 *	0.0000000	1.4069263 *
16	C	3.8826353	2.5006079 *	1.4069263 *	0.0000000
17	C	4.3401392	2.8800421 *	2.4398973 *	1.4286527 *
18	C	3.7901928	2.4971923 *	2.8249633 *	2.4748954 *
19	C	2.4678510 *	1.4436366 *	2.4458067 *	2.8473128 *
20	O	3.0455885	2.5015171 *	1.4651507 *	2.4582366 *
21	N	4.0133771	4.7524795	4.7178510	5.9597674
22	H	7.1197297	8.4970243	9.0768924	10.4787607
23	H	7.6704249	8.8470497	9.0814485	10.4125615
24	H	6.4186612	7.3224439	7.2829418	8.5069463
25	H	6.2185474	7.6637615	8.5380477	9.9202212
26	H	4.9835847	6.3302887	7.4324253	8.7014142

27 H	2.6402812 *	3.8782642	5.0176183	6.2354817
28 H	1.1081093 *	2.1712930 *	3.5274559	4.6698626
29 H	4.7933822	3.5021383	2.1945932 *	1.1062233 *
30 H	5.4441191	3.9842874	3.4389577	2.1925627 *
31 H	4.6538192	3.4926552	3.9284386	3.4760325
32 H	2.6401702 *	2.1990774 *	3.4507597	3.9532595
33 H	4.0104229	3.3205475	2.0356166 *	2.4952156 *
34 H	3.9009473	4.6158267	4.7149388	5.9177133
35 H	4.9775013	5.5793633	5.3422522	6.4738334

C C C O

1 CO	5.4588790	5.6309469	4.7152742	1.9557876 *
2 C	10.3560718	10.0069185	8.6851288	7.3270151
3 C	10.4508612	10.2696402	9.0254601	7.1485698
4 C	9.3516067	9.2899349	8.1276372	5.9536516
5 C	8.0226108	7.9045012	6.7250923	4.7715830
6 C	7.8295482	7.4919241	6.1940076	4.9692807
7 C	9.1518513	8.7106930	7.3622842	6.3880161
8 C	9.4364237	8.8151380	7.4271574	7.0952302
9 C	8.5381323	7.7985182	6.4144881	6.6524473
10 C	7.1209542	6.4289416	5.0510841	5.3126875
11 C	6.6902014	6.2201144	4.8829090	4.3177781
12 N	5.3154272	4.9889088	3.7453855	2.9478247 *
13 C	4.3401392	3.7901928	2.4678510 *	3.0455885
14 C	2.8800421 *	2.4971923 *	1.4436366 *	2.5015171 *
15 C	2.4398973 *	2.8249633 *	2.4458067 *	1.4651507 *
16 C	1.4286527 *	2.4748954 *	2.8473128 *	2.4582366 *
17 C	0.0000000	1.4237375 *	2.4547949 *	3.7685211
18 C	1.4237375 *	0.0000000	1.4151123 *	4.2898394
19 C	2.4547949 *	1.4151123 *	0.0000000	3.7949614
20 O	3.7685211	4.2898394	3.7949614	0.0000000
21 N	7.0595414	7.1201332	6.0966527	3.7428202
22 H	11.3234515	10.9092736	9.5603313	8.3735335
23 H	11.4703626	11.3320804	10.1042256	8.0823780
24 H	9.6668873	9.7396113	8.6680315	6.1586828
25 H	10.5167159	9.8605325	8.4674747	8.1843997
26 H	9.0237224	8.1711782	6.8141461	7.4759388
27 H	6.5281394	5.7237226	4.3795700	5.2677451
28 H	4.8458859	3.9892961	2.5743372 *	4.1386068
29 H	2.2017575 *	3.4758635	3.9534649	2.6845302 *
30 H	1.1042714 *	2.1980329 *	3.4576412	4.6487003
31 H	2.1981279 *	1.1036327 *	2.1865567 *	5.3931968
32 H	3.4564165	2.1849883 *	1.1059521 *	4.6923859
33 H	3.9144451	4.7167283	4.4761529	0.9893584 *
34 H	6.8969847	6.8672231	5.8398867	3.9802225

35 H	7.6630330	7.8674922	6.9415914	4.2105095
	N	H	H	H
1 CO	1.9739922 *	6.4839782	6.1394569	4.3302919
2 C	4.3356703	1.1049099 *	2.1862101 *	3.4411729
3 C	3.8063749	2.1781141 *	1.1030146 *	2.1952748 *
4 C	2.4680967 *	3.4504246	2.1986463 *	1.1083194 *
5 C	1.5085204 *	3.9410092	3.4620367	2.1827616 *
6 C	2.5951269 *	3.5214756	4.0243151	3.5082435
7 C	3.8850554	2.1999698 *	3.4864538	3.9558841
8 C	5.1098388	2.6878869 *	4.6725036	5.3994530
9 C	5.3927630	4.0846031	5.9290951	6.2685198
10 C	4.5748834	4.8949322	6.2520086	6.0058192
11 C	3.1650389	4.6949542	5.4830632	4.8004180
12 N	2.9150319 *	6.0084545	6.4045193	5.1729995
13 C	4.0133771	7.1197297	7.6704249	6.4186612
14 C	4.7524795	8.4970243	8.8470497	7.3224439
15 C	4.7178510	9.0768924	9.0814485	7.2829418
16 C	5.9597674	10.4787607	10.4125615	8.5069463
17 C	7.0595414	11.3234515	11.4703626	9.6668873
18 C	7.1201332	10.9092736	11.3320804	9.7396113
19 C	6.0966527	9.5603313	10.1042256	8.6680315
20 O	3.7428202	8.3735335	8.0823780	6.1586828
21 N	0.0000000	5.4385855	4.6639663	2.6441801 *
22 H	5.4385855	0.0000000	2.5265591 *	4.3593691
23 H	4.6639663	2.5265591 *	0.0000000	2.5183256 *
24 H	2.6441801 *	4.3593691	2.5183256 *	0.0000000
25 H	6.0531940	2.4134948 *	4.7883593	5.9822585
26 H	6.4778105	4.7824320	6.8487172	7.3494521
27 H	5.2732855	5.9652546	7.3353311	6.9605709
28 H	4.7566676	7.1560526	8.0109360	7.0160733
29 H	6.2687128	11.0215736	10.7414825	8.7032695
30 H	8.0389249	12.4126544	12.5033899	10.6317948
31 H	8.1364177	11.7313350	12.2770017	10.7516310
32 H	6.4954387	9.4135286	10.1985646	8.9771721
33 H	4.3518856	9.0844826	8.6215971	6.5959425
34 H	1.0449446 *	5.8187659	5.1553615	3.2137789
35 H	1.0388390 *	5.8051482	4.5643861	2.1907157 *

H H H H

1 CO	6.5520339	6.3114278	4.5280020	3.8740674
2 C	2.6877602 *	4.6678532	5.3857367	6.3660386
3 C	4.0878963	5.9285083	6.2582562	6.9126019
4 C	4.8968313	6.2539779	6.0028703	6.2636827

5 C	4.6726327	5.4698034	4.8021490	4.8876065
6 C	3.5186417	4.0178146	3.5038879	4.0174149
7 C	2.1992203 *	3.4832072	3.9469473	4.9862456
8 C	1.1053202 *	2.1840520 *	3.4288794	4.9273649
9 C	2.1790769 *	1.1046967 *	2.1801642 *	3.9399839
10 C	3.4524252	2.1986063 *	1.1042298 *	2.6261962 *
11 C	3.9643249	3.4756498	2.1900484 *	2.6382332 *
12 N	5.4183554	4.6697938	2.6921326 *	2.0950723 *
13 C	6.2185474	4.9835847	2.6402812 *	1.1081093 *
14 C	7.6637615	6.3302887	3.8782642	2.1712930 *
15 C	8.5380477	7.4324253	5.0176183	3.5274559
16 C	9.9202212	8.7014142	6.2354817	4.6698626
17 C	10.5167159	9.0237224	6.5281394	4.8458859
18 C	9.8605325	8.1711782	5.7237226	3.9892961
19 C	8.4674747	6.8141461	4.3795700	2.5743372 *
20 O	8.1843997	7.4759388	5.2677451	4.1386068
21 N	6.0531940	6.4778105	5.2732855	4.7566676
22 H	2.4134948 *	4.7824320	5.9652546	7.1560526
23 H	4.7883593	6.8487172	7.3353311	8.0109360
24 H	5.9822585	7.3494521	6.9605709	7.0160733
25 H	0.0000000	2.5254115 *	4.3455895	5.9480780
26 H	2.5254115 *	0.0000000	2.4996555 *	4.4304336
27 H	4.3455895	2.4996555 *	0.0000000	2.1568910 *
28 H	5.9480780	4.4304336	2.1568910 *	0.0000000
29 H	10.6446380	9.5704952	7.1414538	5.6667740
30 H	11.6147771	10.0860995	7.5909422	5.9241735
31 H	10.5355813	8.6892492	6.3230532	4.6473427
32 H	8.1042626	6.2778160	3.9856726	2.2585956 *
33 H	9.0141410	8.3607169	6.1680497	5.0945109
34 H	6.2982227	6.6106677	5.3558108	4.5294515
35 H	6.7538977	7.3997604	6.2811354	5.7672288

H H H H

1 CO	4.6280950	6.4395557	6.6980291	5.2983090
2 C	9.9839945	11.4376787	10.8685575	8.6182140
3 C	9.8185878	11.4979047	11.2032426	9.1052466
4 C	8.5890057	10.3672554	10.2691193	8.3381907
5 C	7.4134329	9.0599601	8.8739477	6.9371349
6 C	7.5646248	8.9144413	8.3805447	6.2215363
7 C	8.9765515	10.2464483	9.5347918	7.2419155
8 C	9.5462175	10.5358934	9.5254171	7.1217627
9 C	8.8973887	9.6253509	8.4283524	6.0103199
10 C	7.4843781	8.2118152	7.1176917	4.7529817
11 C	6.7211700	7.7898289	7.0594367	4.8463843
12 N	5.2770399	6.4073279	5.9194757	3.9712045

13 C	4.7933822	5.4441191	4.6538192	2.6401702 *
14 C	3.5021383	3.9842874	3.4926552	2.1990774 *
15 C	2.1945932 *	3.4389577	3.9284386	3.4507597
16 C	1.1062233 *	2.1925627 *	3.4760325	3.9532595
17 C	2.2017575 *	1.1042714 *	2.1981279 *	3.4564165
18 C	3.4758635	2.1980329 *	1.1036327 *	2.1849883 *
19 C	3.9534649	3.4576412	2.1865567 *	1.1059521 *
20 O	2.6845302 *	4.6487003	5.3931968	4.6923859
21 N	6.2687128	8.0389249	8.1364177	6.4954387
22 H	11.0215736	12.4126544	11.7313350	9.4135286
23 H	10.7414825	12.5033899	12.2770017	10.1985646
24 H	8.7032695	10.6317948	10.7516310	8.9771721
25 H	10.6446380	11.6147771	10.5355813	8.1042626
26 H	9.5704952	10.0860995	8.6892492	6.2778160
27 H	7.1414538	7.5909422	6.3230532	3.9856726
28 H	5.6667740	5.9241735	4.6473427	2.2585956 *
29 H	0.0000000	2.5240389 *	4.3886909	5.0594158
30 H	2.5240389 *	0.0000000	2.5376647 *	4.3709692
31 H	4.3886909	2.5376647 *	0.0000000	2.5136268 *
32 H	5.0594158	4.3709692	2.5136268 *	0.0000000
33 H	2.2965008 *	4.6177746	5.8006562	5.4560700
34 H	6.3060277	7.8725826	7.8312579	6.1754719
35 H	6.6249891	8.5803398	8.9073621	7.4166172

H H H

1 CO	2.6590536 *	2.4898379 *	2.6180622 *
2 C	8.0323763	4.7469378	4.7242549
3 C	7.7493562	4.3044844	3.8997970
4 C	6.5140516	3.0515566	2.4690001 *
5 C	5.4466918	2.1084645 *	2.0823785 *
6 C	5.7767716	2.9570478 *	3.4217559
7 C	7.1797300	4.2238524	4.5565314
8 C	7.9396484	5.3522021	5.8840461
9 C	7.5385761	5.5564035	6.3026141
10 C	6.2220178	4.7063925	5.5601277
11 C	5.2224981	3.3528611	4.1570579
12 N	3.8977201	3.0356686	3.9004474
13 C	4.0104229	3.9009473	4.9775013
14 C	3.3205475	4.6158267	5.5793633
15 C	2.0356166 *	4.7149388	5.3422522
16 C	2.4952156 *	5.9177133	6.4738334
17 C	3.9144451	6.8969847	7.6630330
18 C	4.7167283	6.8672231	7.8674922
19 C	4.4761529	5.8398867	6.9415914
20 O	0.9893584 *	3.9802225	4.2105095

4 3	-284.636193765	-0.000001330	0.000431625	0.000046907	134532007
16558011					
5 4	-284.636193701	0.000000063	0.000211793	0.000080715	128132601
17114601					
6 5	-284.636193853	-0.000000151	0.000178464	0.000023408	121758028
17599619					
7 6	-284.636193888	-0.000000035	0.000107051	0.000022918	121270326
17601189					
8 7	-284.636193934	-0.000000046	0.000174535	0.000021230	113477080
18227542					
9 8	-284.636193954	-0.000000021	0.000225810	0.000018897	140920400
16135308					
10 9	-284.636193992	-0.000000038	0.000441756	0.000014979	158941469
14807609					

-----DISABLING FDIFF OPTION-----

11 10	-284.636194023	-0.000000031	0.000245201	0.000020525	197520664
11367407					
12 11	-284.636194045	-0.000000022	0.000207108	0.000019917	197520837
11367408					
13 12	-284.636194063	-0.000000019	0.000183299	0.000013380	197520809
11367412					
14 13	-284.636194073	-0.000000009	0.000061684	0.000005633	197520775
11367407					
15 14	-284.636194074	-0.000000001	0.000034904	0.000004939	197520607
11367412					
16 15	-284.636194076	-0.000000001	0.000021922	0.000002826	197520594
11367410					
17 16	-284.636194076	-0.000000001	0.000041059	0.000002411	197520693
11367404					
18 17	-284.636194077	-0.000000001	0.000087440	0.000001838	197520676
11367408					
19 18	-284.636194078	-0.000000001	0.000059693	0.000002809	197520699
11367410					
20 19	-284.636194078	0.000000000	0.000031421	0.000003295	197520694
11367410					
21 20	-284.636194079	-0.000000001	0.000050865	0.000003346	197520681
11367413					
22 21	-284.636194079	-0.000000001	0.000037474	0.000002659	197520656
11367414					
23 22	-284.636194080	0.000000000	0.000016787	0.000001750	197520504
11367413					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 77.9 SECONDS (3.4 SEC/ITER)

OF THE ABOVE TIME, DFT PART= 24.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.0 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6361940796 AFTER 23 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6022102834
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999461619

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 80.86 , TOTAL = 6151.3 SECONDS (102.5 MIN)
WALL CLOCK TIME: STEP = 74.10 , TOTAL = 5685.5 SECONDS (94.8
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.81 , TOTAL = 6155.2 SECONDS (102.6 MIN)
WALL CLOCK TIME: STEP = 3.78 , TOTAL = 5689.3 SECONDS (94.8
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.87 , TOTAL = 6158.0 SECONDS (102.6 MIN)
WALL CLOCK TIME: STEP = 2.72 , TOTAL = 5692.0 SECONDS (94.9
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 62 ENERGY= -284.6361941

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0010468	-0.0003164	-0.0009790
2 C	6.0	0.0003609	0.0008140	0.0001707
3 C	6.0	-0.0000704	-0.0009787	0.0003626
4 C	6.0	-0.0001821	-0.0006221	0.0007256
5 C	6.0	0.0002693	-0.0001839	0.0001988
6 C	6.0	-0.0000526	0.0001711	0.0001586
7 C	6.0	-0.0004858	0.0003957	-0.0001669
8 C	6.0	-0.0008706	0.0001095	-0.0006527
9 C	6.0	0.0004947	0.0000846	-0.0003886
10 C	6.0	-0.0002361	-0.0001408	-0.0000969
11 C	6.0	0.0005875	0.0004884	0.0003314
12 N	7.0	-0.0004203	-0.0005368	0.0004638
13 C	6.0	-0.0005827	-0.0005401	0.0001354
14 C	6.0	0.0003494	0.0000284	0.0000960
15 C	6.0	0.0002782	0.0004450	-0.0000114
16 C	6.0	-0.0001418	-0.0012418	0.0003786
17 C	6.0	-0.0002219	-0.0002657	-0.0000240
18 C	6.0	-0.0003732	0.0007673	-0.0002430
19 C	6.0	-0.0004603	-0.0000628	-0.0001495
20 O	8.0	-0.0003819	-0.0020852	-0.0002246
21 N	7.0	0.0011814	-0.0006728	0.0004379
22 H	1.0	0.0001938	-0.0004278	0.0000461
23 H	1.0	-0.0007994	0.0002696	-0.0004146
24 H	1.0	-0.0001664	-0.0004046	0.0001168
25 H	1.0	-0.0001040	0.0005534	-0.0006880
26 H	1.0	0.0000633	0.0001259	0.0005926
27 H	1.0	0.0002381	0.0000455	0.0008678
28 H	1.0	-0.0000718	-0.0002664	-0.0007858
29 H	1.0	0.0002143	0.0002732	-0.0003526
30 H	1.0	0.0005188	0.0004805	-0.0002785
31 H	1.0	0.0003026	0.0000801	0.0008100
32 H	1.0	-0.0001516	0.0001053	0.0001639
33 H	1.0	-0.0001682	0.0024965	-0.0005349
34 H	1.0	-0.0006795	0.0003230	-0.0003002
35 H	1.0	0.0005213	0.0006888	0.0002345

MAXIMUM GRADIENT = 0.0024965 RMS GRADIENT = 0.0005590

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0000853940

PREDICTED ENERGY CHANGE WAS -0.0001334361 RATIO= 0.640

GDIIS STEP HAS LENGTH = 0.286996

RADIUS OF STEP TAKEN= 0.05244 CURRENT TRUST RADIUS= 0.05244

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 6158.0 SECONDS (102.6 MIN)

WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5692.1 SECONDS (94.9 MIN)

CPU UTILIZATION: STEP = 91.50% , TOTAL = 100.00%

INSERCH= 63

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1515812526	-1.7641057887	0.8775394466
C	6.0	4.9833892865	0.6559947616	0.5187690865
C	6.0	5.1955601128	-0.7017131836	0.2396751051
C	6.0	4.0663814689	-1.5463397003	-0.0054478712
C	6.0	2.7556456746	-1.0378712412	0.0535254298
C	6.0	2.4727908119	0.3392792226	0.4384638039
C	6.0	3.6483680942	1.1977823251	0.6290444030
C	6.0	3.4881755468	2.5974623910	0.9484153049
C	6.0	2.2182390318	3.1494540520	1.1632468345
C	6.0	1.0630299191	2.3132234464	1.0588739985
C	6.0	1.1631706062	0.9576913519	0.6644820076
N	7.0	-0.0469382305	0.1483591023	0.6230449480
C	6.0	-1.2394249235	0.6812525908	0.3532914202
C	6.0	-2.5514652438	0.0379091256	0.4571911806
C	6.0	-2.8371668348	-1.3084252524	0.8669738191
C	6.0	-4.1430851476	-1.8242863476	0.9589012552
C	6.0	-5.2434726227	-0.9669292002	0.6529916371
C	6.0	-5.0167435552	0.3817272993	0.2564756465
C	6.0	-3.6925896649	0.8685473580	0.1516099431
O	8.0	-1.7261166487	-2.2020581728	1.2048310368
N	7.0	1.6651374457	-1.9905195734	-0.3701692040
H	1.0	5.8441466959	1.3318706876	0.6714010218
H	1.0	6.2155940879	-1.1159212975	0.1706791824
H	1.0	4.2377628872	-2.6045791741	-0.2862022141
H	1.0	4.3922848710	3.2252623295	1.0460154610
H	1.0	2.1035818289	4.2081027884	1.4571767484
H	1.0	0.0850554580	2.7389851192	1.3441478344
H	1.0	-1.2694232624	1.7310297454	0.0002962681
H	1.0	-4.3244422933	-2.8733989855	1.2598380300
H	1.0	-6.2727903071	-1.3609298976	0.7246370892
H	1.0	-5.8682587562	1.0495431790	0.0391225024
H	1.0	-3.5173683708	1.9158754743	-0.1565581964
H	1.0	-2.0616470107	-3.0327824642	1.6254394772

H 1.0 1.3202268674 -1.7373832372 -1.3230476859
H 1.0 2.0768079247 -2.9410038335 -0.4517877501

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C	
1	CO	0.0000000	5.4158999	5.1939649	4.0190483
2	C	5.4158999	0.0000000	1.4022413 *	2.4425364 *
3	C	5.1939649	1.4022413 *	0.0000000	1.4312664 *
4	C	4.0190483	2.4425364 *	1.4312664 *	0.0000000
5	C	2.8262284 *	2.8369835 *	2.4699871 *	1.4071412 *
6	C	3.1630728	2.5317706 *	2.9217554 *	2.5084153 *
7	C	4.5893408	1.4449830 *	2.4806239 *	2.8473709 *
8	C	5.4919179	2.4878819 *	3.7818030	4.2913020
9	C	5.3381433	3.7787229	4.9546861	5.1799572
10	C	4.1818937	4.2903773	5.1806115	5.0049105
11	C	2.9115093 *	3.8348825	4.3811242	3.8919932
12	N	1.9395101 *	5.0569519	5.3247896	4.4929285
13	C	2.8617323 *	6.2250653	6.5828972	5.7656260
14	C	3.2757306	7.5604136	7.7852910	6.8205406
15	C	3.0233047	8.0710155	8.0799941	6.9625212
16	C	4.2958586	9.4677371	9.4333320	8.2705844
17	C	5.4582523	10.3557039	10.4505777	9.3510771
18	C	5.6304441	10.0073312	10.2696286	9.2891984
19	C	4.7154519	8.6863453	9.0262218	8.1276060
20	O	1.9556767 *	7.3250677	7.1478787	5.9538035
21	N	1.9745613 *	4.3364784	3.8074685	2.4690667 *
22	H	6.4832758	1.1049923 *	2.1777317 *	3.4500244
23	H	6.1393848	2.1861340 *	1.1030857 *	2.1989533 *
24	H	4.3310011	3.4402442	2.1942701 *	1.1081811 *
25	H	6.5502477	2.6885924 *	4.0885905	4.8969352
26	H	6.3097988	4.6681229	5.9286535	6.2534360
27	H	4.5276900	5.3864435	6.2590353	6.0030304
28	H	3.8736006	6.3657033	6.9116966	6.2619482
29	H	4.6272530	9.9820605	9.8177084	8.5888275
30	H	6.4388260	11.4373050	11.4975135	10.3665748
31	H	6.6976143	10.8693701	11.2033570	10.2682847
32	H	5.2983782	8.6201071	9.1062558	8.3380471
33	H	2.6584346 *	8.0289684	7.7473403	6.5132203
34	H	2.4917926 *	4.7475579	4.3049881	3.0518735
35	H	2.6189115 *	4.7253142	3.9011740	2.4703664 *

C C C C

1 CO	2.8262284 *	3.1630728	4.5893408	5.4919179
2 C	2.8369835 *	2.5317706 *	1.4449830 *	2.4878819 *
3 C	2.4699871 *	2.9217554 *	2.4806239 *	3.7818030
4 C	1.4071412 *	2.5084153 *	2.8473709 *	4.2913020
5 C	0.0000000	1.4576446 *	2.4751409 *	3.8148497
6 C	1.4576446 *	0.0000000	1.4681044 *	2.5279335 *
7 C	2.4751409 *	1.4681044 *	0.0000000	1.4445635 *
8 C	3.8148497	2.5279335 *	1.4445635 *	0.0000000
9 C	4.3650866	2.9132782 *	2.4778345 *	1.4012802 *
10 C	3.8865807	2.5037553 *	2.8483216 *	2.4442431 *
11 C	2.6251695 *	1.4658182 *	2.4970194 *	2.8592158 *
12 N	3.0961220	2.5336841 *	3.8414338	4.3128879
13 C	4.3595683	3.7289068	4.9227394	5.1357802
14 C	5.4300714	5.0333213	6.3097363	6.5779841
15 C	5.6581313	5.5762175	6.9570001	7.4345509
16 C	7.0021883	6.9800921	8.3635189	8.8197569
17 C	8.0218630	7.8289798	9.1515780	9.4357746
18 C	7.9035741	7.4918654	8.7114243	8.8160031
19 C	6.7248637	6.1947015	7.3638305	7.4288246
20 O	4.7714808	4.9675485	6.3855722	7.0915435
21 N	1.5087293 *	2.5950248 *	3.8854730	5.1099620
22 H	3.9416095	3.5221496	2.2002767 *	2.6886910 *
23 H	3.4628110	4.0246607	3.4862548	4.6725693
24 H	2.1832682 *	3.5080721	3.9551252	5.3988330
25 H	4.6731073	3.5188741	2.1995345 *	1.1050214 *
26 H	5.4695217	4.0176967	3.4834174	2.1840560 *
27 H	4.8023330	3.5043019	3.9476418	3.4289735
28 H	4.8857779	4.0166063	4.9864164	4.9279186
29 H	7.4129615	7.5629581	8.9743035	9.5427620
30 H	9.0591067	8.9139102	10.2462447	10.5354355
31 H	8.8729496	8.3807551	9.5360458	9.5271050
32 H	6.9368192	6.2226774	7.2443501	7.1248279
33 H	5.4458143	5.7741525	7.1759845	7.9346424
34 H	2.1082452 *	2.9570007 *	4.2244647	5.3526099
35 H	2.0828048 *	3.4219303	4.5571428	5.8844826

C C C N

1 CO	5.3381433	4.1818937	2.9115093 *	1.9395101 *
2 C	3.7787229	4.2903773	3.8348825	5.0569519
3 C	4.9546861	5.1806115	4.3811242	5.3247896
4 C	5.1799572	5.0049105	3.8919932	4.4929285
5 C	4.3650866	3.8865807	2.6251695 *	3.0961220
6 C	2.9132782 *	2.5037553 *	1.4658182 *	2.5336841 *
7 C	2.4778345 *	2.8483216 *	2.4970194 *	3.8414338
8 C	1.4012802 *	2.4442431 *	2.8592158 *	4.3128879

9 C	0.0000000	1.4299243 *	2.4830947 *	3.7986072
10 C	1.4299243 *	0.0000000	1.4152881 *	2.4715610 *
11 C	2.4830947 *	1.4152881 *	0.0000000	1.4563994 *
12 N	3.7986072	2.4715610 *	1.4563994 *	0.0000000
13 C	4.3247527	2.9090332 *	2.4383854 *	1.3337042 *
14 C	5.7384933	4.3131952	3.8324259	2.5124415 *
15 C	6.7466728	5.3258520	4.6020633	3.1570710
16 C	8.0775179	6.6507606	5.9985359	4.5587881
17 C	8.5371021	7.1201205	6.6894973	5.3149539
18 C	7.7991999	6.4294763	6.2200919	4.9887673
19 C	6.4159053	5.0523395	4.8835840	3.7458906
20 O	6.6481843	5.3092759	4.3155504	2.9466212 *
21 N	5.3922736	4.5745931	3.1645571	2.9141859 *
22 H	4.0856735	4.8961481	4.6959126	6.0089866
23 H	5.9293731	6.2527467	5.4836752	6.4048693
24 H	6.2680362	6.0060754	4.8006968	5.1733996
25 H	2.1785237 *	3.4519442	3.9641676	5.4178353
26 H	1.1046620 *	2.1981722 *	3.4753292	4.6692645
27 H	2.1798353 *	1.1041233 *	2.1902706 *	2.6923512 *
28 H	3.9405799	2.6267612 *	2.6375572 *	2.0945481 *
29 H	8.8932990	7.4810625	6.7190474	5.2757529
30 H	9.6246310	8.2112956	7.7892964	6.4069890
31 H	8.4299898	7.1189566	7.0597812	5.9195330
32 H	6.0133845	4.7555451	4.8476457	3.9718737
33 H	7.5333323	6.2180690	5.2198438	3.8966021
34 H	5.5560116	4.7060722	3.3523675	3.0352003
35 H	6.3025405	5.5602832	4.1569960	3.8999649

C C C C

1 CO	2.8617323 *	3.2757306	3.0233047	4.2958586
2 C	6.2250653	7.5604136	8.0710155	9.4677371
3 C	6.5828972	7.7852910	8.0799941	9.4333320
4 C	5.7656260	6.8205406	6.9625212	8.2705844
5 C	4.3595683	5.4300714	5.6581313	7.0021883
6 C	3.7289068	5.0333213	5.5762175	6.9800921
7 C	4.9227394	6.3097363	6.9570001	8.3635189
8 C	5.1357802	6.5779841	7.4345509	8.8197569
9 C	4.3247527	5.7384933	6.7466728	8.0775179
10 C	2.9090332 *	4.3131952	5.3258520	6.6507606
11 C	2.4383854 *	3.8324259	4.6020633	5.9985359
12 N	1.3337042 *	2.5124415 *	3.1570710	4.5587881
13 C	0.0000000	1.4649695 *	2.6029727 *	3.8827479
14 C	1.4649695 *	0.0000000	1.4360235 *	2.5005477 *
15 C	2.6029727 *	1.4360235 *	0.0000000	1.4071197 *
16 C	3.8827479	2.5005477 *	1.4071197 *	0.0000000

17 C	4.3403596	2.8800940 *	2.4398187 *	1.4281087 *
18 C	3.7904122	2.4972174 *	2.8248678 *	2.4745054 *
19 C	2.4685567 *	1.4441277 *	2.4459565 *	2.8471071 *
20 O	3.0455655	2.5015234 *	1.4653190 *	2.4586439 *
21 N	4.0122617	4.7517141	4.7187413	5.9606637
22 H	7.1204975	8.4974421	9.0760463	10.4780143
23 H	7.6707555	8.8473015	9.0815398	10.4127475
24 H	6.4191299	7.3231821	7.2845357	8.5086869
25 H	6.2183605	7.6630020	8.5353003	9.9175638
26 H	4.9832649	6.3292930	7.4290927	8.6982093
27 H	2.6401341 *	3.8773374	5.0148389	6.2328994
28 H	1.1079429 *	2.1723356 *	3.5280641	4.6708809
29 H	4.7931938	3.5019144	2.1944187 *	1.1063863 *
30 H	5.4445545	3.9845374	3.4389715	2.1920819 *
31 H	4.6540781	3.4927502	3.9284693	3.4757896
32 H	2.6406943 *	2.1991850 *	3.4505662	3.9527942
33 H	4.0110430	3.3217274	2.0371816 *	2.4974228 *
34 H	3.9002217	4.6163745	4.7184872	5.9213699
35 H	4.9765746	5.5786269	5.3433691	6.4748877

C C C O

1 CO	5.4582523	5.6304441	4.7154519	1.9556767 *
2 C	10.3557039	10.0073312	8.6863453	7.3250677
3 C	10.4505777	10.2696286	9.0262218	7.1478787
4 C	9.3510771	9.2891984	8.1276060	5.9538035
5 C	8.0218630	7.9035741	6.7248637	4.7714808
6 C	7.8289798	7.4918654	6.1947015	4.9675485
7 C	9.1515780	8.7114243	7.3638305	6.3855722
8 C	9.4357746	8.8160031	7.4288246	7.0915435
9 C	8.5371021	7.7991999	6.4159053	6.6481843
10 C	7.1201205	6.4294763	5.0523395	5.3092759
11 C	6.6894973	6.2200919	4.8835840	4.3155504
12 N	5.3149539	4.9887673	3.7458906	2.9466212 *
13 C	4.3403596	3.7904122	2.4685567 *	3.0455655
14 C	2.8800940 *	2.4972174 *	1.4441277 *	2.5015234 *
15 C	2.4398187 *	2.8248678 *	2.4459565 *	1.4653190 *
16 C	1.4281087 *	2.4745054 *	2.8471071 *	2.4586439 *
17 C	0.0000000	1.4239050 *	2.4547089 *	3.7685360
18 C	1.4239050 *	0.0000000	1.4146993 *	4.2899360
19 C	2.4547089 *	1.4146993 *	0.0000000	3.7953800
20 O	3.7685360	4.2899360	3.7953800	0.0000000
21 N	7.0585755	7.1181299	6.0952241	3.7451273
22 H	11.3234324	10.9102646	9.5621228	8.3715045
23 H	11.4701802	11.3320661	10.1049782	8.0820748
24 H	9.6673579	9.7395285	8.6686088	6.1606057

25 H	10.5155485	9.8609777	8.4687226	8.1802119
26 H	9.0225761	8.1720173	6.8156246	7.4713073
27 H	6.5272283	5.7243382	4.3807861	5.2643767
28 H	4.8474800	3.9910718	2.5765301 *	4.1386777
29 H	2.2017053 *	3.4758976	3.9534251	2.6842169 *
30 H	1.1044748 *	2.1985638 *	3.4577976	4.6486906
31 H	2.1984890 *	1.1037656 *	2.1860807 *	5.3934339
32 H	3.4562074	2.1845671 *	1.1056972 *	4.6924771
33 H	3.9163017	4.7186369	4.4780042	0.9897449 *
34 H	6.8978607	6.8660555	5.8389913	3.9857625
35 H	7.6618546	7.8651543	6.9399364	4.2133908

N H H H

1 CO	1.9745613 *	6.4832758	6.1393848	4.3310011
2 C	4.3364784	1.1049923 *	2.1861340 *	3.4402442
3 C	3.8074685	2.1777317 *	1.1030857 *	2.1942701 *
4 C	2.4690667 *	3.4500244	2.1989533 *	1.1081811 *
5 C	1.5087293 *	3.9416095	3.4628110	2.1832682 *
6 C	2.5950248 *	3.5221496	4.0246607	3.5080721
7 C	3.8854730	2.2002767 *	3.4862548	3.9551252
8 C	5.1099620	2.6886910 *	4.6725693	5.3988330
9 C	5.3922736	4.0856735	5.9293731	6.2680362
10 C	4.5745931	4.8961481	6.2527467	6.0060754
11 C	3.1645571	4.6959126	5.4836752	4.8006968
12 N	2.9141859 *	6.0089866	6.4048693	5.1733996
13 C	4.0122617	7.1204975	7.6707555	6.4191299
14 C	4.7517141	8.4974421	8.8473015	7.3231821
15 C	4.7187413	9.0760463	9.0815398	7.2845357
16 C	5.9606637	10.4780143	10.4127475	8.5086869
17 C	7.0585755	11.3234324	11.4701802	9.6673579
18 C	7.1181299	10.9102646	11.3320661	9.7395285
19 C	6.0952241	9.5621228	10.1049782	8.6686088
20 O	3.7451273	8.3715045	8.0820748	6.1606057
21 N	0.0000000	5.4394176	4.6652004	2.6462278 *
22 H	5.4394176	0.0000000	2.5259416 *	4.3581086
23 H	4.6652004	2.5259416 *	0.0000000	2.5172722 *
24 H	2.6462278 *	4.3581086	2.5172722 *	0.0000000
25 H	6.0537008	2.4151958 *	4.7892114	5.9821178
26 H	6.4772174	4.7835113	6.8490111	7.3489274
27 H	5.2729268	5.9665477	7.3362685	6.9610847
28 H	4.7538217	7.1562970	8.0099716	7.0148903
29 H	6.2698856	11.0195623	10.7409200	8.7048183
30 H	8.0377659	12.4126617	12.5030654	10.6320359
31 H	8.1339756	11.7328567	12.2770535	10.7512846
32 H	6.4933750	9.4161851	10.1994821	8.9773815

33 H	4.3540428	9.0808568	8.6199423	6.5969915
34 H	1.0445184 *	5.8192780	5.1557788	3.2154461
35 H	1.0390161 *	5.8061908	4.5659547	2.1932456 *

	H	H	H	H
--	---	---	---	---

1 CO	6.5502477	6.3097988	4.5276900	3.8736006
2 C	2.6885924 *	4.6681229	5.3864435	6.3657033
3 C	4.0885905	5.9286535	6.2590353	6.9116966
4 C	4.8969352	6.2534360	6.0030304	6.2619482
5 C	4.6731073	5.4695217	4.8023330	4.8857779
6 C	3.5188741	4.0176967	3.5043019	4.0166063
7 C	2.1995345 *	3.4834174	3.9476418	4.9864164
8 C	1.1050214 *	2.1840560 *	3.4289735	4.9279186
9 C	2.1785237 *	1.1046620 *	2.1798353 *	3.9405799
10 C	3.4519442	2.1981722 *	1.1041233 *	2.6267612 *
11 C	3.9641676	3.4753292	2.1902706 *	2.6375572 *
12 N	5.4178353	4.6692645	2.6923512 *	2.0945481 *
13 C	6.2183605	4.9832649	2.6401341 *	1.1079429 *
14 C	7.6630020	6.3292930	3.8773374	2.1723356 *
15 C	8.5353003	7.4290927	5.0148389	3.5280641
16 C	9.9175638	8.6982093	6.2328994	4.6708809
17 C	10.5155485	9.0225761	6.5272283	4.8474800
18 C	9.8609777	8.1720173	5.7243382	3.9910718
19 C	8.4687226	6.8156246	4.3807861	2.5765301 *
20 O	8.1802119	7.4713073	5.2643767	4.1386777
21 N	6.0537008	6.4772174	5.2729268	4.7538217
22 H	2.4151958 *	4.7835113	5.9665477	7.1562970
23 H	4.7892114	6.8490111	7.3362685	8.0099716
24 H	5.9821178	7.3489274	6.9610847	7.0148903
25 H	0.0000000	2.5245179 *	4.3448330	5.9482097
26 H	2.5245179 *	0.0000000	2.4991060 *	4.4312024
27 H	4.3448330	2.4991060 *	0.0000000	2.1578980 *
28 H	5.9482097	4.4312024	2.1578980 *	0.0000000
29 H	10.6405227	9.5658823	7.1379012	5.6674819
30 H	11.6137966	10.0853532	7.5904743	5.9260920
31 H	10.5369039	8.6912381	6.3244964	4.6492171
32 H	8.1069903	6.2812043	3.9883688	2.2609795 *
33 H	9.0084457	8.3551100	6.1644754	5.0953524
34 H	6.2990358	6.6099998	5.3551334	4.5263026
35 H	6.7548269	7.3996343	6.2813006	5.7645070

	H	H	H	H
--	---	---	---	---

1 CO	4.6272530	6.4388260	6.6976143	5.2983782
2 C	9.9820605	11.4373050	10.8693701	8.6201071

3 C	9.8177084	11.4975135	11.2033570	9.1062558
4 C	8.5888275	10.3665748	10.2682847	8.3380471
5 C	7.4129615	9.0591067	8.8729496	6.9368192
6 C	7.5629581	8.9139102	8.3807551	6.2226774
7 C	8.9743035	10.2462447	9.5360458	7.2443501
8 C	9.5427620	10.5354355	9.5271050	7.1248279
9 C	8.8932990	9.6246310	8.4299898	6.0133845
10 C	7.4810625	8.2112956	7.1189566	4.7555451
11 C	6.7190474	7.7892964	7.0597812	4.8476457
12 N	5.2757529	6.4069890	5.9195330	3.9718737
13 C	4.7931938	5.4445545	4.6540781	2.6406943 *
14 C	3.5019144	3.9845374	3.4927502	2.1991850 *
15 C	2.1944187 *	3.4389715	3.9284693	3.4505662
16 C	1.1063863 *	2.1920819 *	3.4757896	3.9527942
17 C	2.2017053 *	1.1044748 *	2.1984890 *	3.4562074
18 C	3.4758976	2.1985638 *	1.1037656 *	2.1845671 *
19 C	3.9534251	3.4577976	2.1860807 *	1.1056972 *
20 O	2.6842169 *	4.6486906	5.3934339	4.6924771
21 N	6.2698856	8.0377659	8.1339756	6.4933750
22 H	11.0195623	12.4126617	11.7328567	9.4161851
23 H	10.7409200	12.5030654	12.2770535	10.1994821
24 H	8.7048183	10.6320359	10.7512846	8.9773815
25 H	10.6405227	11.6137966	10.5369039	8.1069903
26 H	9.5658823	10.0853532	8.6912381	6.2812043
27 H	7.1379012	7.5904743	6.3244964	3.9883688
28 H	5.6674819	5.9260920	4.6492171	2.2609795 *
29 H	0.0000000	2.5238983 *	4.3889624	5.0591201
30 H	2.5238983 *	0.0000000	2.5384949 *	4.3710764
31 H	4.3889624	2.5384949 *	0.0000000	2.5130675 *
32 H	5.0591201	4.3710764	2.5130675 *	0.0000000
33 H	2.2976749 *	4.6195523	5.8027646	5.4574587
34 H	6.3106355	7.8732865	7.8292268	6.1732750
35 H	6.6264800	8.5788344	8.9044676	7.4142596

H H H

1 CO	2.6584346 *	2.4917926 *	2.6189115 *
2 C	8.0289684	4.7475579	4.7253142
3 C	7.7473403	4.3049881	3.9011740
4 C	6.5132203	3.0518735	2.4703664 *
5 C	5.4458143	2.1082452 *	2.0828048 *
6 C	5.7741525	2.9570007 *	3.4219303
7 C	7.1759845	4.2244647	4.5571428
8 C	7.9346424	5.3526099	5.8844826
9 C	7.5333323	5.5560116	6.3025405
10 C	6.2180690	4.7060722	5.5602832

11	C	5.2198438	3.3523675	4.1569960
12	N	3.8966021	3.0352003	3.8999649
13	C	4.0110430	3.9002217	4.9765746
14	C	3.3217274	4.6163745	5.5786269
15	C	2.0371816 *	4.7184872	5.3433691
16	C	2.4974228 *	5.9213699	6.4748877
17	C	3.9163017	6.8978607	7.6618546
18	C	4.7186369	6.8660555	7.8651543
19	C	4.4780042	5.8389913	6.9399364
20	O	0.9897449 *	3.9857625	4.2133908
21	N	4.3540428	1.0445184 *	1.0390161 *
22	H	9.0808568	5.8192780	5.8061908
23	H	8.6199423	5.1557788	4.5659547
24	H	6.5969915	3.2154461	2.1932456 *
25	H	9.0084457	6.2990358	6.7548269
26	H	8.3551100	6.6099998	7.3996343
27	H	6.1644754	5.3551334	6.2813006
28	H	5.0953524	4.5263026	5.7645070
29	H	2.2976749 *	6.3106355	6.6264800
30	H	4.6195523	7.8732865	8.5788344
31	H	5.8027646	7.8292268	8.9044676
32	H	5.4574587	6.1732750	7.4142596
33	H	0.0000000	4.6699793	4.6314259
34	H	4.6699793	0.0000000	1.6673966 *
35	H	4.6314259	1.6673966 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 6158.8 SECONDS (102.6 MIN)

WALL CLOCK TIME: STEP = 0.78 , TOTAL = 5692.8 SECONDS (94.9 MIN)

CPU UTILIZATION: STEP = 99.97%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.09 , TOTAL = 6159.9 SECONDS (102.7 MIN)

WALL CLOCK TIME: STEP = 1.09 , TOTAL = 5693.9 SECONDS (94.9 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636185345	-284.636185345	0.004041032	0.000953525	197546682
11365655						
2	1	-284.636242699	-0.000057354	0.001131269	0.000072394	153055182
15160890						
3	2	-284.636242914	-0.000000215	0.000638516	0.000110514	136601294
16453866						
4	3	-284.636243440	-0.000000526	0.000352639	0.000037948	130691271
16876115						
5	4	-284.636243466	-0.000000026	0.000198655	0.000035117	125381869
17322178						
6	5	-284.636243537	-0.000000070	0.000143815	0.000019979	118340291
17834366						
7	6	-284.636243567	-0.000000030	0.000111867	0.000016717	117186134
17961311						
8	7	-284.636243561	0.000000006	0.000129352	0.000016538	112707954
18261492						
9	8	-284.636243578	-0.000000017	0.000249773	0.000016864	136555487
16541732						
10	9	-284.636243600	-0.000000022	0.000300705	0.000015594	161296807
14620704						

-----DISABLING FDIFF OPTION-----

11	10	-284.636243612	-0.000000012	0.000280940	0.000016490	197542579
11366021						
12	11	-284.636243621	-0.000000009	0.000101217	0.000018551	197542636
11366011						
13	12	-284.636243631	-0.000000010	0.000100829	0.000013205	197542668
11366007						
14	13	-284.636243635	-0.000000004	0.000069084	0.000004855	197542588
11366005						
15	14	-284.636243637	-0.000000002	0.000026977	0.000003117	197542587
11366008						
16	15	-284.636243638	0.000000000	0.000019188	0.000002321	197542581
11366008						
17	16	-284.636243638	0.000000000	0.000015678	0.000001648	197542597
11366004						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 56.4 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 18.5 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.3
TIME TO SOLVE SCF EQUATIONS= 1.5 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6362436380 AFTER 17 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6019610326
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999416985

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 59.11 , TOTAL = 6219.0 SECONDS (103.7 MIN)
WALL CLOCK TIME: STEP = 54.24 , TOTAL = 5748.2 SECONDS (95.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.78 , TOTAL = 6222.8 SECONDS (103.7 MIN)
WALL CLOCK TIME: STEP = 3.76 , TOTAL = 5751.9 SECONDS (95.9 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.67 , TOTAL = 6225.5 SECONDS (103.8 MIN)
WALL CLOCK TIME: STEP = 2.67 , TOTAL = 5754.6 SECONDS (95.9 MIN)
CPU UTILIZATION: STEP = 99.82% , TOTAL = 100.00%

NSERCH= 63 ENERGY= -284.6362436

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
------	------	-------	-------	-------

1	CO	27.0	0.0009671	-0.0002927	-0.0008563
2	C	6.0	0.0002083	0.0006876	0.0002105
3	C	6.0	0.0000483	-0.0009429	0.0003523
4	C	6.0	-0.0001672	-0.0004943	0.0006887
5	C	6.0	0.0000931	-0.0000990	0.0001808
6	C	6.0	-0.0000868	-0.0000822	0.0000902
7	C	6.0	-0.0002041	0.0002553	-0.0001333
8	C	6.0	-0.0005634	0.0002330	-0.0006216
9	C	6.0	0.0002630	-0.0000017	-0.0003565
10	C	6.0	-0.0002263	0.0000972	0.0000638
11	C	6.0	0.0003918	0.0004357	0.0002996
12	N	7.0	-0.0003705	-0.0006128	0.0003714
13	C	6.0	-0.0005773	-0.0002687	0.0000768
14	C	6.0	0.0004780	-0.0002944	0.0002311
15	C	6.0	0.0003148	0.0006326	0.0000325
16	C	6.0	-0.0005531	-0.0008538	0.0003311
17	C	6.0	0.0001366	-0.0004242	0.0000498
18	C	6.0	-0.0000209	0.0007625	-0.0003489
19	C	6.0	-0.0009589	0.0001736	-0.0002778
20	O	8.0	-0.0003496	-0.0018280	-0.0003204
21	N	7.0	0.0008686	-0.0004347	0.0001676
22	H	1.0	0.0002852	-0.0004477	-0.0000129
23	H	1.0	-0.0007289	0.0002936	-0.0004295
24	H	1.0	-0.0000443	-0.0002983	0.0002249
25	H	1.0	-0.0003169	0.0005019	-0.0006762
26	H	1.0	0.0000408	0.0001089	0.0005400
27	H	1.0	0.0003052	0.0000548	0.0008075
28	H	1.0	0.0000769	-0.0003763	-0.0007738
29	H	1.0	0.0002466	0.0001593	-0.0003225
30	H	1.0	0.0004070	0.0003705	-0.0002976
31	H	1.0	0.0002608	0.0001766	0.0008193
32	H	1.0	-0.0001824	-0.0000419	0.0002558
33	H	1.0	-0.0001143	0.0021149	-0.0004025
34	H	1.0	-0.0004586	0.0001491	-0.0000765
35	H	1.0	0.0005314	0.0005863	0.0001128

MAXIMUM GRADIENT = 0.0021149 RMS GRADIENT = 0.0004984
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000495584
 PREDICTED ENERGY CHANGE WAS -0.0000719701 RATIO= 0.689
 GDIIS STEP HAS LENGTH = 0.394969
 RADIUS OF STEP TAKEN= 0.05244 CURRENT TRUST RADIUS= 0.05244

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 0.03 , TOTAL = 6225.5 SECONDS (103.8 MIN)

WALL CLOCK TIME: STEP = 0.03 , TOTAL = 5754.6 SECONDS (95.9 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

INSERCH= 64

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1515874780	-1.7633885725	0.8753205449
C	6.0	4.9835488595	0.6548350563	0.5206770272
C	6.0	5.1954622309	-0.7021230479	0.2387097717
C	6.0	4.0659220048	-1.5459253271	-0.0081428010
C	6.0	2.7551169953	-1.0375345258	0.0507149256
C	6.0	2.4726037653	0.3391225122	0.4377127425
C	6.0	3.6485083738	1.1966733835	0.6313919795
C	6.0	3.4883372274	2.5959026140	0.9533838860
C	6.0	2.2181266583	3.1482000152	1.1665973713
C	6.0	1.0626449345	2.3129102613	1.0589851025
C	6.0	1.1628143884	0.9577565609	0.6628555791
N	7.0	-0.0471501352	0.1488710023	0.6201417461
C	6.0	-1.2395073589	0.6818770524	0.3500602812
C	6.0	-2.5517133887	0.0386085406	0.4561171400
C	6.0	-2.8367459698	-1.3065717171	0.8708483304
C	6.0	-4.1421792128	-1.8226060615	0.9644856251
C	6.0	-5.2432673182	-0.9674247541	0.6544282426
C	6.0	-5.0172019596	0.3797015007	0.2532863389
C	6.0	-3.6931618992	0.8673160184	0.1477183761
O	8.0	-1.7250127983	-2.1989258353	1.2104691636
N	7.0	1.6641187935	-1.9892044397	-0.3745446236
H	1.0	5.8445884621	1.3300898316	0.6744256132
H	1.0	6.2155922140	-1.1164985323	0.1690224752
H	1.0	4.2379533189	-2.6038399357	-0.2892294576
H	1.0	4.3921031781	3.2234722711	1.0539047203
H	1.0	2.1034296361	4.2065428854	1.4611745322
H	1.0	0.0843303738	2.7390451194	1.3425553963
H	1.0	-1.2686884777	1.7310286003	-0.0048346784
H	1.0	-4.3227226195	-2.8708122681	1.2691918107
H	1.0	-6.2721754510	-1.3626698674	0.7262293930
H	1.0	-5.8690147684	1.0464399112	0.0331356472
H	1.0	-3.5188845641	1.9140348746	-0.1634741022
H	1.0	-2.0589253758	-3.0290253511	1.6348941688
H	1.0	1.3201808161	-1.7349548120	-1.3273353202
H	1.0	2.0753785885	-2.9398179638	-0.4579899479

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C	
1	CO	0.0000000	5.4149264	5.1934796	4.0186829
2	C	5.4149264	0.0000000	1.4020514 *	2.4423423 *
3	C	5.1934796	1.4020514 *	0.0000000	1.4313628 *
4	C	4.0186829	2.4423423 *	1.4313628 *	0.0000000
5	C	2.8258104 *	2.8374086 *	2.4704509 *	1.4071728 *
6	C	3.1621464	2.5320748 *	2.9219433 *	2.5081578 *
7	C	4.5880196	1.4450535 *	2.4804623 *	2.8469434 *
8	C	5.4903017	2.4880989 *	3.7817996	4.2910228
9	C	5.3365840	3.7791060	4.9548451	5.1796887
10	C	4.1809055	4.2909762	5.1810671	5.0049023
11	C	2.9107305 *	3.8353602	4.3814779	3.8918756
12	N	1.9394199 *	5.0570570	5.3249099	4.4927095
13	C	2.8618818 *	6.2254534	6.5830607	5.7653268
14	C	3.2757840	7.5606931	7.7855430	6.8205119
15	C	3.0230512	8.0701145	8.0796860	6.9625240
16	C	4.2951006	9.4664457	9.4325914	8.2701562
17	C	5.4577294	10.3555485	10.4503723	9.3506507
18	C	5.6299330	10.0081074	10.2698134	9.2886772
19	C	4.7150938	8.6873216	9.0265751	8.1272018
20	O	1.9554145 *	7.3228795	7.1468671	5.9536838
21	N	1.9750713 *	4.3371630	3.8082865	2.4696974 *
22	H	6.4823011	1.1049873 *	2.1774073 *	3.4497851
23	H	6.1391756	2.1861414 *	1.1032808 *	2.1992901 *
24	H	4.3313879	3.4395965	2.1936431 *	1.1080559 *
25	H	6.5484843	2.6892447 *	4.0890374	4.8970902
26	H	6.3081689	4.6684313	5.9287509	6.2530921
27	H	4.5271118	5.3871846	6.2596951	6.0032016
28	H	3.8733459	6.3659113	6.9112072	6.2607114
29	H	4.6261185	9.9798373	9.8163613	8.5881469
30	H	6.4379759	11.4369536	11.4969871	10.3657679
31	H	6.6971683	10.8705652	11.2036773	10.2676692
32	H	5.2985755	8.6223559	9.1074626	8.3381499
33	H	2.6580360 *	8.0255063	7.7453176	6.5125196
34	H	2.4936142 *	4.7483166	4.3054668	3.0520642
35	H	2.6196708 *	4.7261796	3.9022546	2.4713483 *
	C	C	C	C	
1	CO	2.8258104 *	3.1621464	4.5880196	5.4903017
2	C	2.8374086 *	2.5320748 *	1.4450535 *	2.4880989 *
3	C	2.4704509 *	2.9219433 *	2.4804623 *	3.7817996

4 C	1.4071728 *	2.5081578 *	2.8469434 *	4.2910228
5 C	0.0000000	1.4576576 *	2.4752816 *	3.8150083
6 C	1.4576576 *	0.0000000	1.4682155 *	2.5279809 *
7 C	2.4752816 *	1.4682155 *	0.0000000	1.4447062 *
8 C	3.8150083	2.5279809 *	1.4447062 *	0.0000000
9 C	4.3650803	2.9132367 *	2.4780825 *	1.4014019 *
10 C	3.8867146	2.5039571 *	2.8487735 *	2.4444262 *
11 C	2.6251343 *	1.4659282 *	2.4973478 *	2.8593681 *
12 N	3.0958853	2.5335027 *	3.8413420	4.3126193
13 C	4.3592439	3.7289318	4.9230946	5.1361472
14 C	5.4299985	5.0333299	6.3098800	6.5779357
15 C	5.6580855	5.5754023	6.9557242	7.4325497
16 C	7.0017147	6.9789622	8.3619264	8.8174896
17 C	8.0214423	7.8287099	9.1513675	9.4354435
18 C	7.9030712	7.4921859	8.7123443	8.8173625
19 C	6.7244454	6.1951393	7.3649534	7.4304131
20 O	4.7713125	4.9657655	6.3828014	7.0877000
21 N	1.5089064 *	2.5950947 *	3.8858111	5.1102225
22 H	3.9420165	3.5225460	2.2005498 *	2.6892415 *
23 H	3.4633973	4.0250453	3.4863260	4.6728005
24 H	2.1835014 *	3.5079812	3.9546037	5.3984567
25 H	4.6735738	3.5190402	2.1998554 *	1.1048715 *
26 H	5.4694095	4.0175495	3.4835502	2.1840290 *
27 H	4.8025521	3.5045996	3.9481678	3.4291700
28 H	4.8845714	4.0162817	4.9868973	4.9290449
29 H	7.4122471	7.5611837	8.9717196	9.5392538
30 H	9.0583686	8.9135011	10.2459358	10.5351556
31 H	8.8723676	8.3813233	9.5374906	9.5293089
32 H	6.9369110	6.2241230	7.2469263	7.1283569
33 H	5.4452423	5.7716912	7.1720532	7.9294636
34 H	2.1081886 *	2.9572403 *	4.2251823	5.3534016
35 H	2.0831484 *	3.4222101	4.5576366	5.8849495

C C C N

1 CO	5.3365840	4.1809055	2.9107305 *	1.9394199 *
2 C	3.7791060	4.2909762	3.8353602	5.0570570
3 C	4.9548451	5.1810671	4.3814779	5.3249099
4 C	5.1796887	5.0049023	3.8918756	4.4927095
5 C	4.3650803	3.8867146	2.6251343 *	3.0958853
6 C	2.9132367 *	2.5039571 *	1.4659282 *	2.5335027 *
7 C	2.4780825 *	2.8487735 *	2.4973478 *	3.8413420
8 C	1.4014019 *	2.4444262 *	2.8593681 *	4.3126193
9 C	0.0000000	1.4298347 *	2.4830389 *	3.7981663
10 C	1.4298347 *	0.0000000	1.4154130 *	2.4712941 *
11 C	2.4830389 *	1.4154130 *	0.0000000	1.4560682 *

12 N	3.7981663	2.4712941 *	1.4560682 *	0.0000000
13 C	4.3248948	2.9090804 *	2.4382576 *	1.3336998 *
14 C	5.7380934	4.3127119	3.8321392	2.5123493 *
15 C	6.7441972	5.3236543	4.6007528	3.1564240
16 C	8.0748531	6.6484299	5.9970288	4.5579115
17 C	8.5365733	7.1196063	6.6891163	5.3147837
18 C	7.8005578	6.4304731	6.2204901	4.9889158
19 C	6.4174667	5.0534986	4.8840610	3.7460311
20 O	6.6439467	5.3057184	4.3132436	2.9454812 *
21 N	5.3921209	4.5743818	3.1641878	2.9136247 *
22 H	4.0864389	4.8970201	4.6965705	6.0092269
23 H	5.9298010	6.2534585	5.4842474	6.4052018
24 H	6.2677823	6.0062216	4.8008244	5.1736336
25 H	2.1781964 *	3.4517302	3.9641762	5.4174065
26 H	1.1045455 *	2.1979158 *	3.4751522	4.6687290
27 H	2.1797834 *	1.1041297 *	2.1904585 *	2.6922427 *
28 H	3.9418914	2.6278155 *	2.6374166 *	2.0942717 *
29 H	8.8894175	7.4777904	6.7168965	5.2744927
30 H	9.6242974	8.2109808	7.7889325	6.4067894
31 H	8.4323180	7.1206896	7.0605264	5.9198238
32 H	6.0171049	4.7585629	4.8492880	3.9727569
33 H	7.5279871	6.2138674	5.2171732	3.8956370
34 H	5.5561865	4.7059602	3.3520618	3.0349729
35 H	6.3026680	5.5603954	4.1569406	3.8996789

C C C C

1 CO	2.8618818 *	3.2757840	3.0230512	4.2951006
2 C	6.2254534	7.5606931	8.0701145	9.4664457
3 C	6.5830607	7.7855430	8.0796860	9.4325914
4 C	5.7653268	6.8205119	6.9625240	8.2701562
5 C	4.3592439	5.4299985	5.6580855	7.0017147
6 C	3.7289318	5.0333299	5.5754023	6.9789622
7 C	4.9230946	6.3098800	6.9557242	8.3619264
8 C	5.1361472	6.5779357	7.4325497	8.8174896
9 C	4.3248948	5.7380934	6.7441972	8.0748531
10 C	2.9090804 *	4.3127119	5.3236543	6.6484299
11 C	2.4382576 *	3.8321392	4.6007528	5.9970288
12 N	1.3336998 *	2.5123493 *	3.1564240	4.5579115
13 C	0.0000000	1.4652396 *	2.6031365 *	3.8827127
14 C	1.4652396 *	0.0000000	1.4362296 *	2.5004279 *
15 C	2.6031365 *	1.4362296 *	0.0000000	1.4068459 *
16 C	3.8827127	2.5004279 *	1.4068459 *	0.0000000
17 C	4.3408444	2.8802592 *	2.4399187 *	1.4282387 *
18 C	3.7909961	2.4972222 *	2.8247634 *	2.4741924 *
19 C	2.4689574 *	1.4438735 *	2.4458440 *	2.8468239 *

20	O	3.0454957	2.5018075 *	1.4654654 *	2.4586211 *
21	N	4.0113306	4.7513435	4.7196159	5.9610279
22	H	7.1210818	8.4978507	9.0750280	10.4766003
23	H	7.6710781	8.8477310	9.0814929	10.4122418
24	H	6.4192837	7.3237729	7.2856060	8.5093331
25	H	6.2185320	7.6627212	8.5329402	9.9148817
26	H	4.9832792	6.3286787	7.4261870	8.6951117
27	H	2.6399874 *	3.8764490	5.0122061	6.2301671
28	H	1.1079354 *	2.1732269 *	3.5288299	4.6717074
29	H	4.7929762	3.5017558	2.1940038 *	1.1064258 *
30	H	5.4451284	3.9847685	3.4389297	2.1920747 *
31	H	4.6546414	3.4927247	3.9284959	3.4757443
32	H	2.6414941 *	2.1992129 *	3.4507163	3.9526289
33	H	4.0116132	3.3230608	2.0385332 *	2.4989681 *
34	H	3.8995815	4.6171197	4.7218178	5.9243146
35	H	4.9757501	5.5782252	5.3443683	6.4753088

C C C O

1	CO	5.4577294	5.6299330	4.7150938	1.9554145 *
2	C	10.3555485	10.0081074	8.6873216	7.3228795
3	C	10.4503723	10.2698134	9.0265751	7.1468671
4	C	9.3506507	9.2886772	8.1272018	5.9536838
5	C	8.0214423	7.9030712	6.7244454	4.7713125
6	C	7.8287099	7.4921859	6.1951393	4.9657655
7	C	9.1513675	8.7123443	7.3649534	6.3828014
8	C	9.4354435	8.8173625	7.4304131	7.0877000
9	C	8.5365733	7.8005578	6.4174667	6.6439467
10	C	7.1196063	6.4304731	5.0534986	5.3057184
11	C	6.6891163	6.2204901	4.8840610	4.3132436
12	N	5.3147837	4.9889158	3.7460311	2.9454812 *
13	C	4.3408444	3.7909961	2.4689574 *	3.0454957
14	C	2.8802592 *	2.4972222 *	1.4438735 *	2.5018075 *
15	C	2.4399187 *	2.8247634 *	2.4458440 *	1.4654654 *
16	C	1.4282387 *	2.4741924 *	2.8468239 *	2.4586211 *
17	C	0.0000000	1.4236466 *	2.4547618 *	3.7688050
18	C	1.4236466 *	0.0000000	1.4149186 *	4.2899915
19	C	2.4547618 *	1.4149186 *	0.0000000	3.7953773
20	O	3.7688050	4.2899915	3.7953773	0.0000000
21	N	7.0579602	7.1165957	6.0936790	3.7473277
22	H	11.3234058	10.9114200	9.5634859	8.3689998
23	H	11.4701048	11.3323157	10.1054135	8.0814274
24	H	9.6675689	9.7392886	8.6684737	6.1619815
25	H	10.5149210	9.8622029	8.4701923	8.1759416
26	H	9.0219032	8.1735612	6.8173365	7.4665825
27	H	6.5264642	5.7252634	4.3818322	5.2606774

28 H	4.8490778	3.9930020	2.5782442 *	4.1388087
29 H	2.2018676 *	3.4756590	3.9531826	2.6838361 *
30 H	1.1045479 *	2.1987477 *	3.4581531	4.6487095
31 H	2.1984575 *	1.1038983 *	2.1862183 *	5.3936319
32 H	3.4561930	2.1846792 *	1.1058181 *	4.6927755
33 H	3.9181047	4.7201334	4.4792742	0.9903027 *
34 H	6.8989376	6.8653155	5.8379108	3.9911057
35 H	7.6609652	7.8631942	6.9380985	4.2161181

N H H H

1 CO	1.9750713 *	6.4823011	6.1391756	4.3313879
2 C	4.3371630	1.1049873 *	2.1861414 *	3.4395965
3 C	3.8082865	2.1774073 *	1.1032808 *	2.1936431 *
4 C	2.4696974 *	3.4497851	2.1992901 *	1.1080559 *
5 C	1.5089064 *	3.9420165	3.4633973	2.1835014 *
6 C	2.5950947 *	3.5225460	4.0250453	3.5079812
7 C	3.8858111	2.2005498 *	3.4863260	3.9546037
8 C	5.1102225	2.6892415 *	4.6728005	5.3984567
9 C	5.3921209	4.0864389	5.9298010	6.2677823
10 C	4.5743818	4.8970201	6.2534585	6.0062216
11 C	3.1641878	4.6965705	5.4842474	4.8008244
12 N	2.9136247 *	6.0092269	6.4052018	5.1736336
13 C	4.0113306	7.1210818	7.6710781	6.4192837
14 C	4.7513435	8.4978507	8.8477310	7.3237729
15 C	4.7196159	9.0750280	9.0814929	7.2856060
16 C	5.9610279	10.4766003	10.4122418	8.5093331
17 C	7.0579602	11.3234058	11.4701048	9.6675689
18 C	7.1165957	10.9114200	11.3323157	9.7392886
19 C	6.0936790	9.5634859	10.1054135	8.6684737
20 O	3.7473277	8.3689998	8.0814274	6.1619815
21 N	0.0000000	5.4400717	4.6661538	2.6475800 *
22 H	5.4400717	0.0000000	2.5256426 *	4.3572596
23 H	4.6661538	2.5256426 *	0.0000000	2.5165919 *
24 H	2.6475800 *	4.3572596	2.5165919 *	0.0000000
25 H	6.0542848	2.4163226 *	4.7899348	5.9820849
26 H	6.4768931	4.7842685	6.8494020	7.3485658
27 H	5.2726187	5.9675896	7.3372180	6.9614457
28 H	4.7516500	7.1568747	8.0095627	7.0139197
29 H	6.2706756	11.0170568	10.7398356	8.7054652
30 H	8.0367291	12.4124778	12.5026166	10.6317669
31 H	8.1320011	11.7345733	12.2773977	10.7507798
32 H	6.4917911	9.4190071	10.2007218	8.9775019
33 H	4.3566191	9.0768891	8.6182469	6.5980085
34 H	1.0443880 *	5.8199493	5.1562222	3.2165232
35 H	1.0391168 *	5.8070148	4.5671662	2.1950150 *

	H	H	H	H
1 CO	6.5484843	6.3081689	4.5271118	3.8733459
2 C	2.6892447 *	4.6684313	5.3871846	6.3659113
3 C	4.0890374	5.9287509	6.2596951	6.9112072
4 C	4.8970902	6.2530921	6.0032016	6.2607114
5 C	4.6735738	5.4694095	4.8025521	4.8845714
6 C	3.5190402	4.0175495	3.5045996	4.0162817
7 C	2.1998554 *	3.4835502	3.9481678	4.9868973
8 C	1.1048715 *	2.1840290 *	3.4291700	4.9290449
9 C	2.1781964 *	1.1045455 *	2.1797834 *	3.9418914
10 C	3.4517302	2.1979158 *	1.1041297 *	2.6278155 *
11 C	3.9641762	3.4751522	2.1904585 *	2.6374166 *
12 N	5.4174065	4.6687290	2.6922427 *	2.0942717 *
13 C	6.2185320	4.9832792	2.6399874 *	1.1079354 *
14 C	7.6627212	6.3286787	3.8764490	2.1732269 *
15 C	8.5329402	7.4261870	5.0122061	3.5288299
16 C	9.9148817	8.6951117	6.2301671	4.6717074
17 C	10.5149210	9.0219032	6.5264642	4.8490778
18 C	9.8622029	8.1735612	5.7252634	3.9930020
19 C	8.4701923	6.8173365	4.3818322	2.5782442 *
20 O	8.1759416	7.4665825	5.2606774	4.1388087
21 N	6.0542848	6.4768931	5.2726187	4.7516500
22 H	2.4163226 *	4.7842685	5.9675896	7.1568747
23 H	4.7899348	6.8494020	7.3372180	8.0095627
24 H	5.9820849	7.3485658	6.9614457	7.0139197
25 H	0.0000000	2.5239499 *	4.3445248	5.9491915
26 H	2.5239499 *	0.0000000	2.4988762 *	4.4326668
27 H	4.3445248	2.4988762 *	0.0000000	2.1592168 *
28 H	5.9491915	4.4326668	2.1592168 *	0.0000000
29 H	10.6364863	9.5614458	7.1342833	5.6680868
30 H	11.6132213	10.0849906	7.5900652	5.9279260
31 H	10.5390693	8.6939873	6.3262794	4.6511402
32 H	8.1105095	6.2853395	3.9914815	2.2631925 *
33 H	9.0026132	8.3491811	6.1603282	5.0962043
34 H	6.3002389	6.6098911	5.3546539	4.5237477
35 H	6.7556780	7.3996252	6.2813790	5.7623729

	H	H	H	H
1 CO	4.6261185	6.4379759	6.6971683	5.2985755
2 C	9.9798373	11.4369536	10.8705652	8.6223559
3 C	9.8163613	11.4969871	11.2036773	9.1074626
4 C	8.5881469	10.3657679	10.2676692	8.3381499
5 C	7.4122471	9.0583686	8.8723676	6.9369110

6 C	7.5611837	8.9135011	8.3813233	6.2241230
7 C	8.9717196	10.2459358	9.5374906	7.2469263
8 C	9.5392538	10.5351556	9.5293089	7.1283569
9 C	8.8894175	9.6242974	8.4323180	6.0171049
10 C	7.4777904	8.2109808	7.1206896	4.7585629
11 C	6.7168965	7.7889325	7.0605264	4.8492880
12 N	5.2744927	6.4067894	5.9198238	3.9727569
13 C	4.7929762	5.4451284	4.6546414	2.6414941 *
14 C	3.5017558	3.9847685	3.4927247	2.1992129 *
15 C	2.1940038 *	3.4389297	3.9284959	3.4507163
16 C	1.1064258 *	2.1920747 *	3.4757443	3.9526289
17 C	2.2018676 *	1.1045479 *	2.1984575 *	3.4561930
18 C	3.4756590	2.1987477 *	1.1038983 *	2.1846792 *
19 C	3.9531826	3.4581531	2.1862183 *	1.1058181 *
20 O	2.6838361 *	4.6487095	5.3936319	4.6927755
21 N	6.2706756	8.0367291	8.1320011	6.4917911
22 H	11.0170568	12.4124778	11.7345733	9.4190071
23 H	10.7398356	12.5026166	12.2773977	10.2007218
24 H	8.7054652	10.6317669	10.7507798	8.9775019
25 H	10.6364863	11.6132213	10.5390693	8.1105095
26 H	9.5614458	10.0849906	8.6939873	6.2853395
27 H	7.1342833	7.5900652	6.3262794	3.9914815
28 H	5.6680868	5.9279260	4.6511402	2.2631925 *
29 H	0.0000000	2.5238201 *	4.3890453	5.0589969
30 H	2.5238201 *	0.0000000	2.5390406 *	4.3713816
31 H	4.3890453	2.5390406 *	0.0000000	2.5128646 *
32 H	5.0589969	4.3713816	2.5128646 *	0.0000000
33 H	2.2985969 *	4.6210268	5.8044663	5.4588876
34 H	6.3146247	7.8739823	7.8276159	6.1714060
35 H	6.6274895	8.5773790	8.9019572	7.4123146

H H H

1 CO	2.6580360 *	2.4936142 *	2.6196708 *
2 C	8.0255063	4.7483166	4.7261796
3 C	7.7453176	4.3054668	3.9022546
4 C	6.5125196	3.0520642	2.4713483 *
5 C	5.4452423	2.1081886 *	2.0831484 *
6 C	5.7716912	2.9572403 *	3.4222101
7 C	7.1720532	4.2251823	4.5576366
8 C	7.9294636	5.3534016	5.8849495
9 C	7.5279871	5.5561865	6.3026680
10 C	6.2138674	4.7059602	5.5603954
11 C	5.2171732	3.3520618	4.1569406
12 N	3.8956370	3.0349729	3.8996789
13 C	4.0116132	3.8995815	4.9757501

14 C	3.3230608	4.6171197	5.5782252
15 C	2.0385332 *	4.7218178	5.3443683
16 C	2.4989681 *	5.9243146	6.4753088
17 C	3.9181047	6.8989376	7.6609652
18 C	4.7201334	6.8653155	7.8631942
19 C	4.4792742	5.8379108	6.9380985
20 O	0.9903027 *	3.9911057	4.2161181
21 N	4.3566191	1.0443880 *	1.0391168 *
22 H	9.0768891	5.8199493	5.8070148
23 H	8.6182469	5.1562222	4.5671662
24 H	6.5980085	3.2165232	2.1950150 *
25 H	9.0026132	6.3002389	6.7556780
26 H	8.3491811	6.6098911	7.3996252
27 H	6.1603282	5.3546539	6.2813790
28 H	5.0962043	4.5237477	5.7623729
29 H	2.2985969 *	6.3146247	6.6274895
30 H	4.6210268	7.8739823	8.5773790
31 H	5.8044663	7.8276159	8.9019572
32 H	5.4588876	6.1714060	7.4123146
33 H	0.0000000	4.6762999	4.6347159
34 H	4.6762999	0.0000000	1.6666674 *
35 H	4.6347159	1.6666674 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.74, TOTAL = 6226.3 SECONDS (103.8 MIN)
WALL CLOCK TIME: STEP = 0.74, TOTAL = 5755.4 SECONDS (95.9 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.95, TOTAL = 6227.2 SECONDS (103.8 MIN)
WALL CLOCK TIME: STEP = 0.96, TOTAL = 5756.3 SECONDS (95.9 MIN)

CPU UTILIZATION: STEP = 99.30%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636231230	-284.636231230	0.004714490	0.000882301	197560668
11365048						
2	1	-284.636285791	-0.000054561	0.001076785	0.000069744	152415289
15228196						
3	2	-284.636286062	-0.000000271	0.000432344	0.000084195	135595462
16571774						
4	3	-284.636286497	-0.000000435	0.000317381	0.000031147	128954312
17028396						
5	4	-284.636286526	-0.000000028	0.000121630	0.000029539	122321927
17551810						
6	5	-284.636286595	-0.000000069	0.000121406	0.000018907	115437080
18026621						
7	6	-284.636286606	-0.000000011	0.000113905	0.000015301	114043454
18244887						
8	7	-284.636286593	0.000000013	0.000116366	0.000014259	111592491
18380217						
9	8	-284.636286613	-0.000000020	0.000299093	0.000014940	134839337
16714846						
10	9	-284.636286634	-0.000000021	0.000233559	0.000014586	161620358
14617388						
11	10	-284.636286648	-0.000000014	0.000165033	0.000016075	158621715
14860378						
12	11	-284.636286657	-0.000000009	0.000156888	0.000014217	157412732
14927535						
13	12	-284.636286666	-0.000000009	0.000084768	0.000007187	155337063
15071842						
14	13	-284.636286668	-0.000000002	0.000036195	0.000004860	152504189
15273517						
15	14	-284.636286670	-0.000000002	0.000018584	0.000002432	149759068
15420125						
16	15	-284.636286670	0.000000000	0.000013820	0.000001962	145288500
15767480						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 51.1 SECONDS (3.2 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 17.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.8, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.4 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6362866701 AFTER 16 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6014640402
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999372894

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 54.88 , TOTAL = 6282.1 SECONDS (104.7 MIN)
WALL CLOCK TIME: STEP = 50.78 , TOTAL = 5807.1 SECONDS (96.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 4.06 , TOTAL = 6286.1 SECONDS (104.8 MIN)
WALL CLOCK TIME: STEP = 4.04 , TOTAL = 5811.1 SECONDS (96.9 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.87 , TOTAL = 6289.0 SECONDS (104.8 MIN)
WALL CLOCK TIME: STEP = 2.68 , TOTAL = 5813.8 SECONDS (96.9 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 64 ENERGY= -284.6362867

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0008758	-0.0002724	-0.0007512
2 C	6.0	0.0002654	0.0005257	0.0002247
3 C	6.0	0.0000513	-0.0007846	0.0003596
4 C	6.0	-0.0002459	-0.0004326	0.0006390
5 C	6.0	0.0000535	-0.0001016	0.0001507

6 C	6.0	-0.0000809	-0.0001348	0.0000687
7 C	6.0	-0.0001770	0.0001197	-0.0001142
8 C	6.0	-0.0003695	0.0003252	-0.0005832
9 C	6.0	0.0001574	0.0000599	-0.0002972
10 C	6.0	-0.0002383	0.0001822	0.0001504
11 C	6.0	0.0002345	0.0003222	0.0002588
12 N	7.0	-0.0002878	-0.0005884	0.0003084
13 C	6.0	-0.0004871	-0.0001607	0.0000574
14 C	6.0	0.0002348	-0.0002243	0.0002103
15 C	6.0	0.0001330	0.0005847	0.0001081
16 C	6.0	-0.0003794	-0.0006907	0.0003513
17 C	6.0	0.0001095	-0.0002213	-0.0000025
18 C	6.0	-0.0000333	0.0004928	-0.0003234
19 C	6.0	-0.0007934	0.0000476	-0.0002421
20 O	8.0	-0.0002556	-0.0014331	-0.0004833
21 N	7.0	0.0007019	-0.0003337	0.0000933
22 H	1.0	0.0003158	-0.0004803	-0.0000588
23 H	1.0	-0.0005900	0.0002676	-0.0004419
24 H	1.0	0.0000307	-0.0002111	0.0003131
25 H	1.0	-0.0004316	0.0004895	-0.0006598
26 H	1.0	0.0000329	0.0000390	0.0004813
27 H	1.0	0.0003031	0.0000770	0.0007766
28 H	1.0	0.0001734	-0.0003966	-0.0007892
29 H	1.0	0.0002678	0.0001315	-0.0003151
30 H	1.0	0.0003728	0.0003014	-0.0003249
31 H	1.0	0.0001968	0.0002428	0.0008141
32 H	1.0	-0.0001928	0.0000433	0.0002519
33 H	1.0	-0.0001515	0.0016329	-0.0002025
34 H	1.0	-0.0003236	0.0000486	-0.0000407
35 H	1.0	0.0005268	0.0005328	0.0000123

MAXIMUM GRADIENT = 0.0016329 RMS GRADIENT = 0.0004251
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000430322
 PREDICTED ENERGY CHANGE WAS -0.0000545859 RATIO= 0.788
 GDIIS STEP HAS LENGTH = 0.401594
 RADIUS OF STEP TAKEN= 0.07416 CURRENT TRUST RADIUS= 0.07416

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 6289.0 SECONDS (104.8 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5813.8 SECONDS (96.9 MIN)
 CPU UTILIZATION: STEP = 91.60% , TOTAL = 100.00%

INSERCH= 65

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1515163810	-1.7621474779	0.8722405792
C	6.0	4.9836259034	0.6531884448	0.5232961881
C	6.0	5.1952318139	-0.7026869142	0.2371179256
C	6.0	4.0652956097	-1.5453916355	-0.0121427646
C	6.0	2.7543211755	-1.0370490466	0.0467424612
C	6.0	2.4723380620	0.3389476679	0.4366610328
C	6.0	3.6486058782	1.1951485865	0.6348130261
C	6.0	3.4885157783	2.5935511602	0.9607331384
C	6.0	2.2179839296	3.1464124173	1.1713473606
C	6.0	1.0620915161	2.3125355348	1.0588183949
C	6.0	1.1624714062	0.9580358235	0.6604465981
N	7.0	-0.0474947218	0.1497367102	0.6159295806
C	6.0	-1.2396627347	0.6829330270	0.3455338247
C	6.0	-2.5517959827	0.0396673839	0.4545564802
C	6.0	-2.8358477854	-1.3039667463	0.8760930813
C	6.0	-4.1408068936	-1.8202585873	0.9721028508
C	6.0	-5.2428632732	-0.9683072415	0.6564327115
C	6.0	-5.0177625289	0.3769165432	0.2489074167
C	6.0	-3.6939676024	0.8657010840	0.1423664381
O	8.0	-1.7232888118	-2.1943572677	1.2186841562
N	7.0	1.6626440972	-1.9875562360	-0.3806426202
H	1.0	5.8449949116	1.3276618372	0.6787974136
H	1.0	6.2154107926	-1.1173863007	0.1665872218
H	1.0	4.2379778203	-2.6028814102	-0.2937737398
H	1.0	4.3920541396	3.2206570012	1.0655886031
H	1.0	2.1031994565	4.2044297905	1.4666803773
H	1.0	0.0831961758	2.7392207208	1.3397085458
H	1.0	-1.2679582747	1.7313602030	-0.0116016533
H	1.0	-4.3201718508	-2.8671427375	1.2823293575
H	1.0	-6.2712341977	-1.3652878542	0.7285369662
H	1.0	-5.8700737668	1.0417692423	0.0245305037
H	1.0	-3.5209728627	1.9113505239	-0.1730231941
H	1.0	-2.0547853536	-3.0234936633	1.6480274381
H	1.0	1.3200991643	-1.7318441685	-1.3333729952
H	1.0	2.0731096290	-2.9383614148	-0.4661657051

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.000000	5.4133993	5.1927741	4.0183062

2 C	5.4133993	0.0000000	1.4018106 *	2.4420851 *
3 C	5.1927741	1.4018106 *	0.0000000	1.4314461 *
4 C	4.0183062	2.4420851 *	1.4314461 *	0.0000000
5 C	2.8252093 *	2.8379228 *	2.4710495 *	1.4073143 *
6 C	3.1607821	2.5323545 *	2.9221517 *	2.5079221 *
7 C	4.5860230	1.4451420 *	2.4803211 *	2.8465317 *
8 C	5.4877597	2.4883153 *	3.7817567	4.2906888
9 C	5.3342022	3.7795385	4.9550333	5.1794048
10 C	4.1793540	4.2916953	5.1816606	5.0049770
11 C	2.9096879 *	3.8357481	4.3818220	3.8917752
12 N	1.9392271 *	5.0570959	5.3250639	4.4925471
13 C	2.8620304 *	6.2258980	6.5832792	5.7650626
14 C	3.2754991	7.5606690	7.7855513	6.8202728
15 C	3.0222986	8.0684008	8.0788654	6.9622575
16 C	4.2938780	9.4643881	9.4313725	8.2694867
17 C	5.4567469	10.3550980	10.4498903	9.3499648
18 C	5.6289949	10.0089653	10.2699044	9.2879148
19 C	4.7144513	8.6885498	9.0269976	8.1267095
20 O	1.9549228 *	7.3194799	7.1452418	5.9534697
21 N	1.9758624 *	4.3381514	3.8094216	2.4706347 *
22 H	6.4807438	1.1050120 *	2.1770597 *	3.4495165
23 H	6.1387685	2.1862000 *	1.1035014 *	2.1995746 *
24 H	4.3319268	3.4388349	2.1929251 *	1.1078898 *
25 H	6.5458295	2.6899690 *	4.0895092	4.8972947
26 H	6.3057489	4.6688484	5.9289360	6.2527742
27 H	4.5260921	5.3881603	6.2606184	6.0035424
28 H	3.8730713	6.3663863	6.9108084	6.2594488
29 H	4.6244116	9.9764480	9.8142877	8.5871269
30 H	6.4366042	11.4362689	11.4961026	10.3645980
31 H	6.6962758	10.8721000	11.2039863	10.2667576
32 H	5.2985225	8.6253135	9.1089863	8.3382503
33 H	2.6571802 *	8.0201150	7.7420642	6.5112473
34 H	2.4962442 *	4.7494241	4.3060724	3.0522971
35 H	2.6205593 *	4.7275121	3.9039077	2.4729146 *

C C C C

1 CO	2.8252093 *	3.1607821	4.5860230	5.4877597
2 C	2.8379228 *	2.5323545 *	1.4451420 *	2.4883153 *
3 C	2.4710495 *	2.9221517 *	2.4803211 *	3.7817567
4 C	1.4073143 *	2.5079221 *	2.8465317 *	4.2906888
5 C	0.0000000	1.4577098 *	2.4755360 *	3.8151905
6 C	1.4577098 *	0.0000000	1.4683154 *	2.5279449 *
7 C	2.4755360 *	1.4683154 *	0.0000000	1.4447777 *
8 C	3.8151905	2.5279449 *	1.4447777 *	0.0000000
9 C	4.3650594	2.9131286 *	2.4783016 *	1.4015224 *

10	C	3.8868568	2.5041813 *	2.8492790 *	2.4446115 *
11	C	2.6250680 *	1.4659812 *	2.4975476 *	2.8592945 *
12	N	3.0955786	2.5332776 *	3.8411460	4.3121327
13	C	4.3588441	3.7290186	4.9235371	5.1365946
14	C	5.4295957	5.0330718	6.3097236	6.5775302
15	C	5.6576547	5.5739667	6.9535554	7.4293596
16	C	7.0008928	6.9772886	8.3595093	8.8141029
17	C	8.0206862	7.8282531	9.1509143	9.4348510
18	C	7.9022436	7.4925496	8.7134590	8.8191233
19	C	6.7238404	6.1957569	7.3664391	7.4325808
20	O	4.7709329	4.9631118	6.3786290	7.0819145
21	N	1.5092650 *	2.5954210 *	3.8864900	5.1107378
22	H	3.9425392	3.5229249	2.2008224 *	2.6897876 *
23	H	3.4640956	4.0254741	3.4864797	4.6730805
24	H	2.1838084 *	3.5079021	3.9540694	5.3979989
25	H	4.6742141	3.5192483	2.2002198 *	1.1048249 *
26	H	5.4693038	4.0173567	3.4836845	2.1840361 *
27	H	4.8027995	3.5049685	3.9488204	3.4294378
28	H	4.8832597	4.0161634	4.9877829	4.9308066
29	H	7.4110977	7.5585952	8.9678820	9.5340550
30	H	9.0572200	8.9128933	10.2453817	10.5346590
31	H	8.8714242	8.3821027	9.5394566	9.5324551
32	H	6.9369065	6.2260695	7.2504072	7.1332834
33	H	5.4440409	5.7678650	7.1660461	7.9216004
34	H	2.1081868 *	2.9578461 *	4.2264626	5.3548108
35	H	2.0837737 *	3.4227524	4.5585357	5.8857006

C C C N

1	CO	5.3342022	4.1793540	2.9096879 *	1.9392271 *
2	C	3.7795385	4.2916953	3.8357481	5.0570959
3	C	4.9550333	5.1816606	4.3818220	5.3250639
4	C	5.1794048	5.0049770	3.8917752	4.4925471
5	C	4.3650594	3.8868568	2.6250680 *	3.0955786
6	C	2.9131286 *	2.5041813 *	1.4659812 *	2.5332776 *
7	C	2.4783016 *	2.8492790 *	2.4975476 *	3.8411460
8	C	1.4015224 *	2.4446115 *	2.8592945 *	4.3121327
9	C	0.0000000	1.4297205 *	2.4827643 *	3.7974923
10	C	1.4297205 *	0.0000000	1.4154313 *	2.4708361 *
11	C	2.4827643 *	1.4154313 *	0.0000000	1.4557978 *
12	N	3.7974923	2.4708361 *	1.4557978 *	0.0000000
13	C	4.3250456	2.9090294 *	2.4382576 *	1.3336704 *
14	C	5.7372863	4.3117566	3.8316542	2.5119079 *
15	C	6.7404944	5.3203767	4.5988820	3.1552895
16	C	8.0710433	6.6451229	5.9950655	4.5566375
17	C	8.5358243	7.1188692	6.6887313	5.3144630

18	C	7.8023733	6.4317340	6.2211217	4.9889756
19	C	6.4196275	5.0550284	4.8848677	3.7461489
20	O	6.6377475	5.3005644	4.3100839	2.9438708 *
21	N	5.3920969	4.5742213	3.1639456	2.9130314 *
22	H	4.0872568	4.8980156	4.6971253	6.0094005
23	H	5.9303410	6.2543697	5.4848401	6.4055831
24	H	6.2674823	6.0064202	4.8009799	5.1739484
25	H	2.1779069 *	3.4515767	3.9640635	5.4168569
26	H	1.1044446 *	2.1976171 *	3.4747742	4.6679544
27	H	2.1797865 *	1.1041719 *	2.1906281 *	2.6919070 *
28	H	3.9437969	2.6292006 *	2.6375496 *	2.0940056 *
29	H	8.8838417	7.4731374	6.7140231	5.2727052
30	H	9.6238425	8.2105503	7.7886102	6.4064743
31	H	8.4357210	7.1231674	7.0617344	5.9201268
32	H	6.0223197	4.7626529	4.8516112	3.9737615
33	H	7.5200746	6.2076804	5.2133132	3.8940766
34	H	5.5567264	4.7059701	3.3519573	3.0348707
35	H	6.3029287	5.5605443	4.1569735	3.8992619

C C C C

1	CO	2.8620304 *	3.2754991	3.0222986	4.2938780
2	C	6.2258980	7.5606690	8.0684008	9.4643881
3	C	6.5832792	7.7855513	8.0788654	9.4313725
4	C	5.7650626	6.8202728	6.9622575	8.2694867
5	C	4.3588441	5.4295957	5.6576547	7.0008928
6	C	3.7290186	5.0330718	5.5739667	6.9772886
7	C	4.9235371	6.3097236	6.9535554	8.3595093
8	C	5.1365946	6.5775302	7.4293596	8.8141029
9	C	4.3250456	5.7372863	6.7404944	8.0710433
10	C	2.9090294 *	4.3117566	5.3203767	6.6451229
11	C	2.4382576 *	3.8316542	4.5988820	5.9950655
12	N	1.3336704 *	2.5119079 *	3.1552895	4.5566375
13	C	0.0000000	1.4653908 *	2.6032807 *	3.8826788
14	C	1.4653908 *	0.0000000	1.4365692 *	2.5004269 *
15	C	2.6032807 *	1.4365692 *	0.0000000	1.4066604 *
16	C	3.8826788	2.5004269 *	1.4066604 *	0.0000000
17	C	4.3415282	2.8807308 *	2.4402134 *	1.4282846 *
18	C	3.7917042	2.4974026 *	2.8247978 *	2.4737909 *
19	C	2.4694723 *	1.4437279 *	2.4458501 *	2.8464903 *
20	O	3.0455024	2.5022353 *	1.4655891 *	2.4586878 *
21	N	4.0102656	4.7506524	4.7204987	5.9613717
22	H	7.1217353	8.4979592	9.0731155	10.4743338
23	H	7.6714596	8.8479158	9.0809412	10.4112501
24	H	6.4194888	7.3242126	7.2866163	8.5099339
25	H	6.2189032	7.6621870	8.5294018	9.9110689

26 H	4.9832356	6.3276080	7.4219548	8.6907475
27 H	2.6394428 *	3.8748247	5.0083053	6.2262499
28 H	1.1079467 *	2.1742510 *	3.5298002	4.6727861
29 H	4.7927195	3.5017005	2.1935736 *	1.1065165 *
30 H	5.4459721	3.9853714	3.4391006	2.1920409 *
31 H	4.6553746	3.4928639	3.9286338	3.4755518
32 H	2.6424017 *	2.1991721 *	3.4508414	3.9522670
33 H	4.0122953	3.3248080	2.0402730 *	2.5012266 *
34 H	3.8990073	4.6180642	4.7261733	5.9282823
35 H	4.9746447	5.5772876	5.3451630	6.4754559

C C C O

1 CO	5.4567469	5.6289949	4.7144513	1.9549228 *
2 C	10.3550980	10.0089653	8.6885498	7.3194799
3 C	10.4498903	10.2699044	9.0269976	7.1452418
4 C	9.3499648	9.2879148	8.1267095	5.9534697
5 C	8.0206862	7.9022436	6.7238404	4.7709329
6 C	7.8282531	7.4925496	6.1957569	4.9631118
7 C	9.1509143	8.7134590	7.3664391	6.3786290
8 C	9.4348510	8.8191233	7.4325808	7.0819145
9 C	8.5358243	7.8023733	6.4196275	6.6377475
10 C	7.1188692	6.4317340	5.0550284	5.3005644
11 C	6.6887313	6.2211217	4.8848677	4.3100839
12 N	5.3144630	4.9889756	3.7461489	2.9438708 *
13 C	4.3415282	3.7917042	2.4694723 *	3.0455024
14 C	2.8807308 *	2.4974026 *	1.4437279 *	2.5022353 *
15 C	2.4402134 *	2.8247978 *	2.4458501 *	1.4655891 *
16 C	1.4282846 *	2.4737909 *	2.8464903 *	2.4586878 *
17 C	0.0000000	1.4235077 *	2.4549803 *	3.7691816
18 C	1.4235077 *	0.0000000	1.4151658 *	4.2901600
19 C	2.4549803 *	1.4151658 *	0.0000000	3.7955226
20 O	3.7691816	4.2901600	3.7955226	0.0000000
21 N	7.0569417	7.1144148	6.0916258	3.7503539
22 H	11.3230991	10.9127550	9.5651959	8.3651070
23 H	11.4697087	11.3324269	10.1058895	8.0802058
24 H	9.6675267	9.7387077	8.6681625	6.1636938
25 H	10.5141078	9.8639991	8.4724202	8.1696534
26 H	9.0209948	8.1756301	6.8196820	7.4597581
27 H	6.5252999	5.7262647	4.3829979	5.2553046
28 H	4.8512209	3.9954242	2.5804250 *	4.1391046
29 H	2.2019724 *	3.4754157	3.9529445	2.6833733 *
30 H	1.1046897 *	2.1992071 *	3.4587875	4.6488071
31 H	2.1984315 *	1.1039966 *	2.1863951 *	5.3939172
32 H	3.4562020	2.1846950 *	1.1057941 *	4.6931177
33 H	3.9205729	4.7222410	4.4810456	0.9908041 *

34 H	6.9003472	6.8643262	5.8366012	3.9986403
35 H	7.6592950	7.8602077	6.9354439	4.2195856

	N	H	H	H
--	---	---	---	---

1 CO	1.9758624 *	6.4807438	6.1387685	4.3319268
2 C	4.3381514	1.1050120 *	2.1862000 *	3.4388349
3 C	3.8094216	2.1770597 *	1.1035014 *	2.1929251 *
4 C	2.4706347 *	3.4495165	2.1995746 *	1.1078898 *
5 C	1.5092650 *	3.9425392	3.4640956	2.1838084 *
6 C	2.5954210 *	3.5229249	4.0254741	3.5079021
7 C	3.8864900	2.2008224 *	3.4864797	3.9540694
8 C	5.1107378	2.6897876 *	4.6730805	5.3979989
9 C	5.3920969	4.0872568	5.9303410	6.2674823
10 C	4.5742213	4.8980156	6.2543697	6.0064202
11 C	3.1639456	4.6971253	5.4848401	4.8009799
12 N	2.9130314 *	6.0094005	6.4055831	5.1739484
13 C	4.0102656	7.1217353	7.6714596	6.4194888
14 C	4.7506524	8.4979592	8.8479158	7.3242126
15 C	4.7204987	9.0731155	9.0809412	7.2866163
16 C	5.9613717	10.4743338	10.4112501	8.5099339
17 C	7.0569417	11.3230991	11.4697087	9.6675267
18 C	7.1144148	10.9127550	11.3324269	9.7387077
19 C	6.0916258	9.5651959	10.1058895	8.6681625
20 O	3.7503539	8.3651070	8.0802058	6.1636938
21 N	0.0000000	5.4410608	4.6673698	2.6492480 *
22 H	5.4410608	0.0000000	2.5254361 *	4.3563251
23 H	4.6673698	2.5254361 *	0.0000000	2.5157244 *
24 H	2.6492480 *	4.3563251	2.5157244 *	0.0000000
25 H	6.0553075	2.4174522 *	4.7907674	5.9820736
26 H	6.4766799	4.7851423	6.8499818	7.3481945
27 H	5.2722561	5.9688882	7.3385072	6.9619344
28 H	4.7492064	7.1577738	8.0092397	7.0128884
29 H	6.2716214	11.0132307	10.7380180	8.7060818
30 H	8.0351678	12.4119886	12.5017417	10.6311003
31 H	8.1291338	11.7368068	12.2776655	10.7497676
32 H	6.4895658	9.4227195	10.2022423	8.9774265
33 H	4.3598108	9.0707491	8.6153383	6.5989677
34 H	1.0442322 *	5.8210041	5.1566961	3.2176837
35 H	1.0391471 *	5.8083572	4.5689151	2.1974804 *

	H	H	H	H
--	---	---	---	---

1 CO	6.5458295	6.3057489	4.5260921	3.8730713
2 C	2.6899690 *	4.6688484	5.3881603	6.3663863
3 C	4.0895092	5.9289360	6.2606184	6.9108084

4 C	4.8972947	6.2527742	6.0035424	6.2594488
5 C	4.6742141	5.4693038	4.8027995	4.8832597
6 C	3.5192483	4.0173567	3.5049685	4.0161634
7 C	2.2002198 *	3.4836845	3.9488204	4.9877829
8 C	1.1048249 *	2.1840361 *	3.4294378	4.9308066
9 C	2.1779069 *	1.1044446 *	2.1797865 *	3.9437969
10 C	3.4515767	2.1976171 *	1.1041719 *	2.6292006 *
11 C	3.9640635	3.4747742	2.1906281 *	2.6375496 *
12 N	5.4168569	4.6679544	2.6919070 *	2.0940056 *
13 C	6.2189032	4.9832356	2.6394428 *	1.1079467 *
14 C	7.6621870	6.3276080	3.8748247	2.1742510 *
15 C	8.5294018	7.4219548	5.0083053	3.5298002
16 C	9.9110689	8.6907475	6.2262499	4.6727861
17 C	10.5141078	9.0209948	6.5252999	4.8512209
18 C	9.8639991	8.1756301	5.7262647	3.9954242
19 C	8.4724202	6.8196820	4.3829979	2.5804250 *
20 O	8.1696534	7.4597581	5.2553046	4.1391046
21 N	6.0553075	6.4766799	5.2722561	4.7492064
22 H	2.4174522 *	4.7851423	5.9688882	7.1577738
23 H	4.7907674	6.8499818	7.3385072	8.0092397
24 H	5.9820736	7.3481945	6.9619344	7.0128884
25 H	0.0000000	2.5233984 *	4.3443273	5.9509734
26 H	2.5233984 *	0.0000000	2.4986742 *	4.4346472
27 H	4.3443273	2.4986742 *	0.0000000	2.1604260 *
28 H	5.9509734	4.4346472	2.1604260 *	0.0000000
29 H	10.6306709	9.5551464	7.1291131	5.6689059
30 H	11.6125024	10.0845302	7.5894207	5.9304135
31 H	10.5424202	8.6980057	6.3287011	4.6536339
32 H	8.1156909	6.2911171	3.9954675	2.2659497 *
33 H	8.9939086	8.3405397	6.1542589	5.0972641
34 H	6.3023164	6.6100600	5.3540373	4.5209408
35 H	6.7570173	7.3997477	6.2813913	5.7598319

H H H H

1 CO	4.6244116	6.4366042	6.6962758	5.2985225
2 C	9.9764480	11.4362689	10.8721000	8.6253135
3 C	9.8142877	11.4961026	11.2039863	9.1089863
4 C	8.5871269	10.3645980	10.2667576	8.3382503
5 C	7.4110977	9.0572200	8.8714242	6.9369065
6 C	7.5585952	8.9128933	8.3821027	6.2260695
7 C	8.9678820	10.2453817	9.5394566	7.2504072
8 C	9.5340550	10.5346590	9.5324551	7.1332834
9 C	8.8838417	9.6238425	8.4357210	6.0223197
10 C	7.4731374	8.2105503	7.1231674	4.7626529
11 C	6.7140231	7.7886102	7.0617344	4.8516112

12 N	5.2727052	6.4064743	5.9201268	3.9737615
13 C	4.7927195	5.4459721	4.6553746	2.6424017 *
14 C	3.5017005	3.9853714	3.4928639	2.1991721 *
15 C	2.1935736 *	3.4391006	3.9286338	3.4508414
16 C	1.1065165 *	2.1920409 *	3.4755518	3.9522670
17 C	2.2019724 *	1.1046897 *	2.1984315 *	3.4562020
18 C	3.4754157	2.1992071 *	1.1039966 *	2.1846950 *
19 C	3.9529445	3.4587875	2.1863951 *	1.1057941 *
20 O	2.6833733 *	4.6488071	5.3939172	4.6931177
21 N	6.2716214	8.0351678	8.1291338	6.4895658
22 H	11.0132307	12.4119886	11.7368068	9.4227195
23 H	10.7380180	12.5017417	12.2776655	10.2022423
24 H	8.7060818	10.6311003	10.7497676	8.9774265
25 H	10.6306709	11.6125024	10.5424202	8.1156909
26 H	9.5551464	10.0845302	8.6980057	6.2911171
27 H	7.1291131	7.5894207	6.3287011	3.9954675
28 H	5.6689059	5.9304135	4.6536339	2.2659497 *
29 H	0.0000000	2.5236676 *	4.3890599	5.0587318
30 H	2.5236676 *	0.0000000	2.5397793 *	4.3718540
31 H	4.3890599	2.5397793 *	0.0000000	2.5126628 *
32 H	5.0587318	4.3718540	2.5126628 *	0.0000000
33 H	2.3000341 *	4.6231537	5.8067659	5.4606427
34 H	6.3200838	7.8749082	7.8253064	6.1688944
35 H	6.6284504	8.5749606	8.8981113	7.4094128

H H H

1 CO	2.6571802 *	2.4962442 *	2.6205593 *
2 C	8.0201150	4.7494241	4.7275121
3 C	7.7420642	4.3060724	3.9039077
4 C	6.5112473	3.0522971	2.4729146 *
5 C	5.4440409	2.1081868 *	2.0837737 *
6 C	5.7678650	2.9578461 *	3.4227524
7 C	7.1660461	4.2264626	4.5585357
8 C	7.9216004	5.3548108	5.8857006
9 C	7.5200746	5.5567264	6.3029287
10 C	6.2076804	4.7059701	5.5605443
11 C	5.2133132	3.3519573	4.1569735
12 N	3.8940766	3.0348707	3.8992619
13 C	4.0122953	3.8990073	4.9746447
14 C	3.3248080	4.6180642	5.5772876
15 C	2.0402730 *	4.7261733	5.3451630
16 C	2.5012266 *	5.9282823	6.4754559
17 C	3.9205729	6.9003472	7.6592950
18 C	4.7222410	6.8643262	7.8602077
19 C	4.4810456	5.8366012	6.9354439

20	O	0.9908041 *	3.9986403	4.2195856
21	N	4.3598108	1.0442322 *	1.0391471 *
22	H	9.0707491	5.8210041	5.8083572
23	H	8.6153383	5.1566961	4.5689151
24	H	6.5989677	3.2176837	2.1974804 *
25	H	8.9939086	6.3023164	6.7570173
26	H	8.3405397	6.6100600	7.3997477
27	H	6.1542589	5.3540373	6.2813913
28	H	5.0972641	4.5209408	5.7598319
29	H	2.3000341 *	6.3200838	6.6284504
30	H	4.6231537	7.8749082	8.5749606
31	H	5.8067659	7.8253064	8.8981113
32	H	5.4606427	6.1688944	7.4094128
33	H	0.0000000	4.6847575	4.6385965
34	H	4.6847575	0.0000000	1.6657602 *
35	H	4.6385965	1.6657602 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.75 , TOTAL = 6289.8 SECONDS (104.8 MIN)

WALL CLOCK TIME: STEP = 0.75 , TOTAL = 5814.6 SECONDS (96.9 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.83 , TOTAL = 6290.6 SECONDS (104.8 MIN)

WALL CLOCK TIME: STEP = 0.83 , TOTAL = 5815.4 SECONDS (96.9 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636233600	-284.636233600	0.005314034	0.001200279	197589801
11363477						
2	1	-284.636342041	-0.000108440	0.001604688	0.000097297	155419750
14991291						
3	2	-284.636342933	-0.000000893	0.000686097	0.000083362	138192033
16403463						

4 3	-284.636343272	-0.000000339	0.000470555	0.000040104	131584539
16834778					
5 4	-284.636343425	-0.000000153	0.000186353	0.000028910	126244692
17267010					
6 5	-284.636343484	-0.000000060	0.000122444	0.000024976	120009872
17671736					
7 6	-284.636343506	-0.000000022	0.000197104	0.000022989	115290066
18123892					
8 7	-284.636343529	-0.000000022	0.000204520	0.000022950	140757438
16165465					
9 8	-284.636343575	-0.000000046	0.000430660	0.000023209	157164697
14985444					
-----DISABLING FDIFF OPTION-----					
10 9	-284.636343602	-0.000000027	0.000290194	0.000022185	197584505
11363835					
11 10	-284.636343635	-0.000000033	0.000252204	0.000024706	197584533
11363837					
12 11	-284.636343653	-0.000000019	0.000169621	0.000017467	197584512
11363830					
13 12	-284.636343674	-0.000000020	0.000169078	0.000007796	197584517
11363839					
14 13	-284.636343678	-0.000000004	0.000100171	0.000007058	197584462
11363833					
15 14	-284.636343683	-0.000000005	0.000026917	0.000003474	197584406
11363841					
16 15	-284.636343683	-0.000000001	0.000023558	0.000003593	197584382
11363841					
17 16	-284.636343684	-0.000000001	0.000041659	0.000003483	197584388
11363839					
18 17	-284.636343685	-0.000000001	0.000081524	0.000002498	197584520
11363838					
19 18	-284.636343686	-0.000000001	0.000073957	0.000003691	197584541
11363836					
20 19	-284.636343686	-0.000000001	0.000040433	0.000005164	197584502
11363834					
21 20	-284.636343687	-0.000000001	0.000048751	0.000004531	197584510
11363834					
22 21	-284.636343688	-0.000000001	0.000039683	0.000002260	197584497
11363838					
23 22	-284.636343688	0.000000000	0.000031067	0.000001193	197584446
11363838					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 76.8 SECONDS (3.3 SEC/ITER)

OF THE ABOVE TIME, DFT PART= 25.0 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 3.0 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6363436880 AFTER 23 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6008694795
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999313541

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 81.03 , TOTAL = 6371.6 SECONDS (106.2 MIN)
WALL CLOCK TIME: STEP = 74.18 , TOTAL = 5889.6 SECONDS (98.2
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.79 , TOTAL = 6375.4 SECONDS (106.3 MIN)
WALL CLOCK TIME: STEP = 3.76 , TOTAL = 5893.4 SECONDS (98.2
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.86 , TOTAL = 6378.3 SECONDS (106.3 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 5896.1 SECONDS (98.3
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 65 ENERGY= -284.6363437

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0006948	-0.0002393	-0.0005955
2 C	6.0	0.0002936	0.0002899	0.0002223
3 C	6.0	0.0000560	-0.0005698	0.0003525
4 C	6.0	-0.0002148	-0.0003878	0.0005630
5 C	6.0	-0.0000635	-0.0000554	0.0001254
6 C	6.0	-0.0000756	-0.0001483	0.0000610
7 C	6.0	-0.0001639	0.0000562	-0.0000587
8 C	6.0	-0.0002295	0.0003077	-0.0005323
9 C	6.0	0.0000579	0.0000676	-0.0002272
10 C	6.0	-0.0002567	0.0001894	0.0002209
11 C	6.0	0.0001799	0.0003116	0.0002240
12 N	7.0	-0.0002619	-0.0005972	0.0002354
13 C	6.0	-0.0004484	-0.0000745	0.0000253
14 C	6.0	0.0001589	-0.0000666	0.0001663
15 C	6.0	0.0000464	0.0004722	0.0002013
16 C	6.0	-0.0003109	-0.0004434	0.0003367
17 C	6.0	0.0000838	-0.0001217	-0.0000218
18 C	6.0	-0.0000595	0.0003173	-0.0003033
19 C	6.0	-0.0006390	0.0000660	-0.0002343
20 O	8.0	-0.0002037	-0.0010629	-0.0005806
21 N	7.0	0.0005293	-0.0003390	-0.0000500
22 H	1.0	0.0003579	-0.0005004	-0.0001143
23 H	1.0	-0.0004379	0.0002221	-0.0004475
24 H	1.0	0.0001114	-0.0001034	0.0004307
25 H	1.0	-0.0004927	0.0005186	-0.0006307
26 H	1.0	0.0000127	-0.0000156	0.0004007
27 H	1.0	0.0002695	0.0001106	0.0007394
28 H	1.0	0.0002850	-0.0004056	-0.0008035
29 H	1.0	0.0002859	0.0000768	-0.0002878
30 H	1.0	0.0002974	0.0001965	-0.0003549
31 H	1.0	0.0001441	0.0002792	0.0007946
32 H	1.0	-0.0002185	0.0000366	0.0002799
33 H	1.0	-0.0001115	0.0011597	-0.0000296
34 H	1.0	-0.0001482	-0.0000664	-0.0000068
35 H	1.0	0.0004716	0.0005194	-0.0001007

MAXIMUM GRADIENT = 0.0011597 RMS GRADIENT = 0.0003625

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0000570179

PREDICTED ENERGY CHANGE WAS -0.0000644853 RATIO= 0.884

GDIIS STEP HAS LENGTH = 0.405497

RADIUS OF STEP TAKEN= 0.10488 CURRENT TRUST RADIUS= 0.10488

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 6378.3 SECONDS (106.3 MIN)

WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5896.1 SECONDS (98.3 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 66

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1513647723	-1.7599015770	0.8679315572
C	6.0	4.9836327665	0.6508752291	0.5268670113
C	6.0	5.1948543761	-0.7034871373	0.2345485306
C	6.0	4.0643739284	-1.5446701183	-0.0181637062
C	6.0	2.7532788244	-1.0363915289	0.0410395734
C	6.0	2.4719796131	0.3387017304	0.4349766331
C	6.0	3.6487411565	1.1929634000	0.6395841346
C	6.0	3.4889346969	2.5901061582	0.9715311906
C	6.0	2.2179438979	3.1439770891	1.1780389016
C	6.0	1.0614496930	2.3122333157	1.0580381730
C	6.0	1.1619968882	0.9585341442	0.6566968356
N	7.0	-0.0479431616	0.1514563100	0.6097584999
C	6.0	-1.2399131160	0.6848055317	0.3391938734
C	6.0	-2.5519145198	0.0411613420	0.4524644475
C	6.0	-2.8344081030	-1.3001647173	0.8831822981
C	6.0	-4.1386246828	-1.8170249692	0.9824259382
C	6.0	-5.2421643433	-0.9697960606	0.6592870011
C	6.0	-5.0185930059	0.3728709071	0.2431972801
C	6.0	-3.6952750850	0.8633716454	0.1351677084
O	8.0	-1.7205760227	-2.1876017423	1.2303536968
N	7.0	1.6605020361	-1.9852513837	-0.3888116856
H	1.0	5.8452783625	1.3243381798	0.6852437283
H	1.0	6.2150570134	-1.1187448446	0.1631680354
H	1.0	4.2376881460	-2.6016351734	-0.3007798384
H	1.0	4.3923986591	3.2160396204	1.0830389930
H	1.0	2.1030602610	4.2015638414	1.4744363038
H	1.0	0.0816225982	2.7395951588	1.3347605316
H	1.0	-1.2675243424	1.7323619546	-0.0205626326
H	1.0	-4.3162634606	-2.8620079278	1.3002181394
H	1.0	-6.2698363657	-1.3693228814	0.7316843384
H	1.0	-5.8718253654	1.0346788194	0.0125499241
H	1.0	-3.5241006494	1.9074446696	-0.1865369517
H	1.0	-2.0486740360	-3.0152595369	1.6665475708

H 1.0 1.3199408213 -1.7280174913 -1.3417079269
H 1.0 2.0695347487 -2.9366969569 -0.4764811078

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4110058	5.1917216	4.0178514
2 C	5.4110058	0.0000000	1.4015570 *	2.4418261 *
3 C	5.1917216	1.4015570 *	0.0000000	1.4315859 *
4 C	4.0178514	2.4418261 *	1.4315859 *	0.0000000
5 C	2.8243891 *	2.8385518 *	2.4717529 *	1.4074170 *
6 C	3.1586135	2.5326464 *	2.9223922 *	2.5076175 *
7 C	4.5829244	1.4451645 *	2.4801299 *	2.8460534 *
8 C	5.4838557	2.4884664 *	3.7816745	4.2903381
9 C	5.3305667	3.7800287	4.9553154	5.1791522
10 C	4.1769220	4.2925253	5.1824453	5.0051442
11 C	2.9079013 *	3.8361974	4.3822897	3.8916913
12 N	1.9389858 *	5.0569800	5.3252828	4.4924696
13 C	2.8621339 *	6.2264674	6.5836570	5.7648701
14 C	3.2747763	7.5605396	7.7855261	6.8199432
15 C	3.0209982	8.0656854	8.0774876	6.9617096
16 C	4.2918972	9.4611652	9.4293753	8.2682854
17 C	5.4550853	10.3542763	10.4490518	9.3488542
18 C	5.6273861	10.0101087	10.2700111	9.2868488
19 C	4.7132943	8.6903409	9.0276976	8.1261509
20 O	1.9540828 *	7.3142505	7.1426467	5.9529659
21 N	1.9767856 *	4.3394503	3.8109243	2.4718600 *
22 H	6.4781604	1.1050198 *	2.1767529 *	3.4492914
23 H	6.1380890	2.1863755 *	1.1037878 *	2.1999389 *
24 H	4.3327174	3.4380600	2.1921929 *	1.1077386 *
25 H	6.5416076	2.6905303 *	4.0898119	4.8974080
26 H	6.3020658	4.6693656	5.9292527	6.2525044
27 H	4.5241866	5.3893549	6.2618225	6.0039688
28 H	3.8727991	6.3675944	6.9109175	6.2584410
29 H	4.6218191	9.9712833	9.8110257	8.5853709
30 H	6.4345116	11.4351965	11.4947647	10.3628626
31 H	6.6947873	10.8744103	11.2045484	10.2655755
32 H	5.2981486	8.6295678	9.1112268	8.3384886
33 H	2.6559145 *	8.0120381	7.7371582	6.5092427
34 H	2.4998186 *	4.7511411	4.3068784	3.0524250
35 H	2.6213868 *	4.7296246	3.9064577	2.4753135 *

C C C C

1 CO	2.8243891 *	3.1586135	4.5829244	5.4838557
2 C	2.8385518 *	2.5326464 *	1.4451645 *	2.4884664 *
3 C	2.4717529 *	2.9223922 *	2.4801299 *	3.7816745
4 C	1.4074170 *	2.5076175 *	2.8460534 *	4.2903381
5 C	0.0000000	1.4578056 *	2.4759103 *	3.8155589
6 C	1.4578056 *	0.0000000	1.4684669 *	2.5280250 *
7 C	2.4759103 *	1.4684669 *	0.0000000	1.4448996 *
8 C	3.8155589	2.5280250 *	1.4448996 *	0.0000000
9 C	4.3651842	2.9131161 *	2.4786223 *	1.4017261 *
10 C	3.8871404	2.5045214 *	2.8499028 *	2.4448681 *
11 C	2.6250601 *	1.4660855 *	2.4978285 *	2.8593334 *
12 N	3.0953624	2.5329075 *	3.8407163	4.3113104
13 C	4.3585545	3.7292238	4.9241648	5.1373167
14 C	5.4291313	5.0327277	6.3095002	6.5771125
15 C	5.6569449	5.5717611	6.9502699	7.4247341
16 C	6.9995665	6.9747364	8.3558744	8.8092330
17 C	8.0195870	7.8275474	9.1501977	9.4341131
18 C	7.9011949	7.4931052	8.7150649	8.8218269
19 C	6.7232290	6.1967890	7.3686933	7.4359926
20 O	4.7702338	4.9590681	6.3723462	7.0733644
21 N	1.5097246 *	2.5957429 *	3.8873824	5.1115160
22 H	3.9431593	3.5232453	2.2009361 *	2.6900715 *
23 H	3.4649106	4.0259979	3.4866810	4.6734109
24 H	2.1841015 *	3.5077978	3.9534948	5.3975536
25 H	4.6750024	3.5195266	2.2005718 *	1.1047506 *
26 H	5.4693315	4.0172480	3.4839323	2.1841148 *
27 H	4.8030757	3.5053826	3.9496424	3.4298773
28 H	4.8822791	4.0166771	4.9896303	4.9339515
29 H	7.4092398	7.5546958	8.9621721	9.5265262
30 H	9.0556304	8.9120553	10.2446070	10.5341453
31 H	8.8703194	8.3834307	9.5425056	9.5374435
32 H	6.9371072	6.2289816	7.2555234	7.1407152
33 H	5.4421454	5.7621292	7.1571177	7.9100116
34 H	2.1082682 *	2.9589068 *	4.2285883	5.3574062
35 H	2.0848248 *	3.4235878	4.5599988	5.8870186

C C C N

1 CO	5.3305667	4.1769220	2.9079013 *	1.9389858 *
2 C	3.7800287	4.2925253	3.8361974	5.0569800
3 C	4.9553154	5.1824453	4.3822897	5.3252828
4 C	5.1791522	5.0051442	3.8916913	4.4924696
5 C	4.3651842	3.8871404	2.6250601 *	3.0953624
6 C	2.9131161 *	2.5045214 *	1.4660855 *	2.5329075 *
7 C	2.4786223 *	2.8499028 *	2.4978285 *	3.8407163
8 C	1.4017261 *	2.4448681 *	2.8593334 *	4.3113104

9 C	0.0000000	1.4295722 *	2.4825355 *	3.7963624
10 C	1.4295722 *	0.0000000	1.4155162 *	2.4699523 *
11 C	2.4825355 *	1.4155162 *	0.0000000	1.4551745 *
12 N	3.7963624	2.4699523 *	1.4551745 *	0.0000000
13 C	4.3252700	2.9088708 *	2.4382180 *	1.3335888 *
14 C	5.7363292	4.3105555	3.8309818	2.5113301 *
15 C	6.7352504	5.3157974	4.5961146	3.1537836
16 C	8.0657157	6.6405771	5.9921963	4.5549396
17 C	8.5349545	7.1180243	6.6881795	5.3140939
18 C	7.8051537	6.4336624	6.2220314	4.9890632
19 C	6.4229978	5.0574026	4.8861170	3.7463436
20 O	6.6287562	5.2931914	4.3054012	2.9417736 *
21 N	5.3921004	4.5739057	3.1634583	2.9122924 *
22 H	4.0879687	4.8989723	4.6976327	6.0092770
23 H	5.9310770	6.2555633	5.4856244	6.4060928
24 H	6.2672428	6.0067446	4.8011919	5.1744786
25 H	2.1777216 *	3.4514797	3.9640376	5.4159303
26 H	1.1043276 *	2.1972505 *	3.4744121	4.6666749
27 H	2.1798980 *	1.1042077 *	2.1906979 *	2.6908879 *
28 H	3.9468711	2.6313021 *	2.6381932 *	2.0937874 *
29 H	8.8759591	7.4666741	6.7098434	5.2703187
30 H	9.6234881	8.2102447	7.7882403	6.4062150
31 H	8.4410823	7.1270958	7.0636661	5.9206709
32 H	6.0301041	4.7686574	4.8549958	3.9750789
33 H	7.5085861	6.1988171	5.2076139	3.8920196
34 H	5.5580451	4.7062964	3.3520333	3.0350864
35 H	6.3034957	5.5607782	4.1569872	3.8987587

C C C C

1 CO	2.8621339 *	3.2747763	3.0209982	4.2918972
2 C	6.2264674	7.5605396	8.0656854	9.4611652
3 C	6.5836570	7.7855261	8.0774876	9.4293753
4 C	5.7648701	6.8199432	6.9617096	8.2682854
5 C	4.3585545	5.4291313	5.6569449	6.9995665
6 C	3.7292238	5.0327277	5.5717611	6.9747364
7 C	4.9241648	6.3095002	6.9502699	8.3558744
8 C	5.1373167	6.5771125	7.4247341	8.8092330
9 C	4.3252700	5.7363292	6.7352504	8.0657157
10 C	2.9088708 *	4.3105555	5.3157974	6.6405771
11 C	2.4382180 *	3.8309818	4.5961146	5.9921963
12 N	1.3335888 *	2.5113301 *	3.1537836	4.5549396
13 C	0.0000000	1.4657612 *	2.6035446 *	3.8827094
14 C	1.4657612 *	0.0000000	1.4368285 *	2.5002729 *
15 C	2.6035446 *	1.4368285 *	0.0000000	1.4064049 *
16 C	3.8827094	2.5002729 *	1.4064049 *	0.0000000

17 C	4.3426007	2.8813633 *	2.4406070 *	1.4282911 *
18 C	3.7927484	2.4976643 *	2.8247642 *	2.4731452 *
19 C	2.4702864 *	1.4435998 *	2.4457120 *	2.8458622 *
20 O	3.0456405	2.5027226 *	1.4658425 *	2.4588116 *
21 N	4.0089405	4.7495839	4.7213906	5.9614146
22 H	7.1224077	8.4978572	9.0699588	10.4706638
23 H	7.6720505	8.8480995	9.0798762	10.4094910
24 H	6.4198422	7.3246471	7.2876702	8.5102789
25 H	6.2195971	7.6616553	8.5242466	9.9055652
26 H	4.9831552	6.3263074	7.4160092	8.6847059
27 H	2.6381376 *	3.8724035	5.0026811	6.2207245
28 H	1.1079538 *	2.1756774 *	3.5310193	4.6741150
29 H	4.7924299	3.5014290	2.1929816 *	1.1065879 *
30 H	5.4473498	3.9862730	3.4394624	2.1921158 *
31 H	4.6565780	3.4931948	3.9287910	3.4751775
32 H	2.6436248 *	2.1992003 *	3.4509032	3.9516817
33 H	4.0132834	3.3270043	2.0426917 *	2.5043327 *
34 H	3.8987175	4.6195576	4.7319985	5.9334187
35 H	4.9732335	5.5756949	5.3456130	6.4748219

C C C O

1 CO	5.4550853	5.6273861	4.7132943	1.9540828 *
2 C	10.3542763	10.0101087	8.6903409	7.3142505
3 C	10.4490518	10.2700111	9.0276976	7.1426467
4 C	9.3488542	9.2868488	8.1261509	5.9529659
5 C	8.0195870	7.9011949	6.7232290	4.7702338
6 C	7.8275474	7.4931052	6.1967890	4.9590681
7 C	9.1501977	8.7150649	7.3686933	6.3723462
8 C	9.4341131	8.8218269	7.4359926	7.0733644
9 C	8.5349545	7.8051537	6.4229978	6.6287562
10 C	7.1180243	6.4336624	5.0574026	5.2931914
11 C	6.6881795	6.2220314	4.8861170	4.3054012
12 N	5.3140939	4.9890632	3.7463436	2.9417736 *
13 C	4.3426007	3.7927484	2.4702864 *	3.0456405
14 C	2.8813633 *	2.4976643 *	1.4435998 *	2.5027226 *
15 C	2.4406070 *	2.8247642 *	2.4457120 *	1.4658425 *
16 C	1.4282911 *	2.4731452 *	2.8458622 *	2.4588116 *
17 C	0.0000000	1.4233304 *	2.4552131 *	3.7697151
18 C	1.4233304 *	0.0000000	1.4154263 *	4.2903862
19 C	2.4552131 *	1.4154263 *	0.0000000	3.7956959
20 O	3.7697151	4.2903862	3.7956959	0.0000000
21 N	7.0552437	7.1112929	6.0888058	3.7542417
22 H	11.3223280	10.9144123	9.5675093	8.3590083
23 H	11.4689250	11.3325291	10.1066440	8.0780946
24 H	9.6670694	9.7376762	8.6676541	6.1657688

25 H	10.5131152	9.8668995	8.4760824	8.1602390
26 H	9.0199643	8.1788009	6.8233321	7.4499133
27 H	6.5236918	5.7275731	4.3845403	5.2474842
28 H	4.8540310	3.9985374	2.5832866 *	4.1395849
29 H	2.2019425 *	3.4749102	3.9523945	2.6827780 *
30 H	1.1049764 *	2.1998793 *	3.4596420	4.6490882
31 H	2.1983315 *	1.1041709 *	2.1867218 *	5.3943497
32 H	3.4562516	2.1847415 *	1.1058404 *	4.6935792
33 H	3.9238852	4.7250156	4.4833246	0.9914287 *
34 H	6.9021812	6.8631383	5.8351392	4.0089227
35 H	7.6563446	7.8557451	6.9316425	4.2236676

N H H H

1 CO	1.9767856 *	6.4781604	6.1380890	4.3327174
2 C	4.3394503	1.1050198 *	2.1863755 *	3.4380600
3 C	3.8109243	2.1767529 *	1.1037878 *	2.1921929 *
4 C	2.4718600 *	3.4492914	2.1999389 *	1.1077386 *
5 C	1.5097246 *	3.9431593	3.4649106	2.1841015 *
6 C	2.5957429 *	3.5232453	4.0259979	3.5077978
7 C	3.8873824	2.2009361 *	3.4866810	3.9534948
8 C	5.1115160	2.6900715 *	4.6734109	5.3975536
9 C	5.3921004	4.0879687	5.9310770	6.2672428
10 C	4.5739057	4.8989723	6.2555633	6.0067446
11 C	3.1634583	4.6976327	5.4856244	4.8011919
12 N	2.9122924 *	6.0092770	6.4060928	5.1744786
13 C	4.0089405	7.1224077	7.6720505	6.4198422
14 C	4.7495839	8.4978572	8.8480995	7.3246471
15 C	4.7213906	9.0699588	9.0798762	7.2876702
16 C	5.9614146	10.4706638	10.4094910	8.5102789
17 C	7.0552437	11.3223280	11.4689250	9.6670694
18 C	7.1112929	10.9144123	11.3325291	9.7376762
19 C	6.0888058	9.5675093	10.1066440	8.6676541
20 O	3.7542417	8.3590083	8.0780946	6.1657688
21 N	0.0000000	5.4423645	4.6689920	2.6513330 *
22 H	5.4423645	0.0000000	2.5254611 *	4.3554398
23 H	4.6689920	2.5254611 *	0.0000000	2.5147960 *
24 H	2.6513330 *	4.3554398	2.5147960 *	0.0000000
25 H	6.0566519	2.4181883 *	4.7915136	5.9819921
26 H	6.4764368	4.7859637	6.8508121	7.3478939
27 H	5.2714074	5.9703059	7.3401931	6.9625150
28 H	4.7465350	7.1593721	8.0094688	7.0120908
29 H	6.2724198	11.0072985	10.7350156	8.7063814
30 H	8.0327546	12.4110423	12.5003425	10.6298000
31 H	8.1250862	11.7399719	12.2781369	10.7481728
32 H	6.4864553	9.4278989	10.2044749	8.9772055

33 H	4.3638751	9.0614320	8.6108170	6.5999857
34 H	1.0441085 *	5.8227217	5.1573275	3.2186936
35 H	1.0393471 *	5.8105305	4.5715923	2.2009149 *

	H	H	H	H
--	---	---	---	---

1 CO	6.5416076	6.3020658	4.5241866	3.8727991
2 C	2.6905303 *	4.6693656	5.3893549	6.3675944
3 C	4.0898119	5.9292527	6.2618225	6.9109175
4 C	4.8974080	6.2525044	6.0039688	6.2584410
5 C	4.6750024	5.4693315	4.8030757	4.8822791
6 C	3.5195266	4.0172480	3.5053826	4.0166771
7 C	2.2005718 *	3.4839323	3.9496424	4.9896303
8 C	1.1047506 *	2.1841148 *	3.4298773	4.9339515
9 C	2.1777216 *	1.1043276 *	2.1798980 *	3.9468711
10 C	3.4514797	2.1972505 *	1.1042077 *	2.6313021 *
11 C	3.9640376	3.4744121	2.1906979 *	2.6381932 *
12 N	5.4159303	4.6666749	2.6908879 *	2.0937874 *
13 C	6.2195971	4.9831552	2.6381376 *	1.1079538 *
14 C	7.6616553	6.3263074	3.8724035	2.1756774 *
15 C	8.5242466	7.4160092	5.0026811	3.5310193
16 C	9.9055652	8.6847059	6.2207245	4.6741150
17 C	10.5131152	9.0199643	6.5236918	4.8540310
18 C	9.8668995	8.1788009	5.7275731	3.9985374
19 C	8.4760824	6.8233321	4.3845403	2.5832866 *
20 O	8.1602390	7.4499133	5.2474842	4.1395849
21 N	6.0566519	6.4764368	5.2714074	4.7465350
22 H	2.4181883 *	4.7859637	5.9703059	7.1593721
23 H	4.7915136	6.8508121	7.3401931	8.0094688
24 H	5.9819921	7.3478939	6.9625150	7.0120908
25 H	0.0000000	2.5229982 *	4.3443243	5.9543232
26 H	2.5229982 *	0.0000000	2.4986140 *	4.4376593
27 H	4.3443243	2.4986140 *	0.0000000	2.1613924 *
28 H	5.9543232	4.4376593	2.1613924 *	0.0000000
29 H	10.6221761	9.5463142	7.1218363	5.6698771
30 H	11.6117292	10.0842381	7.5886718	5.9337551
31 H	10.5479181	8.7043135	6.3323395	4.6569782
32 H	8.1237433	6.2997424	4.0010074	2.2694356 *
33 H	8.9809236	8.3280456	6.1454535	5.0986710
34 H	6.3057986	6.6108910	5.3531746	4.5182548
35 H	6.7589916	7.4001331	6.2811371	5.7570770

	H	H	H	H
--	---	---	---	---

1 CO	4.6218191	6.4345116	6.6947873	5.2981486
2 C	9.9712833	11.4351965	10.8744103	8.6295678

3 C	9.8110257	11.4947647	11.2045484	9.1112268
4 C	8.5853709	10.3628626	10.2655755	8.3384886
5 C	7.4092398	9.0556304	8.8703194	6.9371072
6 C	7.5546958	8.9120553	8.3834307	6.2289816
7 C	8.9621721	10.2446070	9.5425056	7.2555234
8 C	9.5265262	10.5341453	9.5374435	7.1407152
9 C	8.8759591	9.6234881	8.4410823	6.0301041
10 C	7.4666741	8.2102447	7.1270958	4.7686574
11 C	6.7098434	7.7882403	7.0636661	4.8549958
12 N	5.2703187	6.4062150	5.9206709	3.9750789
13 C	4.7924299	5.4473498	4.6565780	2.6436248 *
14 C	3.5014290	3.9862730	3.4931948	2.1992003 *
15 C	2.1929816 *	3.4394624	3.9287910	3.4509032
16 C	1.1065879 *	2.1921158 *	3.4751775	3.9516817
17 C	2.2019425 *	1.1049764 *	2.1983315 *	3.4562516
18 C	3.4749102	2.1998793 *	1.1041709 *	2.1847415 *
19 C	3.9523945	3.4596420	2.1867218 *	1.1058404 *
20 O	2.6827780 *	4.6490882	5.3943497	4.6935792
21 N	6.2724198	8.0327546	8.1250862	6.4864553
22 H	11.0072985	12.4110423	11.7399719	9.4278989
23 H	10.7350156	12.5003425	12.2781369	10.2044749
24 H	8.7063814	10.6298000	10.7481728	8.9772055
25 H	10.6221761	11.6117292	10.5479181	8.1237433
26 H	9.5463142	10.0842381	8.7043135	6.2997424
27 H	7.1218363	7.5886718	6.3323395	4.0010074
28 H	5.6698771	5.9337551	4.6569782	2.2694356 *
29 H	0.0000000	2.5234473 *	4.3888529	5.0582251
30 H	2.5234473 *	0.0000000	2.5406281 *	4.3725737
31 H	4.3888529	2.5406281 *	0.0000000	2.5126017 *
32 H	5.0582251	4.3725737	2.5126017 *	0.0000000
33 H	2.3020958 *	4.6261526	5.8098361	5.4629500
34 H	6.3271247	7.8760609	7.8222763	6.1656908
35 H	6.6287750	8.5709647	8.8924787	7.4053044

H H H

1 CO	2.6559145 *	2.4998186 *	2.6213868 *
2 C	8.0120381	4.7511411	4.7296246
3 C	7.7371582	4.3068784	3.9064577
4 C	6.5092427	3.0524250	2.4753135 *
5 C	5.4421454	2.1082682 *	2.0848248 *
6 C	5.7621292	2.9589068 *	3.4235878
7 C	7.1571177	4.2285883	4.5599988
8 C	7.9100116	5.3574062	5.8870186
9 C	7.5085861	5.5580451	6.3034957
10 C	6.1988171	4.7062964	5.5607782

11	C	5.2076139	3.3520333	4.1569872
12	N	3.8920196	3.0350864	3.8987587
13	C	4.0132834	3.8987175	4.9732335
14	C	3.3270043	4.6195576	5.5756949
15	C	2.0426917 *	4.7319985	5.3456130
16	C	2.5043327 *	5.9334187	6.4748219
17	C	3.9238852	6.9021812	7.6563446
18	C	4.7250156	6.8631383	7.8557451
19	C	4.4833246	5.8351392	6.9316425
20	O	0.9914287 *	4.0089227	4.2236676
21	N	4.3638751	1.0441085 *	1.0393471 *
22	H	9.0614320	5.8227217	5.8105305
23	H	8.6108170	5.1573275	4.5715923
24	H	6.5999857	3.2186936	2.2009149 *
25	H	8.9809236	6.3057986	6.7589916
26	H	8.3280456	6.6108910	7.4001331
27	H	6.1454535	5.3531746	6.2811371
28	H	5.0986710	4.5182548	5.7570770
29	H	2.3020958 *	6.3271247	6.6287750
30	H	4.6261526	7.8760609	8.5709647
31	H	5.8098361	7.8222763	8.8924787
32	H	5.4629500	6.1656908	7.4053044
33	H	0.0000000	4.6961856	4.6431011
34	H	4.6961856	0.0000000	1.6647566 *
35	H	4.6431011	1.6647566 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 6379.1 SECONDS (106.3 MIN)

WALL CLOCK TIME: STEP = 0.79 , TOTAL = 5896.9 SECONDS (98.3 MIN)

CPU UTILIZATION: STEP = 99.13% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.90 , TOTAL = 6380.0 SECONDS (106.3 MIN)

WALL CLOCK TIME: STEP = 0.90 , TOTAL = 5897.8 SECONDS (98.3 MIN)

CPU UTILIZATION: STEP = 99.93% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636196969	-284.636196969	0.008704702	0.001615079	197631175
11361227						
2	1	-284.636413709	-0.000216739	0.002103917	0.000134911	158515229
14743152						
3	2	-284.636415482	-0.000001773	0.001215870	0.000103496	141852323
16109044						
4	3	-284.636416202	-0.000000720	0.000670510	0.000043677	135735419
16511193						
5	4	-284.636416501	-0.000000299	0.000243814	0.000038401	130376214
16963983						
6	5	-284.636416551	-0.000000050	0.000194098	0.000042965	123613886
17407095						
7	6	-284.636416636	-0.000000086	0.000236788	0.000030652	118757837
17890509						
8	7	-284.636416662	-0.000000026	0.000203689	0.000032227	144891778
15824703						
9	8	-284.636416752	-0.000000090	0.000525352	0.000029622	140046582
16324378						
10	9	-284.636416833	-0.000000081	0.000494476	0.000028207	165912348
14240467						
11	10	-284.636416893	-0.000000060	0.000329983	0.000030819	164534057
14358079						
12	11	-284.636416935	-0.000000042	0.000342808	0.000028090	161247971
14589254						

-----DISABLING FDIFF OPTION-----

13	12	-284.636416967	-0.000000032	0.000167911	0.000024552	197624604
11361697						
14	13	-284.636416978	-0.000000011	0.000103789	0.000013654	197624539
11361702						
15	14	-284.636416988	-0.000000010	0.000044874	0.000005195	197624567
11361697						
16	15	-284.636416989	-0.000000001	0.000040450	0.000004912	197624523
11361697						
17	16	-284.636416991	-0.000000002	0.000073312	0.000004691	197624540
11361698						
18	17	-284.636416993	-0.000000002	0.000127129	0.000003415	197624585
11361700						
19	18	-284.636416995	-0.000000002	0.000095861	0.000005467	197624557
11361703						
20	19	-284.636416996	-0.000000001	0.000044579	0.000007048	197624592
11361698						
21	20	-284.636416997	-0.000000001	0.000077520	0.000005876	197624430
11361702						

22 21	-284.636416999	-0.000000001	0.000055614	0.000002410	197624352
11361703					
23 22	-284.636417000	-0.000000001	0.000060237	0.000002322	197624415
11361704					
24 23	-284.636417000	-0.000000001	0.000038718	0.000002140	197624409
11361703					
25 24	-284.636417001	0.000000000	0.000020582	0.000001553	197624543
11361702					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 84.9 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 27.2 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.5 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6364170006 AFTER 25 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6001045240
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999230054

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 88.40 , TOTAL = 6468.4 SECONDS (107.8 MIN)
WALL CLOCK TIME: STEP = 80.85 , TOTAL = 5978.6 SECONDS (99.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.57 , TOTAL = 6472.0 SECONDS (107.9 MIN)
WALL CLOCK TIME: STEP = 3.54 , TOTAL = 5982.2 SECONDS (99.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.

USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84 , TOTAL = 6474.8 SECONDS (107.9 MIN)

WALL CLOCK TIME: STEP = 2.67 , TOTAL = 5984.8 SECONDS (99.7 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 66 ENERGY= -284.6364170

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0004494	-0.0001942	-0.0004052
2 C	6.0	0.0002936	0.0000598	0.0002110
3 C	6.0	0.0000723	-0.0003088	0.0003177
4 C	6.0	-0.0002337	-0.0002880	0.0004623
5 C	6.0	-0.0001308	-0.0000524	0.0000893
6 C	6.0	-0.0000633	-0.0001694	0.0000402
7 C	6.0	-0.0000788	-0.0000442	0.0000020
8 C	6.0	0.0000093	0.0003197	-0.0004248
9 C	6.0	-0.0001002	0.0000829	-0.0001246
10 C	6.0	-0.0003142	0.0002461	0.0003212
11 C	6.0	-0.0000047	0.0001633	0.0001520
12 N	7.0	-0.0001466	-0.0005147	0.0001578
13 C	6.0	-0.0002801	0.0000911	-0.0000515
14 C	6.0	0.0000031	-0.0000571	0.0001660
15 C	6.0	-0.0000911	0.0004384	0.0002503
16 C	6.0	-0.0001943	-0.0000883	0.0002872
17 C	6.0	0.0001147	0.0000000	-0.0000377
18 C	6.0	-0.0000213	0.0001040	-0.0002160
19 C	6.0	-0.0005125	0.0000426	-0.0001789
20 O	8.0	-0.0001140	-0.0006100	-0.0006641
21 N	7.0	0.0002718	-0.0002262	-0.0001609
22 H	1.0	0.0003809	-0.0005126	-0.0001806
23 H	1.0	-0.0002456	0.0001504	-0.0004338
24 H	1.0	0.0002007	-0.0000088	0.0005700
25 H	1.0	-0.0005604	0.0005269	-0.0005875
26 H	1.0	-0.0000159	-0.0000728	0.0002842
27 H	1.0	0.0002189	0.0001244	0.0006754
28 H	1.0	0.0004119	-0.0004139	-0.0008038
29 H	1.0	0.0003026	0.0000412	-0.0002570

30 H	1.0	0.0001303	0.0000396	-0.0003979
31 H	1.0	0.0000366	0.0003207	0.0007345
32 H	1.0	-0.0002401	0.0000711	0.0002786
33 H	1.0	-0.0000355	0.0005607	0.0001855
34 H	1.0	0.0000637	-0.0002025	-0.0000158
35 H	1.0	0.0004233	0.0003810	-0.0002449

MAXIMUM GRADIENT = 0.0008038 RMS GRADIENT = 0.0003002
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000733125
 PREDICTED ENERGY CHANGE WAS -0.0000785118 RATIO= 0.934
 GDIIS STEP HAS LENGTH = 0.361342
 RADIUS OF STEP TAKEN= 0.20977 CURRENT TRUST RADIUS= 0.20977

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 6474.8 SECONDS (107.9 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 5984.8 SECONDS (99.7 MIN)
 CPU UTILIZATION: STEP = 90.45% , TOTAL = 100.00%

INSERCH= 67

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1510193457	-1.7545097162	0.8599467164
C	6.0	4.9831743231	0.6465745783	0.5334507373
C	6.0	5.1939184666	-0.7049605290	0.2285754238
C	6.0	4.0627392083	-1.5430350266	-0.0311866151
C	6.0	2.7512915301	-1.0349835456	0.0294662725
C	6.0	2.4713046295	0.3379665916	0.4312788804
C	6.0	3.6488093642	1.1884441844	0.6488877699
C	6.0	3.4897606692	2.5827687442	0.9940174835
C	6.0	2.2182048273	3.1390906264	1.1909661669
C	6.0	1.0606642201	2.3117271881	1.0549761577
C	6.0	1.1615343186	0.9597566774	0.6487515958
N	7.0	-0.0488832271	0.1554704035	0.5973312968
C	6.0	-1.2406716775	0.6890564090	0.3277280043
C	6.0	-2.5518813244	0.0442564956	0.4490417998
C	6.0	-2.8310612748	-1.2928386634	0.8973159805
C	6.0	-4.1340920329	-1.8109167470	1.0026990840
C	6.0	-5.2405260725	-0.9729552085	0.6651885799
C	6.0	-5.0198661922	0.3647061167	0.2322599515
C	6.0	-3.6975635314	0.8586492838	0.1215170200
O	8.0	-1.7146611749	-2.1737392526	1.2539258158

N	7.0	1.6559437385	-1.9806383346	-0.4042982242
H	1.0	5.8449357971	1.3187163983	0.6984248483
H	1.0	6.2141346250	-1.1211484518	0.1569261557
H	1.0	4.2366543989	-2.5991251327	-0.3164494306
H	1.0	4.3938092107	3.2049195397	1.1204588443
H	1.0	2.1027173507	4.1959604676	1.4888749757
H	1.0	0.0785272694	2.7403104950	1.3222345408
H	1.0	-1.2680459895	1.7356052842	-0.0354269956
H	1.0	-4.3085883965	-2.8517909829	1.3351984612
H	1.0	-6.2665569118	-1.3773766980	0.7379609524
H	1.0	-5.8748992895	1.0197208848	-0.0124737251
H	1.0	-3.5296096366	1.8990311858	-0.2141036235
H	1.0	-2.0359888427	-2.9987988043	1.7016367933
H	1.0	1.3190853875	-1.7207266196	-1.3576009774
H	1.0	2.0606638939	-2.9340828418	-0.4946137169

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.4056940	5.1895101	4.0175107
2 C	5.4056940	0.0000000	1.4014311 *	2.4413943 *
3 C	5.1895101	1.4014311 *	0.0000000	1.4315766 *
4 C	4.0175107	2.4413943 *	1.4315766 *	0.0000000
5 C	2.8229118 *	2.8395315 *	2.4728498 *	1.4077251 *
6 C	3.1537180	2.5328181 *	2.9225694 *	2.5069315 *
7 C	4.5760309	1.4448108 *	2.4797189 *	2.8451393 *
8 C	5.4751395	2.4882230 *	3.7814308	4.2897092
9 C	5.3226078	3.7802142	4.9555824	5.1786355
10 C	4.1713035	4.2931116	5.1833516	5.0051369
11 C	2.9039604 *	3.8361843	4.3826879	3.8914357
12 N	1.9382858 *	5.0563690	5.3257198	4.4928159
13 C	2.8620056 *	6.2273899	6.5846082	5.7651729
14 C	3.2726251	7.5595619	7.7850720	6.8193342
15 C	3.0178372	8.0595285	8.0742253	6.9605460
16 C	4.2878595	9.4543114	9.4251889	8.2661190
17 C	5.4513778	10.3520182	10.4470132	9.3466932
18 C	5.6234441	10.0115426	10.2696445	9.2845356
19 C	4.7101453	8.6930935	9.0285541	8.1248818
20 O	1.9523670 *	7.3030305	7.1370251	5.9521137
21 N	1.9784456 *	4.3418987	3.8138102	2.4745451 *
22 H	6.4723638	1.1052710 *	2.1771197 *	3.4493737
23 H	6.1365097	2.1867507 *	1.1041680 *	2.2004265 *
24 H	4.3347084	3.4371775	2.1911792 *	1.1076767 *
25 H	6.5318505	2.6901782 *	4.0893512	4.8968324

26 H	6.2938678	4.6699045	5.9298319	6.2520670
27 H	4.5191121	5.3908694	6.2636419	6.0043936
28 H	3.8725112	6.3708214	6.9125280	6.2583361
29 H	4.6171411	9.9608341	9.8046485	8.5824808
30 H	6.4298052	11.4321763	11.4914800	10.3592176
31 H	6.6909766	10.8781908	11.2049702	10.2627836
32 H	5.2961283	8.6368383	9.1146410	8.3381676
33 H	2.6532437 *	7.9951271	7.7267822	6.5051064
34 H	2.5065988 *	4.7545493	4.3083718	3.0526359
35 H	2.6216348 *	4.7348803	3.9127066	2.4815488 *

C C C C

1 CO	2.8229118 *	3.1537180	4.5760309	5.4751395
2 C	2.8395315 *	2.5328181 *	1.4448108 *	2.4882230 *
3 C	2.4728498 *	2.9225694 *	2.4797189 *	3.7814308
4 C	1.4077251 *	2.5069315 *	2.8451393 *	4.2897092
5 C	0.0000000	1.4576824 *	2.4764596 *	3.8162583
6 C	1.4576824 *	0.0000000	1.4687352 *	2.5284509 *
7 C	2.4764596 *	1.4687352 *	0.0000000	1.4451823 *
8 C	3.8162583	2.5284509 *	1.4451823 *	0.0000000
9 C	4.3653360	2.9133280 *	2.4790119 *	1.4018335 *
10 C	3.8872052	2.5049223 *	2.8504680 *	2.4449313 *
11 C	2.6248487 *	1.4660885 *	2.4977660 *	2.8590234 *
12 N	3.0952593	2.5322372 *	3.8396124	4.3094243
13 C	4.3585599	3.7299806	4.9253991	5.1387818
14 C	5.4281162	5.0317967	6.3085394	6.5759015
15 C	5.6552909	5.5670280	6.9431408	7.4150168
16 C	6.9969823	6.9696116	8.3483473	8.7992998
17 C	8.0173025	7.8259544	9.1483440	9.4323490
18 C	7.8988068	7.4938617	8.7176866	8.8268809
19 C	6.7217595	6.1985480	7.3726575	7.4425449
20 O	4.7687314	4.9505276	6.3590223	7.0553474
21 N	1.5106957 *	2.5959452 *	3.8889328	5.1130085
22 H	3.9443686	3.5234393	2.2005445 *	2.6892477 *
23 H	3.4662592	4.0265447	3.4867088	4.6735359
24 H	2.1846051 *	3.5074300	3.9526091	5.3969619
25 H	4.6759927	3.5200017	2.2008128 *	1.1047003 *
26 H	5.4693050	4.0172731	3.4844129	2.1842987 *
27 H	4.8028912	3.5057726	3.9507720	3.4306062
28 H	4.8821561	4.0191978	4.9943106	4.9410693
29 H	7.4059186	7.5470904	8.9506816	9.5113139
30 H	9.0521151	8.9099204	10.2423561	10.5325234
31 H	8.8676230	8.3857513	9.5481356	9.5474080
32 H	6.9366770	6.2341329	7.2649424	7.1553206
33 H	5.4379020	5.7500876	7.1385023	7.8859704

34 H	2.1084149 *	2.9607293 *	4.2328342	5.3630227
35 H	2.0876313 *	3.4252314	4.5634451	5.8901606

	C	C	C	N
--	---	---	---	---

1 CO	5.3226078	4.1713035	2.9039604 *	1.9382858 *
2 C	3.7802142	4.2931116	3.8361843	5.0563690
3 C	4.9555824	5.1833516	4.3826879	5.3257198
4 C	5.1786355	5.0051369	3.8914357	4.4928159
5 C	4.3653360	3.8872052	2.6248487 *	3.0952593
6 C	2.9133280 *	2.5049223 *	1.4660885 *	2.5322372 *
7 C	2.4790119 *	2.8504680 *	2.4977660 *	3.8396124
8 C	1.4018335 *	2.4449313 *	2.8590234 *	4.3094243
9 C	0.0000000	1.4293089 *	2.4819439 *	3.7939531
10 C	1.4293089 *	0.0000000	1.4152800 *	2.4677880 *
11 C	2.4819439 *	1.4152800 *	0.0000000	1.4541771 *
12 N	3.7939531	2.4677880 *	1.4541771 *	0.0000000
13 C	4.3256993	2.9082808 *	2.4386325 *	1.3333265 *
14 C	5.7342979	4.3080233	3.8298147	2.5098521 *
15 C	6.7248283	5.3069086	4.5909465	3.1508895
16 C	8.0554139	6.6320750	5.9871169	4.5519153
17 C	8.5333481	7.1166054	6.6874526	5.3132951
18 C	7.8106337	6.4374376	6.2239266	4.9887602
19 C	6.4296539	5.0619673	4.8886635	3.7461617
20 O	6.6104130	5.2783919	4.2962231	2.9378819 *
21 N	5.3919042	4.5725530	3.1621634	2.9107829 *
22 H	4.0877300	4.8992299	4.6974002	6.0083662
23 H	5.9318067	6.2569470	5.4864222	6.4069575
24 H	6.2668621	6.0070119	4.8014182	5.1757728
25 H	2.1777418 *	3.4513673	3.9636934	5.4139005
26 H	1.1041109 *	2.1964694 *	3.4734202	4.6636676
27 H	2.1804763 *	1.1044020 *	2.1901725 *	2.6875856 *
28 H	3.9531957	2.6351066 *	2.6406253 *	2.0936970 *
29 H	8.8606148	7.4544831	6.7023389	5.2662280
30 H	9.6226230	8.2096380	7.7875985	6.4053777
31 H	8.4521198	7.1351784	7.0676879	5.9212544
32 H	6.0456050	4.7803238	4.8614388	3.9766678
33 H	7.4854950	6.1813523	5.1964298	3.8881221
34 H	5.5607044	4.7061655	3.3519045	3.0353276
35 H	6.3047153	5.5605531	4.1566458	3.8971621

	C	C	C	C
--	---	---	---	---

1 CO	2.8620056 *	3.2726251	3.0178372	4.2878595
2 C	6.2273899	7.5595619	8.0595285	9.4543114
3 C	6.5846082	7.7850720	8.0742253	9.4251889

4 C	5.7651729	6.8193342	6.9605460	8.2661190
5 C	4.3585599	5.4281162	5.6552909	6.9969823
6 C	3.7299806	5.0317967	5.5670280	6.9696116
7 C	4.9253991	6.3085394	6.9431408	8.3483473
8 C	5.1387818	6.5759015	7.4150168	8.7992998
9 C	4.3256993	5.7342979	6.7248283	8.0554139
10 C	2.9082808 *	4.3080233	5.3069086	6.6320750
11 C	2.4386325 *	3.8298147	4.5909465	5.9871169
12 N	1.3333265 *	2.5098521 *	3.1508895	4.5519153
13 C	0.0000000	1.4662042 *	2.6041654 *	3.8829542
14 C	1.4662042 *	0.0000000	1.4376073 *	2.5003190 *
15 C	2.6041654 *	1.4376073 *	0.0000000	1.4062004 *
16 C	3.8829542	2.5003190 *	1.4062004 *	0.0000000
17 C	4.3445365	2.8827504 *	2.4416652 *	1.4283869 *
18 C	3.7942889	2.4981256 *	2.8249993 *	2.4721463 *
19 C	2.4713564 *	1.4432934 *	2.4457290 *	2.8449291 *
20 O	3.0459986	2.5036535 *	1.4661192 *	2.4593497 *
21 N	4.0066836	4.7470180	4.7223386	5.9609530
22 H	7.1231820	8.4966451	9.0627095	10.4627044
23 H	7.6733403	8.8479679	9.0770713	10.4056190
24 H	6.4209192	7.3251389	7.2891848	8.5106299
25 H	6.2213635	7.6604966	8.5134232	9.8943206
26 H	4.9824581	6.3232261	7.4039874	8.6727580
27 H	2.6338133 *	3.8665517	4.9912477	6.2098256
28 H	1.1081044 *	2.1779816 *	3.5333411	4.6765098
29 H	4.7921509	3.5011976	2.1920675 *	1.1065369 *
30 H	5.4495834	3.9878979	3.4402283	2.1921336 *
31 H	4.6584484	3.4938483	3.9294527	3.4746935
32 H	2.6451574 *	2.1990688 *	3.4512688	3.9509140
33 H	4.0150256	3.3309645	2.0467956 *	2.5103017 *
34 H	3.8986849	4.6220674	4.7425158	5.9427514
35 H	4.9701308	5.5710470	5.3441675	6.4713560

C C C O

1 CO	5.4513778	5.6234441	4.7101453	1.9523670 *
2 C	10.3520182	10.0115426	8.6930935	7.3030305
3 C	10.4470132	10.2696445	9.0285541	7.1370251
4 C	9.3466932	9.2845356	8.1248818	5.9521137
5 C	8.0173025	7.8988068	6.7217595	4.7687314
6 C	7.8259544	7.4938617	6.1985480	4.9505276
7 C	9.1483440	8.7176866	7.3726575	6.3590223
8 C	9.4323490	8.8268809	7.4425449	7.0553474
9 C	8.5333481	7.8106337	6.4296539	6.6104130
10 C	7.1166054	6.4374376	5.0619673	5.2783919
11 C	6.6874526	6.2239266	4.8886635	4.2962231

12 N	5.3132951	4.9887602	3.7461617	2.9378819 *
13 C	4.3445365	3.7942889	2.4713564 *	3.0459986
14 C	2.8827504 *	2.4981256 *	1.4432934 *	2.5036535 *
15 C	2.4416652 *	2.8249993 *	2.4457290 *	1.4661192 *
16 C	1.4283869 *	2.4721463 *	2.8449291 *	2.4593497 *
17 C	0.0000000	1.4231851 *	2.4558272 *	3.7709703
18 C	1.4231851 *	0.0000000	1.4158842 *	4.2909074
19 C	2.4558272 *	1.4158842 *	0.0000000	3.7960021
20 O	3.7709703	4.2909074	3.7960021	0.0000000
21 N	7.0512781	7.1043849	6.0826044	3.7613791
22 H	11.3199085	10.9165639	9.5709863	8.3458573
23 H	11.4668890	11.3320878	10.1075523	8.0732372
24 H	9.6656604	9.7349140	8.6660160	6.1696992
25 H	10.5110573	9.8728412	8.4837009	8.1400979
26 H	9.0177255	8.1846678	6.8301224	7.4297143
27 H	6.5201518	5.7293243	4.3864830	5.2314506
28 H	4.8587818	4.0033955	2.5877092 *	4.1406365
29 H	2.2016914 *	3.4739377	3.9514227	2.6823158 *
30 H	1.1052565 *	2.2010960 *	3.4611475	4.6497492
31 H	2.1982751 *	1.1045454 *	2.1873931 *	5.3953254
32 H	3.4566885	2.1850077 *	1.1060037 *	4.6943165
33 H	3.9303086	4.7303021	4.4874842	0.9921793 *
34 H	6.9050230	6.8599559	5.8316153	4.0285122
35 H	7.6484337	7.8450150	6.9225441	4.2294908

N H H H

1 CO	1.9784456 *	6.4723638	6.1365097	4.3347084
2 C	4.3418987	1.1052710 *	2.1867507 *	3.4371775
3 C	3.8138102	2.1771197 *	1.1041680 *	2.1911792 *
4 C	2.4745451 *	3.4493737	2.2004265 *	1.1076767 *
5 C	1.5106957 *	3.9443686	3.4662592	2.1846051 *
6 C	2.5959452 *	3.5234393	4.0265447	3.5074300
7 C	3.8889328	2.2005445 *	3.4867088	3.9526091
8 C	5.1130085	2.6892477 *	4.6735359	5.3969619
9 C	5.3919042	4.0877300	5.9318067	6.2668621
10 C	4.5725530	4.8992299	6.2569470	6.0070119
11 C	3.1621634	4.6974002	5.4864222	4.8014182
12 N	2.9107829 *	6.0083662	6.4069575	5.1757728
13 C	4.0066836	7.1231820	7.6733403	6.4209192
14 C	4.7470180	8.4966451	8.8479679	7.3251389
15 C	4.7223386	9.0627095	9.0770713	7.2891848
16 C	5.9609530	10.4627044	10.4056190	8.5106299
17 C	7.0512781	11.3199085	11.4668890	9.6656604
18 C	7.1043849	10.9165639	11.3320878	9.7349140
19 C	6.0826044	9.5709863	10.1075523	8.6660160

20	O	3.7613791	8.3458573	8.0732372	6.1696992
21	N	0.0000000	5.4451257	4.6723441	2.6552421 *
22	H	5.4451257	0.0000000	2.5263549 *	4.3549996
23	H	4.6723441	2.5263549 *	0.0000000	2.5137477 *
24	H	2.6552421 *	4.3549996	2.5137477 *	0.0000000
25	H	6.0589440	2.4169492 *	4.7913301	5.9813324
26	H	6.4756532	4.7861826	6.8519696	7.3475215
27	H	5.2684453	5.9717280	7.3426485	6.9631084
28	H	4.7430210	7.1628796	8.0113088	7.0121743
29	H	6.2737867	10.9951201	10.7289864	8.7070635
30	H	8.0271226	12.4080110	12.4968362	10.6264716
31	H	8.1159891	11.7451824	12.2783044	10.7439269
32	H	6.4790411	9.4367142	10.2078254	8.9754522
33	H	4.3705811	9.0419215	8.6009441	6.6013987
34	H	1.0439415 *	5.8265580	5.1589527	3.2199052
35	H	1.0397171 *	5.8163869	4.5784882	2.2088173 *

H H H H

1	CO	6.5318505	6.2938678	4.5191121	3.8725112
2	C	2.6901782 *	4.6699045	5.3908694	6.3708214
3	C	4.0893512	5.9298319	6.2636419	6.9125280
4	C	4.8968324	6.2520670	6.0043936	6.2583361
5	C	4.6759927	5.4693050	4.8028912	4.8821561
6	C	3.5200017	4.0172731	3.5057726	4.0191978
7	C	2.2008128 *	3.4844129	3.9507720	4.9943106
8	C	1.1047003 *	2.1842987 *	3.4306062	4.9410693
9	C	2.1777418 *	1.1041109 *	2.1804763 *	3.9531957
10	C	3.4513673	2.1964694 *	1.1044020 *	2.6351066 *
11	C	3.9636934	3.4734202	2.1901725 *	2.6406253 *
12	N	5.4139005	4.6636676	2.6875856 *	2.0936970 *
13	C	6.2213635	4.9824581	2.6338133 *	1.1081044 *
14	C	7.6604966	6.3232261	3.8665517	2.1779816 *
15	C	8.5134232	7.4039874	4.9912477	3.5333411
16	C	9.8943206	8.6727580	6.2098256	4.6765098
17	C	10.5110573	9.0177255	6.5201518	4.8587818
18	C	9.8728412	8.1846678	5.7293243	4.0033955
19	C	8.4837009	6.8301224	4.3864830	2.5877092 *
20	O	8.1400979	7.4297143	5.2314506	4.1406365
21	N	6.0589440	6.4756532	5.2684453	4.7430210
22	H	2.4169492 *	4.7861826	5.9717280	7.1628796
23	H	4.7913301	6.8519696	7.3426485	8.0113088
24	H	5.9813324	7.3475215	6.9631084	7.0121743
25	H	0.0000000	2.5232904 *	4.3449089	5.9625130
26	H	2.5232904 *	0.0000000	2.4988060 *	4.4428470
27	H	4.3449089	2.4988060 *	0.0000000	2.1600780 *

28 H	5.9625130	4.4428470	2.1600780 *	0.0000000
29 H	10.6047904	9.5288645	7.1076403	5.6716591
30 H	11.6097868	10.0831895	7.5866209	5.9391832
31 H	10.5595930	8.7169325	6.3391768	4.6622006
32 H	8.1404525	6.3165756	4.0108276	2.2744897 *
33 H	8.9535575	8.3029343	6.1280095	5.1011478
34 H	6.3132161	6.6123892	5.3498930	4.5152656
35 H	6.7630893	7.4009130	6.2792152	5.7530122

H H H H

1 CO	4.6171411	6.4298052	6.6909766	5.2961283
2 C	9.9608341	11.4321763	10.8781908	8.6368383
3 C	9.8046485	11.4914800	11.2049702	9.1146410
4 C	8.5824808	10.3592176	10.2627836	8.3381676
5 C	7.4059186	9.0521151	8.8676230	6.9366770
6 C	7.5470904	8.9099204	8.3857513	6.2341329
7 C	8.9506816	10.2423561	9.5481356	7.2649424
8 C	9.5113139	10.5325234	9.5474080	7.1553206
9 C	8.8606148	9.6226230	8.4521198	6.0456050
10 C	7.4544831	8.2096380	7.1351784	4.7803238
11 C	6.7023389	7.7875985	7.0676879	4.8614388
12 N	5.2662280	6.4053777	5.9212544	3.9766678
13 C	4.7921509	5.4495834	4.6584484	2.6451574 *
14 C	3.5011976	3.9878979	3.4938483	2.1990688 *
15 C	2.1920675 *	3.4402283	3.9294527	3.4512688
16 C	1.1065369 *	2.1921336 *	3.4746935	3.9509140
17 C	2.2016914 *	1.1052565 *	2.1982751 *	3.4566885
18 C	3.4739377	2.2010960 *	1.1045454 *	2.1850077 *
19 C	3.9514227	3.4611475	2.1873931 *	1.1060037 *
20 O	2.6823158 *	4.6497492	5.3953254	4.6943165
21 N	6.2737867	8.0271226	8.1159891	6.4790411
22 H	10.9951201	12.4080110	11.7451824	9.4367142
23 H	10.7289864	12.4968362	12.2783044	10.2078254
24 H	8.7070635	10.6264716	10.7439269	8.9754522
25 H	10.6047904	11.6097868	10.5595930	8.1404525
26 H	9.5288645	10.0831895	8.7169325	6.3165756
27 H	7.1076403	7.5866209	6.3391768	4.0108276
28 H	5.6716591	5.9391832	4.6622006	2.2744897 *
29 H	0.0000000	2.5227427 *	4.3884114	5.0574160
30 H	2.5227427 *	0.0000000	2.5421693 *	4.3740320
31 H	4.3884114	2.5421693 *	0.0000000	2.5128121 *
32 H	5.0574160	4.3740320	2.5128121 *	0.0000000
33 H	2.3066419 *	4.6319960	5.8158326	5.4671476
34 H	6.3404406	7.8772608	7.8149111	6.1579279
35 H	6.6273946	8.5606764	8.8790870	7.3951900

	H	H	H
1 CO	2.6532437 *	2.5065988 *	2.6216348 *
2 C	7.9951271	4.7545493	4.7348803
3 C	7.7267822	4.3083718	3.9127066
4 C	6.5051064	3.0526359	2.4815488 *
5 C	5.4379020	2.1084149 *	2.0876313 *
6 C	5.7500876	2.9607293 *	3.4252314
7 C	7.1385023	4.2328342	4.5634451
8 C	7.8859704	5.3630227	5.8901606
9 C	7.4854950	5.5607044	6.3047153
10 C	6.1813523	4.7061655	5.5605531
11 C	5.1964298	3.3519045	4.1566458
12 N	3.8881221	3.0353276	3.8971621
13 C	4.0150256	3.8986849	4.9701308
14 C	3.3309645	4.6220674	5.5710470
15 C	2.0467956 *	4.7425158	5.3441675
16 C	2.5103017 *	5.9427514	6.4713560
17 C	3.9303086	6.9050230	7.6484337
18 C	4.7303021	6.8599559	7.8450150
19 C	4.4874842	5.8316153	6.9225441
20 O	0.9921793 *	4.0285122	4.2294908
21 N	4.3705811	1.0439415 *	1.0397171 *
22 H	9.0419215	5.8265580	5.8163869
23 H	8.6009441	5.1589527	4.5784882
24 H	6.6013987	3.2199052	2.2088173 *
25 H	8.9535575	6.3132161	6.7630893
26 H	8.3029343	6.6123892	7.4009130
27 H	6.1280095	5.3498930	6.2792152
28 H	5.1011478	4.5152656	5.7530122
29 H	2.3066419 *	6.3404406	6.6273946
30 H	4.6319960	7.8772608	8.5606764
31 H	5.8158326	7.8149111	8.8790870
32 H	5.4671476	6.1579279	7.3951900
33 H	0.0000000	4.7168769	4.6486846
34 H	4.7168769	0.0000000	1.6634058 *
35 H	4.6486846	1.6634058 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.79 , TOTAL = 6475.6 SECONDS (107.9 MIN)

WALL CLOCK TIME: STEP = 0.79 , TOTAL = 5985.6 SECONDS (99.8 MIN)

CPU UTILIZATION: STEP = 99.66%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.99 , TOTAL = 6476.6 SECONDS (107.9 MIN)

WALL CLOCK TIME: STEP = 0.98 , TOTAL = 5986.6 SECONDS (99.8 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.635651222 -284.635651222 0.024514442 0.003122795 197772039
11353825

2 1 -284.636526699 -0.000875477 0.004574145 0.000268315 164716256
14237787

3 2 -284.636534246 -0.000007547 0.004222287 0.000152615 149710080
15485982

4 3 -284.636536513 -0.000002267 0.001625110 0.000141191 143554143
15921350

5 4 -284.636537793 -0.000001280 0.000740366 0.000133523 139007790
16331497

6 5 -284.636537822 -0.000000029 0.000652771 0.000141185 134511084
16625134

7 6 -284.636538483 -0.000000661 0.000399382 0.000065327 131206901
16940146

8 7 -284.636538528 -0.000000045 0.000331207 0.000055195 129304943
17012606

9 8 -284.636538836 -0.000000308 0.000895756 0.000054704 124443580
17482573

10 9 -284.636539126 -0.000000289 0.001123533 0.000054032 152000411
15340475

11 10 -284.636539447 -0.000000322 0.000798434 0.000050625 170294073
13908973

12 11 -284.636539676 -0.000000229 0.000933622 0.000057151 168911781
13976227

-----DISABLING FDIFF OPTION-----

13 12 -284.636539860 -0.000000184 0.000312936 0.000047483 197765782
11354324

14 13 -284.636539934 -0.000000074 0.000370093 0.000027316 197765717
11354328

15	14	-284.636539990	-0.000000056	0.000150410	0.000011530	197765762
11354331						
16	15	-284.636540001	-0.000000011	0.000096226	0.000010111	197765758
11354324						
17	16	-284.636540008	-0.000000006	0.000117757	0.000009838	197765850
11354315						
18	17	-284.636540016	-0.000000008	0.000329601	0.000008634	197765748
11354323						
19	18	-284.636540030	-0.000000014	0.000221850	0.000011376	197765754
11354326						
20	19	-284.636540036	-0.000000006	0.000093281	0.000015031	197766121
11354318						
21	20	-284.636540041	-0.000000005	0.000200083	0.000013022	197766129
11354323						
22	21	-284.636540048	-0.000000007	0.000118422	0.000004887	197765933
11354326						
23	22	-284.636540052	-0.000000004	0.000095863	0.000004883	197766008
11354328						
24	23	-284.636540054	-0.000000002	0.000064164	0.000004184	197765981
11354328						
25	24	-284.636540055	-0.000000001	0.000046169	0.000002619	197765972
11354327						
26	25	-284.636540056	-0.000000001	0.000027932	0.000002368	197765972
11354326						
27	26	-284.636540056	0.000000000	0.000008882	0.000001062	197765918
11354326						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 92.1 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 29.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6365400563 AFTER 27 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.5990967432
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9999062364

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!

PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 95.73 , TOTAL = 6572.3 SECONDS (109.5 MIN)
WALL CLOCK TIME: STEP = 87.61 , TOTAL = 6074.2 SECONDS (101.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.82 , TOTAL = 6576.2 SECONDS (109.6 MIN)
WALL CLOCK TIME: STEP = 3.80 , TOTAL = 6078.0 SECONDS (101.3 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.87 , TOTAL = 6579.0 SECONDS (109.7 MIN)
WALL CLOCK TIME: STEP = 2.71 , TOTAL = 6080.7 SECONDS (101.3 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 67 ENERGY= -284.6365401

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000526	-0.0000856	-0.0000690
2 C	6.0	0.0000094	-0.0001603	0.0001384
3 C	6.0	0.0000418	-0.0001781	0.0001041
4 C	6.0	-0.0000582	0.0001218	0.0003150
5 C	6.0	-0.0002561	0.0001480	0.0000897
6 C	6.0	-0.0001065	-0.0003402	-0.0000282
7 C	6.0	0.0002050	-0.0002720	0.0000788
8 C	6.0	0.0002125	0.0004246	-0.0001226
9 C	6.0	-0.0002362	-0.0000325	0.0000465
10 C	6.0	-0.0002880	0.0001110	0.0003893
11 C	6.0	-0.0000779	0.0001077	0.0000876

12 N	7.0	-0.0000258	-0.0003542	-0.0000028
13 C	6.0	-0.0000535	0.0002380	-0.0001636
14 C	6.0	-0.0001336	0.0002487	0.0000671
15 C	6.0	-0.0000881	0.0001409	0.0003678
16 C	6.0	-0.0001555	0.0003312	0.0002076
17 C	6.0	-0.0001125	0.0000727	-0.0000085
18 C	6.0	0.0001485	-0.0001425	0.0000313
19 C	6.0	-0.0002722	-0.0000241	0.0000388
20 O	8.0	-0.0000464	0.0000214	-0.0006112
21 N	7.0	-0.0001682	-0.0000684	-0.0003742
22 H	1.0	0.0004821	-0.0003482	-0.0002544
23 H	1.0	0.0000174	0.0000479	-0.0003121
24 H	1.0	0.0003337	0.0000144	0.0007707
25 H	1.0	-0.0005767	0.0004925	-0.0004615
26 H	1.0	-0.0000972	-0.0001655	0.0000175
27 H	1.0	-0.0000070	0.0001134	0.0005453
28 H	1.0	0.0005914	-0.0003204	-0.0007835
29 H	1.0	0.0003268	0.0000976	-0.0002302
30 H	1.0	-0.0000158	-0.0001966	-0.0004908
31 H	1.0	-0.0001860	0.0003806	0.0005289
32 H	1.0	-0.0002311	0.0001535	0.0001903
33 H	1.0	0.0002243	-0.0002558	0.0004056
34 H	1.0	0.0004277	-0.0003779	-0.0000727
35 H	1.0	0.0002246	0.0000565	-0.0004348

MAXIMUM GRADIENT = 0.0007835 RMS GRADIENT = 0.0002719
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0001230557
 PREDICTED ENERGY CHANGE WAS -0.0001187868 RATIO= 1.036
 GDIIS STEP HAS LENGTH = 0.238059
 RADIUS OF STEP TAKEN= 0.23806 CURRENT TRUST RADIUS= 0.41953

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 6579.0 SECONDS (109.7 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6080.8 SECONDS (101.3
 MIN)
 CPU UTILIZATION: STEP = 91.15%, TOTAL = 100.00%

INSERCH= 68

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1508207036	-1.7453998133	0.8518274193
C	6.0	4.9819383319	0.6420440656	0.5396151349

C	6.0	5.1921301761	-0.7058124179	0.2202646513
C	6.0	4.0604783448	-1.5418371750	-0.0484408159
C	6.0	2.7495045406	-1.0338222065	0.0158691231
C	6.0	2.4707852038	0.3376707909	0.4261532616
C	6.0	3.6477409890	1.1835232769	0.6584961374
C	6.0	3.4911103223	2.5731166384	1.0210557141
C	6.0	2.2196213193	3.1344304548	1.2045868447
C	6.0	1.0612058607	2.3124771828	1.0474990251
C	6.0	1.1618001234	0.9619898532	0.6379903865
N	7.0	-0.0500273632	0.1626431427	0.5823596005
C	6.0	-1.2421712760	0.6958316354	0.3168292596
C	6.0	-2.5510533411	0.0474660698	0.4458195317
C	6.0	-2.8259172392	-1.2848256268	0.9104476357
C	6.0	-4.1272081820	-1.8053305232	1.0218953293
C	6.0	-5.2370882821	-0.9775294388	0.6717625970
C	6.0	-5.0209090052	0.3552037375	0.2220844909
C	6.0	-3.6998620798	0.8531199195	0.1079160911
O	8.0	-1.7061819677	-2.1567492235	1.2807376992
N	7.0	1.6504350042	-1.9759628333	-0.4184764868
H	1.0	5.8416494637	1.3140046999	0.7145931170
H	1.0	6.2120501362	-1.1239221614	0.1513193824
H	1.0	4.2332345687	-2.5965591536	-0.3390662553
H	1.0	4.3980991629	3.1876980938	1.1683624864
H	1.0	2.1032873336	4.1906248825	1.5039339378
H	1.0	0.0756995449	2.7417629476	1.3014822899
H	1.0	-1.2736348634	1.7432030209	-0.0446608913
H	1.0	-4.2994148351	-2.8416149672	1.3697762725
H	1.0	-6.2617212795	-1.3870927732	0.7461635841
H	1.0	-5.8780749222	0.9999928743	-0.0401845477
H	1.0	-3.5350547048	1.8882827205	-0.2448249515
H	1.0	-2.0209567414	-2.9785854974	1.7384279918
H	1.0	1.3165109655	-1.7155741682	-1.3729985903
H	1.0	2.0471709873	-2.9333630274	-0.5057294559

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3978757	5.1859825	4.0171313
2 C	5.3978757	0.0000000	1.4010291 *	2.4421785 *
3 C	5.1859825	1.4010291 *	0.0000000	1.4324021 *
4 C	4.0171313	2.4421785 *	1.4324021 *	0.0000000
5 C	2.8210506 *	2.8401757 *	2.4730119 *	1.4074329 *
6 C	3.1468424	2.5320756 *	2.9218086 *	2.5069731 *
7 C	4.5655689	1.4447889 *	2.4792689 *	2.8456461 *

8 C	5.4622118	2.4866432 *	3.7796972	4.2896209
9 C	5.3119788	3.7794937	4.9550141	5.1794123
10 C	4.1633465	4.2919035	5.1825596	5.0052431
11 C	2.8978897 *	3.8347750	4.3817370	3.8913588
12 N	1.9374160 *	5.0549314	5.3259312	4.4943764
13 C	2.8611642 *	6.2283278	6.5859066	5.7670336
14 C	3.2679250	7.5570023	7.7830068	6.8178097
15 C	3.0127286	8.0506492	8.0685001	6.9575834
16 C	4.2818274	9.4445109	9.4181537	8.2615531
17 C	5.4453293	10.3474145	10.4425226	9.3424773
18 C	5.6174638	10.0119957	10.2680051	9.2813547
19 C	4.7046219	8.6950892	9.0283121	8.1230013
20 O	1.9497772 *	7.2878982	7.1285715	5.9497230
21 N	1.9788063 *	4.3440550	3.8163958	2.4766309 *
22 H	6.4625321	1.1051025 *	2.1785080 *	3.4511772
23 H	6.1331434	2.1869123 *	1.1044482 *	2.2008676 *
24 H	4.3369117	3.4381956	2.1925453 *	1.1075858 *
25 H	6.5172865	2.6863629 *	4.0851926	4.8952121
26 H	6.2828145	4.6700073	5.9299119	6.2531260
27 H	4.5102619	5.3907736	6.2635988	6.0041639
28 H	3.8733854	6.3785677	6.9191025	6.2645245
29 H	4.6124348	9.9482945	9.7965533	8.5783784
30 H	6.4234137	11.4271580	11.4861406	10.3538953
31 H	6.6843436	10.8813686	11.2038853	10.2584506
32 H	5.2907441	8.6433574	9.1164354	8.3364508
33 H	2.6501745 *	7.9741238	7.7135556	6.4993075
34 H	2.5118866 *	4.7593921	4.3102820	3.0518838
35 H	2.6173196 *	4.7422717	3.9217110	2.4897517 *

C C C C

1 CO	2.8210506 *	3.1468424	4.5655689	5.4622118
2 C	2.8401757 *	2.5320756 *	1.4447889 *	2.4866432 *
3 C	2.4730119 *	2.9218086 *	2.4792689 *	3.7796972
4 C	1.4074329 *	2.5069731 *	2.8456461 *	4.2896209
5 C	0.0000000	1.4584274 *	2.4771797 *	3.8171176
6 C	1.4584274 *	0.0000000	1.4678810 *	2.5282782 *
7 C	2.4771797 *	1.4678810 *	0.0000000	1.4446288 *
8 C	3.8171176	2.5282782 *	1.4446288 *	0.0000000
9 C	4.3667100	2.9139161 *	2.4786649 *	1.4019419 *
10 C	3.8874583	2.5045648 *	2.8488637 *	2.4439861 *
11 C	2.6250916 *	1.4656368 *	2.4958765 *	2.8579983 *
12 N	3.0967434	2.5317052 *	3.8368586	4.3060995
13 C	4.3607058	3.7317927	4.9260351	5.1404366
14 C	5.4267813	5.0302553	6.3056251	6.5740056
15 C	5.6523094	5.5607637	6.9328549	7.4027556

16 C	6.9926026	6.9628213	8.3375740	8.7868980
17 C	8.0136777	7.8231317	9.1438786	9.4292388
18 C	7.8962804	7.4944936	8.7190631	8.8324383
19 C	6.7203685	6.2003105	7.3756068	7.4499864
20 O	4.7659207	4.9395851	6.3410643	7.0321343
21 N	1.5113699 *	2.5960112 *	3.8899169	5.1141434
22 H	3.9448532	3.5212429	2.1985010 *	2.6840858 *
23 H	3.4663651	4.0260217	3.4867197	4.6720499
24 H	2.1839370 *	3.5073486	3.9530946	5.3968721
25 H	4.6762526	3.5196689	2.1999359 *	1.1054585 *
26 H	5.4705375	4.0177010	3.4846466	2.1853048 *
27 H	4.8017786	3.5046106	3.9498129	3.4310511
28 H	4.8888837	4.0271415	5.0027604	4.9525049
29 H	7.4019216	7.5388256	8.9367188	9.4938510
30 H	9.0476694	8.9069571	10.2378316	10.5297934
31 H	8.8642356	8.3880634	9.5531674	9.5594237
32 H	6.9355853	6.2389680	7.2735981	7.1720601
33 H	5.4319991	5.7354482	7.1150219	7.8561379
34 H	2.1088409 *	2.9639688 *	4.2386755	5.3715219
35 H	2.0913137 *	3.4274650	4.5679315	5.8938402

C C C N

1 CO	5.3119788	4.1633465	2.8978897 *	1.9374160 *
2 C	3.7794937	4.2919035	3.8347750	5.0549314
3 C	4.9550141	5.1825596	4.3817370	5.3259312
4 C	5.1794123	5.0052431	3.8913588	4.4943764
5 C	4.3667100	3.8874583	2.6250916 *	3.0967434
6 C	2.9139161 *	2.5045648 *	1.4656368 *	2.5317052 *
7 C	2.4786649 *	2.8488637 *	2.4958765 *	3.8368586
8 C	1.4019419 *	2.4439861 *	2.8579983 *	4.3060995
9 C	0.0000000	1.4290592 *	2.4818371 *	3.7907772
10 C	1.4290592 *	0.0000000	1.4147906 *	2.4643418 *
11 C	2.4818371 *	1.4147906 *	0.0000000	1.4527821 *
12 N	3.7907772	2.4643418 *	1.4527821 *	0.0000000
13 C	4.3265328	2.9073987 *	2.4398900 *	1.3326678 *
14 C	5.7327492	4.3058925	3.8286504	2.5073970 *
15 C	6.7137025	5.2980276	4.5852266	3.1477567
16 C	8.0446790	6.6239442	5.9815595	4.5485729
17 C	8.5319771	7.1157453	6.6864526	5.3116464
18 C	7.8175886	6.4423870	6.2263199	4.9876389
19 C	6.4379615	5.0675741	4.8916859	3.7447494
20 O	6.5889538	5.2618267	4.2854380	2.9343076 *
21 N	5.3920708	4.5702290	3.1601349	2.9097905 *
22 H	4.0832746	4.8949377	4.6936949	6.0045795
23 H	5.9314777	6.2564507	5.4856998	6.4073911

24 H	6.2675151	6.0069100	4.8012103	5.1776979
25 H	2.1794301 *	3.4518801	3.9634206	5.4111169
26 H	1.1039425 *	2.1958382 *	3.4728001	4.6594743
27 H	2.1817372 *	1.1045436 *	2.1880193 *	2.6804484 *
28 H	3.9621929	2.6397666 *	2.6471967 *	2.0948841 *
29 H	8.8452382	7.4434389	6.6953558	5.2633531
30 H	9.6222397	8.2099259	7.7870765	6.4041904
31 H	8.4662840	7.1455782	7.0725672	5.9207140
32 H	6.0638251	4.7932925	4.8680414	3.9758624
33 H	7.4589847	6.1621793	5.1835353	3.8843756
34 H	5.5661566	4.7062923	3.3522174	3.0362070
35 H	6.3065869	5.5590903	4.1552077	3.8945389

C C C C

1 CO	2.8611642 *	3.2679250	3.0127286	4.2818274
2 C	6.2283278	7.5570023	8.0506492	9.4445109
3 C	6.5859066	7.7830068	8.0685001	9.4181537
4 C	5.7670336	6.8178097	6.9575834	8.2615531
5 C	4.3607058	5.4267813	5.6523094	6.9926026
6 C	3.7317927	5.0302553	5.5607637	6.9628213
7 C	4.9260351	6.3056251	6.9328549	8.3375740
8 C	5.1404366	6.5740056	7.4027556	8.7868980
9 C	4.3265328	5.7327492	6.7137025	8.0446790
10 C	2.9073987 *	4.3058925	5.2980276	6.6239442
11 C	2.4398900 *	3.8286504	4.5852266	5.9815595
12 N	1.3326678 *	2.5073970 *	3.1477567	4.5485729
13 C	0.0000000	1.4663522 *	2.6045417 *	3.8828299
14 C	1.4663522 *	0.0000000	1.4375085 *	2.4997965 *
15 C	2.6045417 *	1.4375085 *	0.0000000	1.4059531 *
16 C	3.8828299	2.4997965 *	1.4059531 *	0.0000000
17 C	4.3457424	2.8838255 *	2.4423651 *	1.4281741 *
18 C	3.7952421	2.4989892 *	2.8251600 *	2.4710943 *
19 C	2.4715640 *	1.4432666 *	2.4451273 *	2.8434735 *
20 O	3.0465789	2.5038892 *	1.4666876 *	2.4600533 *
21 N	4.0057872	4.7427604	4.7203220	5.9569243
22 H	7.1218586	8.4919856	9.0509110	10.4500148
23 H	7.6749146	8.8459518	9.0712193	10.3981961
24 H	6.4226245	7.3234881	7.2879046	8.5073652
25 H	6.2247215	7.6598855	8.5003765	9.8809237
26 H	4.9814547	6.3204634	7.3912003	8.6604224
27 H	2.6252924 *	3.8589150	4.9785242	6.1982789
28 H	1.1084457 *	2.1789660 *	3.5342284	4.6768059
29 H	4.7925947	3.5010360	2.1922069 *	1.1065992 *
30 H	5.4514938	3.9896394	3.4412494	2.1925093 *
31 H	4.6595682	3.4946502	3.9293465	3.4732387

32 H	2.6447513 *	2.1986028 *	3.4505286	3.9494309
33 H	4.0160666	3.3329907	2.0499598 *	2.5152021 *
34 H	3.9009295	4.6232525	4.7496718	5.9479115
35 H	4.9666316	5.5618751	5.3357494	6.4598029

C C C O

1 CO	5.4453293	5.6174638	4.7046219	1.9497772 *
2 C	10.3474145	10.0119957	8.6950892	7.2878982
3 C	10.4425226	10.2680051	9.0283121	7.1285715
4 C	9.3424773	9.2813547	8.1230013	5.9497230
5 C	8.0136777	7.8962804	6.7203685	4.7659207
6 C	7.8231317	7.4944936	6.2003105	4.9395851
7 C	9.1438786	8.7190631	7.3756068	6.3410643
8 C	9.4292388	8.8324383	7.4499864	7.0321343
9 C	8.5319771	7.8175886	6.4379615	6.5889538
10 C	7.1157453	6.4423870	5.0675741	5.2618267
11 C	6.6864526	6.2263199	4.8916859	4.2854380
12 N	5.3116464	4.9876389	3.7447494	2.9343076 *
13 C	4.3457424	3.7952421	2.4715640 *	3.0465789
14 C	2.8838255 *	2.4989892 *	1.4432666 *	2.5038892 *
15 C	2.4423651 *	2.8251600 *	2.4451273 *	1.4666876 *
16 C	1.4281741 *	2.4710943 *	2.8434735 *	2.4600533 *
17 C	0.0000000	1.4230677 *	2.4560668 *	3.7720962
18 C	1.4230677 *	0.0000000	1.4163756 *	4.2916279
19 C	2.4560668 *	1.4163756 *	0.0000000	3.7959957
20 O	3.7720962	4.2916279	3.7959957	0.0000000
21 N	7.0443926	7.0958782	6.0750701	3.7665488
22 H	11.3133281	10.9159077	9.5718814	8.3268489
23 H	11.4618961	11.3301453	10.1072540	8.0647825
24 H	9.6607477	9.7296951	8.6622227	6.1720229
25 H	10.5086902	9.8811022	8.4942203	8.1140615
26 H	9.0157330	8.1919330	6.8384463	7.4061482
27 H	6.5157806	5.7302865	4.3870763	5.2125765
28 H	4.8605155	4.0049667	2.5888426 *	4.1416670
29 H	2.2002885 *	3.4723767	3.9500406	2.6836217 *
30 H	1.1059613 *	2.2022423 *	3.4625186	4.6509224
31 H	2.1973455 *	1.1042063 *	2.1881766 *	5.3957898
32 H	3.4568671	2.1854287 *	1.1059610 *	4.6940814
33 H	3.9351623	4.7342541	4.4899063	0.9919569 *
34 H	6.9047391	6.8553120	5.8271173	4.0464335
35 H	7.6336234	7.8295683	6.9095878	4.2287412

N H H H

1 CO	1.9788063 *	6.4625321	6.1331434	4.3369117
------	-------------	-----------	-----------	-----------

2 C	4.3440550	1.1051025 *	2.1869123 *	3.4381956
3 C	3.8163958	2.1785080 *	1.1044482 *	2.1925453 *
4 C	2.4766309 *	3.4511772	2.2008676 *	1.1075858 *
5 C	1.5113699 *	3.9448532	3.4663651	2.1839370 *
6 C	2.5960112 *	3.5212429	4.0260217	3.5073486
7 C	3.8899169	2.1985010 *	3.4867197	3.9530946
8 C	5.1141434	2.6840858 *	4.6720499	5.3968721
9 C	5.3920708	4.0832746	5.9314777	6.2675151
10 C	4.5702290	4.8949377	6.2564507	6.0069100
11 C	3.1601349	4.6936949	5.4856998	4.8012103
12 N	2.9097905 *	6.0045795	6.4073911	5.1776979
13 C	4.0057872	7.1218586	7.6749146	6.4226245
14 C	4.7427604	8.4919856	8.8459518	7.3234881
15 C	4.7203220	9.0509110	9.0712193	7.2879046
16 C	5.9569243	10.4500148	10.3981961	8.5073652
17 C	7.0443926	11.3133281	11.4618961	9.6607477
18 C	7.0958782	10.9159077	11.3301453	9.7296951
19 C	6.0750701	9.5718814	10.1072540	8.6622227
20 O	3.7665488	8.3268489	8.0647825	6.1720229
21 N	0.0000000	5.4473858	4.6753581	2.6574987 *
22 H	5.4473858	0.0000000	2.5294192 *	4.3577180
23 H	4.6753581	2.5294192 *	0.0000000	2.5149252 *
24 H	2.6574987 *	4.3577180	2.5149252 *	0.0000000
25 H	6.0606196	2.4084167 *	4.7869473	5.9797286
26 H	6.4751480	4.7826095	6.8524381	7.3484143
27 H	5.2626026	5.9690126	7.3431052	6.9623401
28 H	4.7457473	7.1685388	8.0183723	7.0175367
29 H	6.2727916	10.9790539	10.7203545	8.7055328
30 H	8.0190630	12.4011494	12.4907194	10.6200109
31 H	8.1041890	11.7482012	12.2767590	10.7360652
32 H	6.4693007	9.4431382	10.2096210	8.9704518
33 H	4.3745407	9.0163820	8.5872634	6.6012753
34 H	1.0442318 *	5.8320893	5.1613856	3.2175188
35 H	1.0400133 *	5.8247220	4.5882467	2.2181270 *

H H H H

1 CO	6.5172865	6.2828145	4.5102619	3.8733854
2 C	2.6863629 *	4.6700073	5.3907736	6.3785677
3 C	4.0851926	5.9299119	6.2635988	6.9191025
4 C	4.8952121	6.2531260	6.0041639	6.2645245
5 C	4.6762526	5.4705375	4.8017786	4.8888837
6 C	3.5196689	4.0177010	3.5046106	4.0271415
7 C	2.1999359 *	3.4846466	3.9498129	5.0027604
8 C	1.1054585 *	2.1853048 *	3.4310511	4.9525049
9 C	2.1794301 *	1.1039425 *	2.1817372 *	3.9621929

10 C	3.4518801	2.1958382 *	1.1045436 *	2.6397666 *
11 C	3.9634206	3.4728001	2.1880193 *	2.6471967 *
12 N	5.4111169	4.6594743	2.6804484 *	2.0948841 *
13 C	6.2247215	4.9814547	2.6252924 *	1.1084457 *
14 C	7.6598855	6.3204634	3.8589150	2.1789660 *
15 C	8.5003765	7.3912003	4.9785242	3.5342284
16 C	9.8809237	8.6604224	6.1982789	4.6768059
17 C	10.5086902	9.0157330	6.5157806	4.8605155
18 C	9.8811022	8.1919330	5.7302865	4.0049667
19 C	8.4942203	6.8384463	4.3870763	2.5888426 *
20 O	8.1140615	7.4061482	5.2125765	4.1416670
21 N	6.0606196	6.4751480	5.2626026	4.7457473
22 H	2.4084167 *	4.7826095	5.9690126	7.1685388
23 H	4.7869473	6.8524381	7.3431052	8.0183723
24 H	5.9797286	7.3484143	6.9623401	7.0175367
25 H	0.0000000	2.5267829 *	4.3473805	5.9771698
26 H	2.5267829 *	0.0000000	2.5002599 *	4.4487777
27 H	4.3473805	2.5002599 *	0.0000000	2.1517265 *
28 H	5.9771698	4.4487777	2.1517265 *	0.0000000
29 H	10.5848917	9.5113086	7.0936873	5.6724362
30 H	11.6077015	10.0825849	7.5841104	5.9418146
31 H	10.5757455	8.7330738	6.3467522	4.6640379
32 H	8.1621388	6.3363900	4.0195822	2.2748920 *
33 H	8.9192100	8.2741739	6.1081319	5.1022723
34 H	6.3243008	6.6165660	5.3441852	4.5206721
35 H	6.7673360	7.4022361	6.2737364	5.7541816

H H H H

1 CO	4.6124348	6.4234137	6.6843436	5.2907441
2 C	9.9482945	11.4271580	10.8813686	8.6433574
3 C	9.7965533	11.4861406	11.2038853	9.1164354
4 C	8.5783784	10.3538953	10.2584506	8.3364508
5 C	7.4019216	9.0476694	8.8642356	6.9355853
6 C	7.5388256	8.9069571	8.3880634	6.2389680
7 C	8.9367188	10.2378316	9.5531674	7.2735981
8 C	9.4938510	10.5297934	9.5594237	7.1720601
9 C	8.8452382	9.6222397	8.4662840	6.0638251
10 C	7.4434389	8.2099259	7.1455782	4.7932925
11 C	6.6953558	7.7870765	7.0725672	4.8680414
12 N	5.2633531	6.4041904	5.9207140	3.9758624
13 C	4.7925947	5.4514938	4.6595682	2.6447513 *
14 C	3.5010360	3.9896394	3.4946502	2.1986028 *
15 C	2.1922069 *	3.4412494	3.9293465	3.4505286
16 C	1.1065992 *	2.1925093 *	3.4732387	3.9494309
17 C	2.2002885 *	1.1059613 *	2.1973455 *	3.4568671

18 C	3.4723767	2.2022423 *	1.1042063 *	2.1854287 *
19 C	3.9500406	3.4625186	2.1881766 *	1.1059610 *
20 O	2.6836217 *	4.6509224	5.3957898	4.6940814
21 N	6.2727916	8.0190630	8.1041890	6.4693007
22 H	10.9790539	12.4011494	11.7482012	9.4431382
23 H	10.7203545	12.4907194	12.2767590	10.2096210
24 H	8.7055328	10.6200109	10.7360652	8.9704518
25 H	10.5848917	11.6077015	10.5757455	8.1621388
26 H	9.5113086	10.0825849	8.7330738	6.3363900
27 H	7.0936873	7.5841104	6.3467522	4.0195822
28 H	5.6724362	5.9418146	4.6640379	2.2748920 *
29 H	0.0000000	2.5209471 *	4.3861268	5.0559980
30 H	2.5209471 *	0.0000000	2.5423819 *	4.3754832
31 H	4.3861268	2.5423819 *	0.0000000	2.5140963 *
32 H	5.0559980	4.3754832	2.5140963 *	0.0000000
33 H	2.3121497 *	4.6369733	5.8197860	5.4692039
34 H	6.3505436	7.8758080	7.8046629	6.1480281
35 H	6.6185415	8.5437626	8.8598839	7.3808931

H H H

1 CO	2.6501745 *	2.5118866 *	2.6173196 *
2 C	7.9741238	4.7593921	4.7422717
3 C	7.7135556	4.3102820	3.9217110
4 C	6.4993075	3.0518838	2.4897517 *
5 C	5.4319991	2.1088409 *	2.0913137 *
6 C	5.7354482	2.9639688 *	3.4274650
7 C	7.1150219	4.2386755	4.5679315
8 C	7.8561379	5.3715219	5.8938402
9 C	7.4589847	5.5661566	6.3065869
10 C	6.1621793	4.7062923	5.5590903
11 C	5.1835353	3.3522174	4.1552077
12 N	3.8843756	3.0362070	3.8945389
13 C	4.0160666	3.9009295	4.9666316
14 C	3.3329907	4.6232525	5.5618751
15 C	2.0499598 *	4.7496718	5.3357494
16 C	2.5152021 *	5.9479115	6.4598029
17 C	3.9351623	6.9047391	7.6336234
18 C	4.7342541	6.8553120	7.8295683
19 C	4.4899063	5.8271173	6.9095878
20 O	0.9919569 *	4.0464335	4.2287412
21 N	4.3745407	1.0442318 *	1.0400133 *
22 H	9.0163820	5.8320893	5.8247220
23 H	8.5872634	5.1613856	4.5882467
24 H	6.6012753	3.2175188	2.2181270 *
25 H	8.9192100	6.3243008	6.7673360

26 H	8.2741739	6.6165660	7.4022361
27 H	6.1081319	5.3441852	6.2737364
28 H	5.1022723	4.5206721	5.7541816
29 H	2.3121497 *	6.3505436	6.6185415
30 H	4.6369733	7.8758080	8.5437626
31 H	5.8197860	7.8046629	8.8598839
32 H	5.4692039	6.1480281	7.3808931
33 H	0.0000000	4.7344338	4.6462836
34 H	4.7344338	0.0000000	1.6640401 *
35 H	4.6462836	1.6640401 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 6579.8 SECONDS (109.7 MIN)
WALL CLOCK TIME: STEP = 0.77 , TOTAL = 6081.5 SECONDS (101.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.93 , TOTAL = 6580.8 SECONDS (109.7 MIN)
WALL CLOCK TIME: STEP = 0.93 , TOTAL = 6082.5 SECONDS (101.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.635479912	-284.635479912	0.042041848	0.003058612	197941238
11343069					
2 1	-284.636634893	-0.001154981	0.007824716	0.000277628	166500900
14091000					
3 2	-284.636641029	-0.000006136	0.005991791	0.000537714	152636836
15226468					
4 3	-284.636647676	-0.000006648	0.002551988	0.000369877	147160295
15650168					
5 4	-284.636648712	-0.000001036	0.002603975	0.000272351	143947227
15943708					
6 5	-284.636650416	-0.000001704	0.001321977	0.000081871	139625715
16209369					

7 6	-284.636650945	-0.000000529	0.000422882	0.000076753	137020956
16450685					
8 7	-284.636651198	-0.000000253	0.000486400	0.000063170	131481057
16835565					
9 8	-284.636651498	-0.000000300	0.000707475	0.000058649	151753584
15331535					
10 9	-284.636651812	-0.000000314	0.001236383	0.000048479	171828599
13694204					

-----DISABLING FDIFF OPTION-----

11 10	-284.636652388	-0.000000576	0.002309451	0.000048498	197941830
11342776					
12 11	-284.636652913	-0.000000524	0.000888296	0.000083037	197942262
11342761					
13 12	-284.636653113	-0.000000201	0.000496858	0.000074457	197942496
11342738					
14 13	-284.636653294	-0.000000181	0.000856038	0.000043649	197942391
11342735					
15 14	-284.636653405	-0.000000111	0.000224081	0.000021152	197942493
11342725					
16 15	-284.636653443	-0.000000038	0.000122017	0.000019132	197942411
11342734					
17 16	-284.636653457	-0.000000014	0.000139851	0.000014993	197942411
11342736					
18 17	-284.636653472	-0.000000014	0.000313469	0.000013430	197942569
11342733					
19 18	-284.636653496	-0.000000024	0.000385961	0.000011261	197942649
11342730					
20 19	-284.636653511	-0.000000015	0.000190556	0.000015701	197942852
11342722					
21 20	-284.636653519	-0.000000008	0.000102108	0.000016542	197942886
11342723					
22 21	-284.636653527	-0.000000008	0.000268678	0.000011915	197942787
11342728					
23 22	-284.636653537	-0.000000010	0.000120289	0.000006394	197942657
11342730					
24 23	-284.636653540	-0.000000003	0.000070072	0.000005792	197942684
11342728					
25 24	-284.636653542	-0.000000002	0.000070075	0.000004308	197942646
11342725					
26 25	-284.636653544	-0.000000002	0.000042596	0.000002780	197942667
11342726					
27 26	-284.636653545	-0.000000001	0.000031015	0.000001282	197942641
11342726					
28 27	-284.636653545	0.000000000	0.000016372	0.000001092	197942644
11342727					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 95.1 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 30.5 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 3.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6366535449 AFTER 28 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6000730225
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998889453

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 99.59 , TOTAL = 6680.3 SECONDS (111.3 MIN)
WALL CLOCK TIME: STEP = 91.46 , TOTAL = 6173.9 SECONDS (102.9
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.77 , TOTAL = 6684.1 SECONDS (111.4 MIN)
WALL CLOCK TIME: STEP = 3.83 , TOTAL = 6177.8 SECONDS (103.0
MIN)
CPU UTILIZATION: STEP = 98.47% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.85 , TOTAL = 6687.0 SECONDS (111.4 MIN)
WALL CLOCK TIME: STEP = 2.68 , TOTAL = 6180.4 SECONDS (103.0
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 68 ENERGY= -284.6366535

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0004906	0.0000515	0.0000234
2 C	6.0	0.0002800	-0.0002817	-0.0001474
3 C	6.0	0.0000026	0.0005503	-0.0000860
4 C	6.0	-0.0002407	-0.0000705	-0.0000236
5 C	6.0	0.0000537	-0.0001335	-0.0000130
6 C	6.0	0.0001524	0.0002942	0.0001402
7 C	6.0	-0.0002398	-0.0000476	0.0001790
8 C	6.0	-0.0000381	-0.0002834	0.0001336
9 C	6.0	-0.0002229	-0.0000801	0.0002625
10 C	6.0	-0.0001646	-0.0002543	0.0002628
11 C	6.0	0.0000023	-0.0002063	0.0000043
12 N	7.0	0.0000292	0.0001436	-0.0000736
13 C	6.0	0.0002378	0.0001152	-0.0003094
14 C	6.0	0.0001569	-0.0000358	0.0001676
15 C	6.0	-0.0001641	0.0003131	0.0000265
16 C	6.0	0.0000376	0.0008976	-0.0001392
17 C	6.0	0.0001240	0.0000557	0.0000934
18 C	6.0	-0.0001929	0.0000754	0.0005106
19 C	6.0	-0.0000132	0.0001408	0.0003716
20 O	8.0	0.0000575	0.0000336	0.0000696
21 N	7.0	-0.0002982	0.0000100	-0.0002730
22 H	1.0	0.0001674	-0.0001004	-0.0002692
23 H	1.0	0.0001584	-0.0001306	0.0000017
24 H	1.0	0.0002165	-0.0000011	0.0008502
25 H	1.0	-0.0000133	0.0005650	-0.0001770
26 H	1.0	-0.0002324	-0.0001926	-0.0003088
27 H	1.0	-0.0003345	-0.0001086	0.0003407
28 H	1.0	0.0005011	-0.0000278	-0.0006573
29 H	1.0	0.0001463	0.0001184	-0.0001631
30 H	1.0	-0.0004557	-0.0004657	-0.0005233
31 H	1.0	-0.0000883	0.0000018	0.0002265
32 H	1.0	-0.0001692	0.0000457	0.0000075
33 H	1.0	0.0006514	-0.0003567	0.0001829
34 H	1.0	0.0005553	-0.0002762	-0.0003800
35 H	1.0	-0.0001718	-0.0003589	-0.0003107

MAXIMUM GRADIENT = 0.0008976 RMS GRADIENT = 0.0002748
HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0001134887
PREDICTED ENERGY CHANGE WAS -0.0000508404 RATIO= 2.232
GDIIS STEP HAS LENGTH = 0.107297
RADIUS OF STEP TAKEN= 0.10730 CURRENT TRUST RADIUS= 0.23806

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 6687.0 SECONDS (111.4 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6180.5 SECONDS (103.0 MIN)
CPU UTILIZATION: STEP = 89.88% , TOTAL = 100.00%

INSERCH= 69

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1516475506	-1.7421568782	0.8478834100
C	6.0	4.9808889191	0.6403751897	0.5424554243
C	6.0	5.1909892746	-0.7064470770	0.2174234636
C	6.0	4.0596207054	-1.5412675533	-0.0559817529
C	6.0	2.7486840395	-1.0329651687	0.0095974339
C	6.0	2.4704164263	0.3373494029	0.4234138586
C	6.0	3.6473710487	1.1817043829	0.6618859420
C	6.0	3.4916775227	2.5692822968	1.0320397182
C	6.0	2.2204120668	3.1325792292	1.2103434051
C	6.0	1.0616454389	2.3127335073	1.0444859870
C	6.0	1.1618592167	0.9629270089	0.6334303723
N	7.0	-0.0503362776	0.1653047053	0.5761278489
C	6.0	-1.2427835799	0.6982061912	0.3123904443
C	6.0	-2.5508237673	0.0482979449	0.4437303588
C	6.0	-2.8235925580	-1.2822002547	0.9160275006
C	6.0	-4.1241580407	-1.8039182240	1.0306812670
C	6.0	-5.2351120193	-0.9792613615	0.6750595545
C	6.0	-5.0206335671	0.3509847902	0.2165721272
C	6.0	-3.7001303263	0.8503407776	0.1002098709
O	8.0	-1.7026130587	-2.1496775211	1.2928816753
N	7.0	1.6482956254	-1.9732639672	-0.4250716596
H	1.0	5.8396451651	1.3123701590	0.7223913825
H	1.0	6.2108024730	-1.1249646263	0.1503047599
H	1.0	4.2311623414	-2.5953621217	-0.3506276495
H	1.0	4.3998829709	3.1795025893	1.1888104023
H	1.0	2.1037419660	4.1883892105	1.5117535340
H	1.0	0.0751806776	2.7417731697	1.2935116945
H	1.0	-1.2768473072	1.7460959945	-0.0478202538
H	1.0	-4.2962517786	-2.8378369834	1.3856983413

H	1.0	-6.2590333118	-1.3897903414	0.7521352538
H	1.0	-5.8786746884	0.9916870448	-0.0529924792
H	1.0	-3.5363062789	1.8829906981	-0.2606328410
H	1.0	-2.0161129756	-2.9691560863	1.7557464311
H	1.0	1.3137882489	-1.7113798051	-1.3793836409
H	1.0	2.0416948578	-2.9321413230	-0.5115941847

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3936368	5.1831592	4.0161652
2 C	5.3936368	0.0000000	1.4013273 *	2.4426271 *
3 C	5.1831592	1.4013273 *	0.0000000	1.4323653 *
4 C	4.0161652	2.4426271 *	1.4323653 *	0.0000000
5 C	2.8196232 *	2.8402014 *	2.4727840 *	1.4075606 *
6 C	3.1434392	2.5314951 *	2.9212086 *	2.5069089 *
7 C	4.5611010	1.4441506 *	2.4789958 *	2.8460253 *
8 C	5.4569425	2.4855836 *	3.7791088	4.2898683
9 C	5.3079390	3.7785431	4.9546283	5.1798756
10 C	4.1603948	4.2906044	5.1817916	5.0052182
11 C	2.8955132 *	3.8337063	4.3810684	3.8914395
12 N	1.9372811 *	5.0537167	5.3254214	4.4948524
13 C	2.8612170 *	6.2281918	6.5860081	5.7677060
14 C	3.2668669	7.5555938	7.7818072	6.8172140
15 C	3.0113547	8.0464765	8.0655478	6.9563311
16 C	4.2801569	9.4400643	9.4147650	8.2597855
17 C	5.4432579	10.3444421	10.4397053	9.3403602
18 C	5.6153618	10.0110139	10.2662264	9.2793277
19 C	4.7027920	8.6948124	9.0271444	8.1214483
20 O	1.9499690 *	7.2812590	7.1246949	5.9491960
21 N	1.9783277 *	4.3443522	3.8168447	2.4773649 *
22 H	6.4574918	1.1051771 *	2.1797638 *	3.4521877
23 H	6.1303263	2.1869829 *	1.1043916 *	2.2007829 *
24 H	4.3366841	3.4394307	2.1936157 *	1.1078619 *
25 H	6.5104890	2.6837494 *	4.0828968	4.8939715
26 H	6.2787557	4.6696806	5.9300766	6.2539765
27 H	4.5066684	5.3894278	6.2625623	6.0034434
28 H	3.8743762	6.3820300	6.9222996	6.2677521
29 H	4.6123279	9.9435586	9.7936424	8.5778866
30 H	6.4210715	11.4237205	11.4828521	10.3513583
31 H	6.6820855	10.8815486	11.2024214	10.2560023
32 H	5.2888096	8.6447474	9.1158880	8.3345986
33 H	2.6512126 *	7.9661049	7.7089956	6.4989049
34 H	2.5124165 *	4.7614960	4.3118871	3.0528555

35 H 2.6146742 * 4.7447610 3.9246958 2.4928171 *

C C C C

1 CO 2.8196232 * 3.1434392 4.5611010 5.4569425
2 C 2.8402014 * 2.5314951 * 1.4441506 * 2.4855836 *
3 C 2.4727840 * 2.9212086 * 2.4789958 * 3.7791088
4 C 1.4075606 * 2.5069089 * 2.8460253 * 4.2898683
5 C 0.0000000 1.4582314 * 2.4774745 * 3.8175404
6 C 1.4582314 * 0.0000000 1.4680008 * 2.5288187 *
7 C 2.4774745 * 1.4680008 * 0.0000000 1.4445161 *
8 C 3.8175404 2.5288187 * 1.4445161 * 0.0000000
9 C 4.3672213 2.9146303 * 2.4784935 * 1.4018600 *
10 C 3.8872604 2.5044977 * 2.8480847 * 2.4435687 *
11 C 2.6250269 * 1.4655293 * 2.4952840 * 2.8578524 *
12 N 3.0969860 2.5312280 * 3.8358131 4.3049768
13 C 4.3612443 3.7323449 4.9264115 5.1413950
14 C 5.4260837 5.0295941 6.3047459 6.5736818
15 C 5.6510176 5.5580698 6.9288371 7.3979736
16 C 6.9909183 6.9600440 8.3334637 8.7821316
17 C 8.0116617 7.8212504 9.1415782 9.4274309
18 C 7.8943304 7.4939175 8.7190999 8.8343235
19 C 6.7187989 6.2002636 7.3763852 7.4528630
20 O 4.7652818 4.9351243 6.3339238 7.0226259
21 N 1.5112755 * 2.5951386 * 3.8899363 5.1142895
22 H 3.9449605 3.5201925 2.1969980 * 2.6811681 *
23 H 3.4661977 4.0253495 3.4862039 4.6710339
24 H 2.1837097 * 3.5071589 3.9537612 5.3974215
25 H 4.6756696 3.5194471 2.1988909 * 1.1053429 *
26 H 5.4712855 4.0186367 3.4849992 2.1858631 *
27 H 4.8004901 3.5036379 3.9488365 3.4308266
28 H 4.8919710 4.0309570 5.0070098 4.9580805
29 H 7.4015091 7.5362855 8.9320636 9.4875632
30 H 9.0453114 8.9047382 10.2351149 10.5275336
31 H 8.8619666 8.3882324 9.5547216 9.5639742
32 H 6.9337527 6.2400036 7.2765420 7.1787572
33 H 5.4314972 5.7303608 7.1064214 7.8443487
34 H 2.1091327 * 2.9639769 * 4.2405573 5.3742192
35 H 2.0924494 * 3.4274789 4.5693520 5.8949909

C C C N

1 CO 5.3079390 4.1603948 2.8955132 * 1.9372811 *
2 C 3.7785431 4.2906044 3.8337063 5.0537167
3 C 4.9546283 5.1817916 4.3810684 5.3254214
4 C 5.1798756 5.0052182 3.8914395 4.4948524

5 C	4.3672213	3.8872604	2.6250269 *	3.0969860
6 C	2.9146303 *	2.5044977 *	1.4655293 *	2.5312280 *
7 C	2.4784935 *	2.8480847 *	2.4952840 *	3.8358131
8 C	1.4018600 *	2.4435687 *	2.8578524 *	4.3049768
9 C	0.0000000	1.4291241 *	2.4820865 *	3.7898873
10 C	1.4291241 *	0.0000000	1.4145625 *	2.4631917 *
11 C	2.4820865 *	1.4145625 *	0.0000000	1.4522062 *
12 N	3.7898873	2.4631917 *	1.4522062 *	0.0000000
13 C	4.3273798	2.9074139 *	2.4403792 *	1.3324684 *
14 C	5.7328159	4.3056369	3.8283870	2.5067224 *
15 C	6.7096112	5.2948205	4.5830430	3.1467051
16 C	8.0408243	6.6211457	5.9795668	4.5475797
17 C	8.5310375	7.1149744	6.6854371	5.3105290
18 C	7.8203319	6.4442236	6.2266734	4.9867437
19 C	6.4415705	5.0699860	4.8924372	3.7438976
20 O	6.5802109	5.2550868	4.2811662	2.9330696 *
21 N	5.3918025	4.5687561	3.1588391	2.9088188 *
22 H	4.0804542	4.8922135	4.6916635	6.0024190
23 H	5.9307316	6.2554893	5.4849366	6.4068696
24 H	6.2680985	6.0067947	4.8010846	5.1779714
25 H	2.1800823 *	3.4519484	3.9631367	5.4097338
26 H	1.1041715 *	2.1959937 *	3.4730680	4.6583964
27 H	2.1821237 *	1.1041746 *	2.1865204 *	2.6774211 *
28 H	3.9668797	2.6424911 *	2.6504237 *	2.0958391 *
29 H	8.8398827	7.4398834	6.6934811	5.2632749
30 H	9.6209550	8.2089274	7.7858215	6.4029070
31 H	8.4719917	7.1496620	7.0739749	5.9201545
32 H	6.0716595	4.7988722	4.8701771	3.9752485
33 H	7.4482738	6.1544168	5.1788395	3.8833777
34 H	5.5670991	4.7044881	3.3505850	3.0342719
35 H	6.3069679	5.5579308	4.1541244	3.8928017

C C C C

1 CO	2.8612170 *	3.2668669	3.0113547	4.2801569
2 C	6.2281918	7.5555938	8.0464765	9.4400643
3 C	6.5860081	7.7818072	8.0655478	9.4147650
4 C	5.7677060	6.8172140	6.9563311	8.2597855
5 C	4.3612443	5.4260837	5.6510176	6.9909183
6 C	3.7323449	5.0295941	5.5580698	6.9600440
7 C	4.9264115	6.3047459	6.9288371	8.3334637
8 C	5.1413950	6.5736818	7.3979736	8.7821316
9 C	4.3273798	5.7328159	6.7096112	8.0408243
10 C	2.9074139 *	4.3056369	5.2948205	6.6211457
11 C	2.4403792 *	3.8283870	4.5830430	5.9795668
12 N	1.3324684 *	2.5067224 *	3.1467051	4.5475797

13 C	0.0000000	1.4664924 *	2.6048694 *	3.8831543
14 C	1.4664924 *	0.0000000	1.4379474 *	2.5001194 *
15 C	2.6048694 *	1.4379474 *	0.0000000	1.4059892 *
16 C	3.8831543	2.5001194 *	1.4059892 *	0.0000000
17 C	4.3455854	2.8835386 *	2.4423889 *	1.4285463 *
18 C	3.7949828	2.4986358 *	2.8255124 *	2.4718513 *
19 C	2.4711776 *	1.4429777 *	2.4457326 *	2.8444098 *
20 O	3.0468423	2.5043194 *	1.4666734 *	2.4601176 *
21 N	4.0048648	4.7406891	4.7195233	5.9555953
22 H	7.1208212	8.4897291	9.0454949	10.4443128
23 H	7.6750354	8.8447011	9.0681502	10.3945875
24 H	6.4227151	7.3222455	7.2868633	8.5056320
25 H	6.2261248	7.6597592	8.4946925	9.8751589
26 H	4.9818754	6.3202857	7.3865326	8.6559758
27 H	2.6221737 *	3.8565317	4.9737051	6.1940968
28 H	1.1085960 *	2.1787970 *	3.5344026	4.6768520
29 H	4.7936687	3.5019420	2.1930165 *	1.1066352 *
30 H	5.4512261	3.9892392	3.4410303	2.1924375 *
31 H	4.6595195	3.4944682	3.9297697	3.4739151
32 H	2.6442988 *	2.1984997 *	3.4512207	3.9504885
33 H	4.0163243	3.3335163	2.0501149 *	2.5154230 *
34 H	3.8992645	4.6211943	4.7508975	5.9488012
35 H	4.9644911	5.5575976	5.3321132	6.4551718

C C C O

1 CO	5.4432579	5.6153618	4.7027920	1.9499690 *
2 C	10.3444421	10.0110139	8.6948124	7.2812590
3 C	10.4397053	10.2662264	9.0271444	7.1246949
4 C	9.3403602	9.2793277	8.1214483	5.9491960
5 C	8.0116617	7.8943304	6.7187989	4.7652818
6 C	7.8212504	7.4939175	6.2002636	4.9351243
7 C	9.1415782	8.7190999	7.3763852	6.3339238
8 C	9.4274309	8.8343235	7.4528630	7.0226259
9 C	8.5310375	7.8203319	6.4415705	6.5802109
10 C	7.1149744	6.4442236	5.0699860	5.2550868
11 C	6.6854371	6.2266734	4.8924372	4.2811662
12 N	5.3105290	4.9867437	3.7438976	2.9330696 *
13 C	4.3455854	3.7949828	2.4711776 *	3.0468423
14 C	2.8835386 *	2.4986358 *	1.4429777 *	2.5043194 *
15 C	2.4423889 *	2.8255124 *	2.4457326 *	1.4666734 *
16 C	1.4285463 *	2.4718513 *	2.8444098 *	2.4601176 *
17 C	0.0000000	1.4232943 *	2.4564334 *	3.7722841
18 C	1.4232943 *	0.0000000	1.4165541 *	4.2919709
19 C	2.4564334 *	1.4165541 *	0.0000000	3.7963997
20 O	3.7722841	4.2919709	3.7963997	0.0000000

21 N	7.0412805	7.0914354	6.0707763	3.7697579
22 H	11.3094678	10.9144752	9.5712015	8.3184670
23 H	11.4588636	11.3281937	10.1059849	8.0608724
24 H	9.6578552	9.7261710	8.6591874	6.1732850
25 H	10.5067781	9.8839209	8.4982505	8.1025582
26 H	9.0146241	8.1951141	6.8425110	7.3964406
27 H	6.5136618	5.7308804	4.3879903	5.2045020
28 H	4.8598341	4.0040198	2.5877772 *	4.1419572
29 H	2.2001749 *	3.4727755	3.9510121	2.6849842 *
30 H	1.1058434 *	2.2024441 *	3.4628281	4.6508925
31 H	2.1974691 *	1.1042640 *	2.1884938 *	5.3962060
32 H	3.4574482	2.1858623 *	1.1060794 *	4.6944916
33 H	3.9356727	4.7349273	4.4905759	0.9920036 *
34 H	6.9025234	6.8502060	5.8215968	4.0536137
35 H	7.6271755	7.8221241	6.9029002	4.2294473

N H H H

1 CO	1.9783277 *	6.4574918	6.1303263	4.3366841
2 C	4.3443522	1.1051771 *	2.1869829 *	3.4394307
3 C	3.8168447	2.1797638 *	1.1043916 *	2.1936157 *
4 C	2.4773649 *	3.4521877	2.2007829 *	1.1078619 *
5 C	1.5112755 *	3.9449605	3.4661977	2.1837097 *
6 C	2.5951386 *	3.5201925	4.0253495	3.5071589
7 C	3.8899363	2.1969980 *	3.4862039	3.9537612
8 C	5.1142895	2.6811681 *	4.6710339	5.3974215
9 C	5.3918025	4.0804542	5.9307316	6.2680985
10 C	4.5687561	4.8922135	6.2554893	6.0067947
11 C	3.1588391	4.6916635	5.4849366	4.8010846
12 N	2.9088188 *	6.0024190	6.4068696	5.1779714
13 C	4.0048648	7.1208212	7.6750354	6.4227151
14 C	4.7406891	8.4897291	8.8447011	7.3222455
15 C	4.7195233	9.0454949	9.0681502	7.2868633
16 C	5.9555953	10.4443128	10.3945875	8.5056320
17 C	7.0412805	11.3094678	11.4588636	9.6578552
18 C	7.0914354	10.9144752	11.3281937	9.7261710
19 C	6.0707763	9.5712015	10.1059849	8.6591874
20 O	3.7697579	8.3184670	8.0608724	6.1732850
21 N	0.0000000	5.4478871	4.6762312	2.6577713 *
22 H	5.4478871	0.0000000	2.5309369 *	4.3599264
23 H	4.6762312	2.5309369 *	0.0000000	2.5163420 *
24 H	2.6577713 *	4.3599264	2.5163420 *	0.0000000
25 H	6.0602683	2.4034653 *	4.7839692	5.9789128
26 H	6.4749280	4.7803296	6.8522418	7.3493988
27 H	5.2592580	5.9664413	7.3419642	6.9613498
28 H	4.7468325	7.1711791	8.0216670	7.0198377

29 H	6.2740751	10.9727208	10.7171973	8.7057690
30 H	8.0157413	12.3967970	12.4871589	10.6166706
31 H	8.0984356	11.7483223	12.2750561	10.7314637
32 H	6.4635777	9.4445969	10.2089566	8.9664548
33 H	4.3790021	9.0062326	8.5825767	6.6034069
34 H	1.0446003 *	5.8347153	5.1637755	3.2172714
35 H	1.0400456 *	5.8277804	4.5918903	2.2210579 *

H H H H

1 CO	6.5104890	6.2787557	4.5066684	3.8743762
2 C	2.6837494 *	4.6696806	5.3894278	6.3820300
3 C	4.0828968	5.9300766	6.2625623	6.9222996
4 C	4.8939715	6.2539765	6.0034434	6.2677521
5 C	4.6756696	5.4712855	4.8004901	4.8919710
6 C	3.5194471	4.0186367	3.5036379	4.0309570
7 C	2.1988909 *	3.4849992	3.9488365	5.0070098
8 C	1.1053429 *	2.1858631 *	3.4308266	4.9580805
9 C	2.1800823 *	1.1041715 *	2.1821237 *	3.9668797
10 C	3.4519484	2.1959937 *	1.1041746 *	2.6424911 *
11 C	3.9631367	3.4730680	2.1865204 *	2.6504237 *
12 N	5.4097338	4.6583964	2.6774211 *	2.0958391 *
13 C	6.2261248	4.9818754	2.6221737 *	1.1085960 *
14 C	7.6597592	6.3202857	3.8565317	2.1787970 *
15 C	8.4946925	7.3865326	4.9737051	3.5344026
16 C	9.8751589	8.6559758	6.1940968	4.6768520
17 C	10.5067781	9.0146241	6.5136618	4.8598341
18 C	9.8839209	8.1951141	5.7308804	4.0040198
19 C	8.4982505	6.8425110	4.3879903	2.5877772 *
20 O	8.1025582	7.3964406	5.2045020	4.1419572
21 N	6.0602683	6.4749280	5.2592580	4.7468325
22 H	2.4034653 *	4.7803296	5.9664413	7.1711791
23 H	4.7839692	6.8522418	7.3419642	8.0216670
24 H	5.9789128	7.3493988	6.9613498	7.0198377
25 H	0.0000000	2.5287167 *	4.3480593	5.9840769
26 H	2.5287167 *	0.0000000	2.5010774 *	4.4525779
27 H	4.3480593	2.5010774 *	0.0000000	2.1490752 *
28 H	5.9840769	4.4525779	2.1490752 *	0.0000000
29 H	10.5768568	9.5049284	7.0887213	5.6731138
30 H	11.6052410	10.0811268	7.5818977	5.9410344
31 H	10.5819355	8.7399262	6.3501393	4.6632580
32 H	8.1709809	6.3455780	4.0243895	2.2735840 *
33 H	8.9046294	8.2621542	6.0993346	5.1022513
34 H	6.3277430	6.6173994	5.3393904	4.5209062
35 H	6.7679109	7.4026847	6.2704777	5.7544516

	H	H	H	H
1 CO	4.6123279	6.4210715	6.6820855	5.2888096
2 C	9.9435586	11.4237205	10.8815486	8.6447474
3 C	9.7936424	11.4828521	11.2024214	9.1158880
4 C	8.5778866	10.3513583	10.2560023	8.3345986
5 C	7.4015091	9.0453114	8.8619666	6.9337527
6 C	7.5362855	8.9047382	8.3882324	6.2400036
7 C	8.9320636	10.2351149	9.5547216	7.2765420
8 C	9.4875632	10.5275336	9.5639742	7.1787572
9 C	8.8398827	9.6209550	8.4719917	6.0716595
10 C	7.4398834	8.2089274	7.1496620	4.7988722
11 C	6.6934811	7.7858215	7.0739749	4.8701771
12 N	5.2632749	6.4029070	5.9201545	3.9752485
13 C	4.7936687	5.4512261	4.6595195	2.6442988 *
14 C	3.5019420	3.9892392	3.4944682	2.1984997 *
15 C	2.1930165 *	3.4410303	3.9297697	3.4512207
16 C	1.1066352 *	2.1924375 *	3.4739151	3.9504885
17 C	2.2001749 *	1.1058434 *	2.1974691 *	3.4574482
18 C	3.4727755	2.2024441 *	1.1042640 *	2.1858623 *
19 C	3.9510121	3.4628281	2.1884938 *	1.1060794 *
20 O	2.6849842 *	4.6508925	5.3962060	4.6944916
21 N	6.2740751	8.0157413	8.0984356	6.4635777
22 H	10.9727208	12.3967970	11.7483223	9.4445969
23 H	10.7171973	12.4871589	12.2750561	10.2089566
24 H	8.7057690	10.6166706	10.7314637	8.9664548
25 H	10.5768568	11.6052410	10.5819355	8.1709809
26 H	9.5049284	10.0811268	8.7399262	6.3455780
27 H	7.0887213	7.5818977	6.3501393	4.0243895
28 H	5.6731138	5.9410344	4.6632580	2.2735840 *
29 H	0.0000000	2.5200700 *	4.3862453	5.0570879
30 H	2.5200700 *	0.0000000	2.5425062 *	4.3760756
31 H	4.3862453	2.5425062 *	0.0000000	2.5148015 *
32 H	5.0570879	4.3760756	2.5148015 *	0.0000000
33 H	2.3137012 *	4.6372410	5.8205840	5.4699270
34 H	6.3550872	7.8736535	7.7972692	6.1395863
35 H	6.6165081	8.5368581	8.8509321	7.3730980

	H	H	H
1 CO	2.6512126 *	2.5124165 *	2.6146742 *
2 C	7.9661049	4.7614960	4.7447610
3 C	7.7089956	4.3118871	3.9246958
4 C	6.4989049	3.0528555	2.4928171 *
5 C	5.4314972	2.1091327 *	2.0924494 *
6 C	5.7303608	2.9639769 *	3.4274789

7 C	7.1064214	4.2405573	4.5693520
8 C	7.8443487	5.3742192	5.8949909
9 C	7.4482738	5.5670991	6.3069679
10 C	6.1544168	4.7044881	5.5579308
11 C	5.1788395	3.3505850	4.1541244
12 N	3.8833777	3.0342719	3.8928017
13 C	4.0163243	3.8992645	4.9644911
14 C	3.3335163	4.6211943	5.5575976
15 C	2.0501149 *	4.7508975	5.3321132
16 C	2.5154230 *	5.9488012	6.4551718
17 C	3.9356727	6.9025234	7.6271755
18 C	4.7349273	6.8502060	7.8221241
19 C	4.4905759	5.8215968	6.9029002
20 O	0.9920036 *	4.0536137	4.2294473
21 N	4.3790021	1.0446003 *	1.0400456 *
22 H	9.0062326	5.8347153	5.8277804
23 H	8.5825767	5.1637755	4.5918903
24 H	6.6034069	3.2172714	2.2210579 *
25 H	8.9046294	6.3277430	6.7679109
26 H	8.2621542	6.6173994	7.4026847
27 H	6.0993346	5.3393904	6.2704777
28 H	5.1022513	4.5209062	5.7544516
29 H	2.3137012 *	6.3550872	6.6165081
30 H	4.6372410	7.8736535	8.5368581
31 H	5.8205840	7.7972692	8.8509321
32 H	5.4699270	6.1395863	7.3730980
33 H	0.0000000	4.7433410	4.6484415
34 H	4.7433410	0.0000000	1.6652823 *
35 H	4.6484415	1.6652823 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 6687.8 SECONDS (111.5 MIN)
WALL CLOCK TIME: STEP = 0.77 , TOTAL = 6181.2 SECONDS (103.0 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.92 , TOTAL = 6688.7 SECONDS (111.5 MIN)
WALL CLOCK TIME: STEP = 0.92 , TOTAL = 6182.1 SECONDS (103.0 MIN)

CPU UTILIZATION: STEP = 99.69% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

		NONZERO BLOCKS				
ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD	
INTEGRALS SKIPPED						
-----START SECOND ORDER SCF-----						
1	0	-284.636459710	-284.636459710	0.017238511	0.001478866	198015145
11337964						
2	1	-284.636683987	-0.000224277	0.002354049	0.000138190	159504921
14649575						
3	2	-284.636685505	-0.000001518	0.002592656	0.000127854	144053982
15912476						
4	3	-284.636686733	-0.000001229	0.000863802	0.000066825	138366057
16316026						
5	4	-284.636686987	-0.000000253	0.000602387	0.000066565	133369327
16751098						
6	5	-284.636687106	-0.000000119	0.000294656	0.000051421	128204086
17104243						
7	6	-284.636687258	-0.000000153	0.000212089	0.000029507	125143893
17382597						
8	7	-284.636687251	0.000000008	0.000190175	0.000028519	122990523
17515494						
9	8	-284.636687321	-0.000000071	0.000349902	0.000021519	142674952
16077502						
10	9	-284.636687377	-0.000000055	0.000408864	0.000021272	165965740
14188363						
-----DISABLING FDIFF OPTION-----						
11	10	-284.636687456	-0.000000079	0.000761698	0.000020811	198013139
11337953						
12	11	-284.636687536	-0.000000080	0.000521856	0.000036382	198012976
11337946						
13	12	-284.636687583	-0.000000047	0.000292133	0.000035380	198012930
11337953						
14	13	-284.636687624	-0.000000041	0.000374834	0.000021922	198013065
11337946						
15	14	-284.636687644	-0.000000020	0.000091818	0.000011596	198013131
11337944						
16	15	-284.636687653	-0.000000009	0.000063353	0.000010171	198013096
11337947						
17	16	-284.636687656	-0.000000003	0.000094237	0.000007736	198013077
11337947						
18	17	-284.636687661	-0.000000005	0.000184092	0.000005781	198013085
11337945						
19	18	-284.636687666	-0.000000005	0.000093081	0.000004951	198013121
11337945						

20	19	-284.636687667	-0.000000001	0.000039866	0.000005987	198013104
11337945						
21	20	-284.636687668	-0.000000001	0.000058976	0.000005268	198013110
11337943						
22	21	-284.636687670	-0.000000002	0.000088393	0.000002826	198013119
11337945						
23	22	-284.636687672	-0.000000002	0.000072177	0.000003546	198013095
11337944						
24	23	-284.636687673	-0.000000001	0.000036414	0.000003259	198013080
11337946						
25	24	-284.636687673	-0.000000001	0.000044462	0.000002198	198013080
11337946						
26	25	-284.636687674	0.000000000	0.000016858	0.000001773	198013101
11337947						
27	26	-284.636687674	0.000000000	0.000009061	0.000000890	198013044
11337948						

 DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 90.6 SECONDS (3.4 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 29.3 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.1
 TIME TO SOLVE SCF EQUATIONS= 3.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6366876737 AFTER 27 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6001566782
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998801542

 SPIN SZ = 1.500
 S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
 PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 95.21 , TOTAL = 6783.9 SECONDS (113.1 MIN)
 WALL CLOCK TIME: STEP = 87.13 , TOTAL = 6269.3 SECONDS (104.5
 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
 END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 4.08 , TOTAL = 6788.0 SECONDS (113.1 MIN)
 WALL CLOCK TIME: STEP = 4.05 , TOTAL = 6273.3 SECONDS (104.6 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
 USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.89 , TOTAL = 6790.9 SECONDS (113.2 MIN)
 WALL CLOCK TIME: STEP = 2.70 , TOTAL = 6276.0 SECONDS (104.6 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 69 ENERGY= -284.6366877

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0003198	0.0000995	-0.0001516
2 C	6.0	0.0000121	-0.0000023	-0.0002256
3 C	6.0	-0.0000953	0.0004319	-0.0002094
4 C	6.0	-0.0000461	0.0000420	-0.0000238
5 C	6.0	0.0000295	-0.0001075	-0.0000402
6 C	6.0	0.0000842	0.0000730	0.0000822
7 C	6.0	0.0001065	0.0000922	0.0001695
8 C	6.0	0.0000024	-0.0002693	0.0002611
9 C	6.0	-0.0000960	-0.0002355	0.0002479
10 C	6.0	-0.0003583	-0.0003042	0.0002502
11 C	6.0	-0.0000694	-0.0002758	0.0000083
12 N	7.0	0.0001724	0.0002627	-0.0000643
13 C	6.0	0.0004127	0.0001305	-0.0003623
14 C	6.0	-0.0000147	0.0001817	0.0000863
15 C	6.0	-0.0000615	0.0001098	-0.0000258
16 C	6.0	0.0002573	0.0005752	-0.0001116
17 C	6.0	-0.0001497	-0.0000120	0.0001169
18 C	6.0	-0.0001986	0.0002843	0.0006253
19 C	6.0	0.0002324	0.0002242	0.0004721
20 O	8.0	-0.0000279	0.0001127	0.0003559
21 N	7.0	-0.0001893	0.0000248	-0.0000274

22 H	1.0	0.0000653	0.0001131	-0.0002266
23 H	1.0	0.0001114	-0.0001415	0.0001438
24 H	1.0	0.0001200	-0.0002038	0.0007471
25 H	1.0	0.0000225	0.0003620	-0.0000687
26 H	1.0	-0.0002921	-0.0000194	-0.0003412
27 H	1.0	-0.0002133	-0.0003396	0.0001980
28 H	1.0	0.0003456	0.0000954	-0.0005972
29 H	1.0	0.0000377	0.0001102	-0.0001388
30 H	1.0	-0.0003637	-0.0004653	-0.0004906
31 H	1.0	-0.0001148	-0.0000311	0.0000812
32 H	1.0	-0.0001266	0.0000924	-0.0001057
33 H	1.0	0.0006162	-0.0004296	0.0001301
34 H	1.0	0.0004416	-0.0000880	-0.0006317
35 H	1.0	-0.0003328	-0.0004928	-0.0001336

MAXIMUM GRADIENT = 0.0007471 RMS GRADIENT = 0.0002596
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000341288
 PREDICTED ENERGY CHANGE WAS -0.0000225281 RATIO= 1.515
 GDIIS STEP HAS LENGTH = 0.052780
 RADIUS OF STEP TAKEN= 0.05278 CURRENT TRUST RADIUS= 0.10730

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 6790.9 SECONDS (113.2 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6276.1 SECONDS (104.6 MIN)
 CPU UTILIZATION: STEP = 91.25% , TOTAL = 100.00%

INSERCH= 70

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1525656246	-1.7399744840	0.8485387980
C	6.0	4.9793181672	0.6399819181	0.5427545436
C	6.0	5.1902724839	-0.7067071304	0.2163411234
C	6.0	4.0595870785	-1.5409150358	-0.0600075326
C	6.0	2.7485833205	-1.0322932830	0.0077101266
C	6.0	2.4701925068	0.3372474028	0.4216970807
C	6.0	3.6463235671	1.1811688570	0.6613275114
C	6.0	3.4919423979	2.5677459124	1.0350925613
C	6.0	2.2218869820	3.1331271944	1.2102942096
C	6.0	1.0638410071	2.3139093161	1.0403019959
C	6.0	1.1626267913	0.9638793998	0.6311485651
N	7.0	-0.0505799920	0.1670687282	0.5743341862

C	6.0	-1.2439286712	0.6993720517	0.3143609076
C	6.0	-2.5504594606	0.0474042500	0.4432654312
C	6.0	-2.8221040062	-1.2831591899	0.9158293472
C	6.0	-4.1227334270	-1.8057014841	1.0312662978
C	6.0	-5.2328325368	-0.9801327485	0.6759091806
C	6.0	-5.0190647514	0.3489668275	0.2140919492
C	6.0	-3.6991215540	0.8486327128	0.0974699774
O	8.0	-1.7006133468	-2.1471875769	1.2956014594
N	7.0	1.6476074967	-1.9720028565	-0.4243690814
H	1.0	5.8362769855	1.3138041577	0.7261102429
H	1.0	6.2097938325	-1.1245666326	0.1518688141
H	1.0	4.2286526480	-2.5942887055	-0.3602447475
H	1.0	4.4022594323	3.1723802534	1.1982240554
H	1.0	2.1050577550	4.1884155305	1.5135868073
H	1.0	0.0763063240	2.7424547750	1.2862440395
H	1.0	-1.2824683995	1.7489445325	-0.0400938967
H	1.0	-4.2964114292	-2.8385020713	1.3885285155
H	1.0	-6.2564956433	-1.3884851792	0.7572220149
H	1.0	-5.8773878781	0.9878859799	-0.0583267527
H	1.0	-3.5344287542	1.8799156458	-0.2656366057
H	1.0	-2.0168429449	-2.9652295106	1.7574447202
H	1.0	1.3099343741	-1.7100815576	-1.3774738068
H	1.0	2.0384410201	-2.9319729998	-0.5075250385

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3902910	5.1812938	4.0162044
2 C	5.3902910	0.0000000	1.4016486 *	2.4424453 *
3 C	5.1812938	1.4016486 *	0.0000000	1.4320338 *
4 C	4.0162044	2.4424453 *	1.4320338 *	0.0000000
5 C	2.8190625 *	2.8388298 *	2.4721204 *	1.4078397 *
6 C	3.1414072	2.5302203 *	2.9207614 *	2.5071315 *
7 C	4.5579020	1.4435434 *	2.4790859 *	2.8461995 *
8 C	5.4536863	2.4841412 *	3.7784549	4.2898204
9 C	5.3066070	3.7768783	4.9541480	5.1804902
10 C	4.1594675	4.2872541	5.1798139	5.0044826
11 C	2.8945307 *	3.8314300	4.3800519	3.8915384
12 N	1.9373358 *	5.0521797	5.3252397	4.4958949
13 C	2.8611106 *	6.2277197	6.5867755	5.7694295
14 C	3.2657792	7.5537142	7.7806883	6.8167996
15 C	3.0102936	8.0436214	8.0634830	6.9553122
16 C	4.2797069	9.4375502	9.4129682	8.2590168
17 C	5.4414772	10.3407216	10.4368138	9.3383678

18	C	5.6135514	10.0080153	10.2637722	9.2773220
19	C	4.7011154	8.6923604	9.0252168	8.1198705
20	O	1.9493486 *	7.2771270	7.1220850	5.9485419
21	N	1.9771904 *	4.3425901	3.8160134	2.4771438 *
22	H	6.4533036	1.1054565 *	2.1816627 *	3.4531189
23	H	6.1281392	2.1864340 *	1.1037151 *	2.2003697 *
24	H	4.3365304	3.4408448	2.1954790 *	1.1082967 *
25	H	6.5048756	2.6787457 *	4.0782812	4.8903705
26	H	6.2769676	4.6685404	5.9298923	6.2547272
27	H	4.5043949	5.3863433	6.2605160	6.0021809
28	H	3.8757640	6.3858814	6.9276517	6.2738449
29	H	4.6142983	9.9425522	9.7936584	8.5793181
30	H	6.4193419	11.4194653	11.4798029	10.3495247
31	H	6.6801173	10.8788971	11.2000087	10.2536973
32	H	5.2857279	8.6414593	9.1128114	8.3314730
33	H	2.6521111 *	7.9636230	7.7083355	6.5003697
34	H	2.5090891 *	4.7617699	4.3132389	3.0536740
35	H	2.6108036 *	4.7445450	3.9255359	2.4940621 *

C C C C

1	CO	2.8190625 *	3.1414072	4.5579020	5.4536863
2	C	2.8388298 *	2.5302203 *	1.4435434 *	2.4841412 *
3	C	2.4721204 *	2.9207614 *	2.4790859 *	3.7784549
4	C	1.4078397 *	2.5071315 *	2.8461995 *	4.2898204
5	C	0.0000000	1.4575762 *	2.4764022 *	3.8168547
6	C	1.4575762 *	0.0000000	1.4672799 *	2.5289030 *
7	C	2.4764022 *	1.4672799 *	0.0000000	1.4443441 *
8	C	3.8168547	2.5289030 *	1.4443441 *	0.0000000
9	C	4.3674186	2.9155591 *	2.4780083 *	1.4012110 *
10	C	3.8860873	2.5035353 *	2.8453363 *	2.4413391 *
11	C	2.6246217 *	1.4650139 *	2.4933662 *	2.8567936 *
12	N	3.0975551	2.5311169 *	3.8344573	4.3040695
13	C	4.3626656	3.7332762	4.9261629	5.1418625
14	C	5.4254317	5.0290576	6.3034192	6.5736597
15	C	5.6497939	5.5568234	6.9266326	7.3966801
16	C	6.9900516	6.9592009	8.3316562	8.7812496
17	C	8.0095075	7.8189967	9.1384271	9.4253994
18	C	7.8922005	7.4921433	8.7167388	8.8337005
19	C	6.7170557	6.1989575	7.3745562	7.4529113
20	O	4.7641373	4.9327221	6.3300864	7.0186251
21	N	1.5105940 *	2.5932819 *	3.8879422	5.1128190
22	H	3.9438717	3.5180755	2.1949225 *	2.6765173 *
23	H	3.4654400	4.0242174	3.4853040	4.6690441
24	H	2.1830771 *	3.5067819	3.9543390	5.3978060
25	H	4.6723921	3.5176491	2.1965017 *	1.1049306 *

26 H	5.4715254	4.0195824	3.4850221	2.1860869 *
27 H	4.7983785	3.5018788	3.9462840	3.4293104
28 H	4.8976471	4.0359142	5.0107236	4.9620016
29 H	7.4027698	7.5370469	8.9316076	9.4874069
30 H	9.0432344	8.9020119	10.2312338	10.5243062
31 H	8.8596199	8.3866472	9.5528184	9.5643020
32 H	6.9305065	6.2376061	7.2739751	7.1787811
33 H	5.4320439	5.7292288	7.1039107	7.8410666
34 H	2.1089908 *	2.9622239 *	4.2396644	5.3741458
35 H	2.0924991 *	3.4260276	4.5683081	5.8940006

C C C N

1 CO	5.3066070	4.1594675	2.8945307 *	1.9373358 *
2 C	3.7768783	4.2872541	3.8314300	5.0521797
3 C	4.9541480	5.1798139	4.3800519	5.3252397
4 C	5.1804902	5.0044826	3.8915384	4.4958949
5 C	4.3674186	3.8860873	2.6246217 *	3.0975551
6 C	2.9155591 *	2.5035353 *	1.4650139 *	2.5311169 *
7 C	2.4780083 *	2.8453363 *	2.4933662 *	3.8344573
8 C	1.4012110 *	2.4413391 *	2.8567936 *	4.3040695
9 C	0.0000000	1.4286657 *	2.4825547 *	3.7902578
10 C	1.4286657 *	0.0000000	1.4141237 *	2.4633280 *
11 C	2.4825547 *	1.4141237 *	0.0000000	1.4525859 *
12 N	3.7902578	2.4633280 *	1.4525859 *	0.0000000
13 C	4.3287110	2.9085257 *	2.4416854 *	1.3322965 *
14 C	5.7345715	4.3077449	3.8291300	2.5061716 *
15 C	6.7105991	5.2966937	4.5834818	3.1466054
16 C	8.0422813	6.6235813	5.9804436	4.5478614
17 C	8.5309623	7.1155880	6.6845409	5.3086844
18 C	7.8214672	6.4455694	6.2261837	4.9848473
19 C	6.4432628	5.0716644	4.8923094	3.7421631
20 O	6.5783744	5.2544049	4.2799976	2.9323402 *
21 N	5.3911292	4.5667371	3.1573293	2.9080709 *
22 H	4.0753142	4.8862124	4.6876936	5.9994269
23 H	5.9288803	6.2524604	5.4831753	6.4061751
24 H	6.2687314	6.0056616	4.8004099	5.1778726
25 H	2.1807592 *	3.4506448	3.9615995	5.4082266
26 H	1.1042051 *	2.1958835 *	3.4733999	4.6583473
27 H	2.1821800 *	1.1042479 *	2.1846218 *	2.6749821 *
28 H	3.9698789	2.6441650 *	2.6543143 *	2.0969983 *
29 H	8.8419646	7.4431788	6.6957320	5.2653065
30 H	9.6194192	8.2082390	7.7841436	6.4005144
31 H	8.4740611	7.1516419	7.0737373	5.9182507
32 H	6.0732266	4.7997824	4.8688476	3.9719765
33 H	7.4468893	6.1542030	5.1783653	3.8829413

34 H	5.5664057	4.7009259	3.3475858	3.0305523
35 H	6.3063457	5.5556183	4.1522637	3.8908210

	C	C	C	C
--	---	---	---	---

1 CO	2.8611106 *	3.2657792	3.0102936	4.2797069
2 C	6.2277197	7.5537142	8.0436214	9.4375502
3 C	6.5867755	7.7806883	8.0634830	9.4129682
4 C	5.7694295	6.8167996	6.9553122	8.2590168
5 C	4.3626656	5.4254317	5.6497939	6.9900516
6 C	3.7332762	5.0290576	5.5568234	6.9592009
7 C	4.9261629	6.3034192	6.9266326	8.3316562
8 C	5.1418625	6.5736597	7.3966801	8.7812496
9 C	4.3287110	5.7345715	6.7105991	8.0422813
10 C	2.9085257 *	4.3077449	5.2966937	6.6235813
11 C	2.4416854 *	3.8291300	4.5834818	5.9804436
12 N	1.3322965 *	2.5061716 *	3.1466054	4.5478614
13 C	0.0000000	1.4658448 *	2.6043870 *	3.8828937
14 C	1.4658448 *	0.0000000	1.4378826 *	2.5003582 *
15 C	2.6043870 *	1.4378826 *	0.0000000	1.4064185 *
16 C	3.8828937	2.5003582 *	1.4064185 *	0.0000000
17 C	4.3431334	2.8818537 *	2.4415157 *	1.4283426 *
18 C	3.7926890	2.4974933 *	2.8254039 *	2.4726058 *
19 C	2.4692696 *	1.4425554 *	2.4461007 *	2.8455074 *
20 O	3.0453728	2.5029879 *	1.4657808 *	2.4603153 *
21 N	4.0053648	4.7386244	4.7168801	5.9534330
22 H	7.1187342	8.4865257	9.0414475	10.4406094
23 H	7.6753590	8.8431027	9.0655373	10.3922281
24 H	6.4228063	7.3198724	7.2842704	8.5031654
25 H	6.2270718	7.6600090	8.4925265	9.8734328
26 H	4.9826978	6.3219778	7.3873112	8.6572198
27 H	2.6194970 *	3.8566577	4.9742896	6.1953752
28 H	1.1084791 *	2.1763908 *	3.5324099	4.6744440
29 H	4.7945845	3.5029025	2.1945656 *	1.1065611 *
30 H	5.4480365	3.9868598	3.4396651	2.1913719 *
31 H	4.6573684	3.4935016	3.9295529	3.4742130
32 H	2.6413010 *	2.1974612 *	3.4508420	3.9511812
33 H	4.0136258	3.3298312	2.0460016 *	2.5112975 *
34 H	3.8974335	4.6158952	4.7450230	5.9434882
35 H	4.9634780	5.5532602	5.3262954	6.4495300

	C	C	C	O
--	---	---	---	---

1 CO	5.4414772	5.6135514	4.7011154	1.9493486 *
2 C	10.3407216	10.0080153	8.6923604	7.2771270
3 C	10.4368138	10.2637722	9.0252168	7.1220850

4 C	9.3383678	9.2773220	8.1198705	5.9485419
5 C	8.0095075	7.8922005	6.7170557	4.7641373
6 C	7.8189967	7.4921433	6.1989575	4.9327221
7 C	9.1384271	8.7167388	7.3745562	6.3300864
8 C	9.4253994	8.8337005	7.4529113	7.0186251
9 C	8.5309623	7.8214672	6.4432628	6.5783744
10 C	7.1155880	6.4455694	5.0716644	5.2544049
11 C	6.6845409	6.2261837	4.8923094	4.2799976
12 N	5.3086844	4.9848473	3.7421631	2.9323402 *
13 C	4.3431334	3.7926890	2.4692696 *	3.0453728
14 C	2.8818537 *	2.4974933 *	1.4425554 *	2.5029879 *
15 C	2.4415157 *	2.8254039 *	2.4461007 *	1.4657808 *
16 C	1.4283426 *	2.4726058 *	2.8455074 *	2.4603153 *
17 C	0.0000000	1.4231927 *	2.4558592 *	3.7712873
18 C	1.4231927 *	0.0000000	1.4161627 *	4.2909870
19 C	2.4558592 *	1.4161627 *	0.0000000	3.7953252
20 O	3.7712873	4.2909870	3.7953252	0.0000000
21 N	7.0381016	7.0879512	6.0676035	3.7682318
22 H	11.3044174	10.9101566	9.5674134	8.3130921
23 H	11.4555304	11.3253008	10.1036171	8.0578173
24 H	9.6539534	9.7217742	8.6552189	6.1723514
25 H	10.5048167	9.8844084	8.4996374	8.0964400
26 H	9.0144456	8.1965343	6.8445623	7.3939514
27 H	6.5128428	5.7307156	4.3878926	5.2025122
28 H	4.8544722	3.9983372	2.5825758 *	4.1399001
29 H	2.1996016 *	3.4729652	3.9520312	2.6878837 *
30 H	1.1051016 *	2.2011281 *	3.4612326	4.6498973
31 H	2.1971918 *	1.1041505 *	2.1882660 *	5.3951138
32 H	3.4570162	2.1858838 *	1.1056738 *	4.6923239
33 H	3.9310199	4.7306628	4.4867719	0.9912078 *
34 H	6.8961588	6.8431712	5.8149049	4.0496655
35 H	7.6211296	7.8162449	6.8977259	4.2246516

N H H H

1 CO	1.9771904 *	6.4533036	6.1281392	4.3365304
2 C	4.3425901	1.1054565 *	2.1864340 *	3.4408448
3 C	3.8160134	2.1816627 *	1.1037151 *	2.1954790 *
4 C	2.4771438 *	3.4531189	2.2003697 *	1.1082967 *
5 C	1.5105940 *	3.9438717	3.4654400	2.1830771 *
6 C	2.5932819 *	3.5180755	4.0242174	3.5067819
7 C	3.8879422	2.1949225 *	3.4853040	3.9543390
8 C	5.1128190	2.6765173 *	4.6690441	5.3978060
9 C	5.3911292	4.0753142	5.9288803	6.2687314
10 C	4.5667371	4.8862124	6.2524604	6.0056616
11 C	3.1573293	4.6876936	5.4831753	4.8004099

12 N	2.9080709 *	5.9994269	6.4061751	5.1778726
13 C	4.0053648	7.1187342	7.6753590	6.4228063
14 C	4.7386244	8.4865257	8.8431027	7.3198724
15 C	4.7168801	9.0414475	9.0655373	7.2842704
16 C	5.9534330	10.4406094	10.3922281	8.5031654
17 C	7.0381016	11.3044174	11.4555304	9.6539534
18 C	7.0879512	10.9101566	11.3253008	9.7217742
19 C	6.0676035	9.5674134	10.1036171	8.6552189
20 O	3.7682318	8.3130921	8.0578173	6.1723514
21 N	0.0000000	5.4465661	4.6758681	2.6557759 *
22 H	5.4465661	0.0000000	2.5327693 *	4.3632342
23 H	4.6758681	2.5327693 *	0.0000000	2.5193776 *
24 H	2.6557759 *	4.3632342	2.5193776 *	0.0000000
25 H	6.0568633	2.3944943 *	4.7776346	5.9760719
26 H	6.4742327	4.7755112	6.8506141	7.3502365
27 H	5.2555966	5.9608770	7.3389598	6.9594351
28 H	4.7516799	7.1730713	8.0266998	7.0241460
29 H	6.2744545	10.9704977	10.7166810	8.7060074
30 H	8.0132077	12.3910647	12.4837686	10.6132478
31 H	8.0944725	11.7444246	12.2721881	10.7263780
32 H	6.4587903	9.4400302	10.2054445	8.9606299
33 H	4.3789277	9.0025148	8.5815772	6.6051814
34 H	1.0445260 *	5.8358143	5.1662694	3.2148863
35 H	1.0398117 *	5.8285537	4.5936589	2.2209793 *

H H H H

1 CO	6.5048756	6.2769676	4.5043949	3.8757640
2 C	2.6787457 *	4.6685404	5.3863433	6.3858814
3 C	4.0782812	5.9298923	6.2605160	6.9276517
4 C	4.8903705	6.2547272	6.0021809	6.2738449
5 C	4.6723921	5.4715254	4.7983785	4.8976471
6 C	3.5176491	4.0195824	3.5018788	4.0359142
7 C	2.1965017 *	3.4850221	3.9462840	5.0107236
8 C	1.1049306 *	2.1860869 *	3.4293104	4.9620016
9 C	2.1807592 *	1.1042051 *	2.1821800 *	3.9698789
10 C	3.4506448	2.1958835 *	1.1042479 *	2.6441650 *
11 C	3.9615995	3.4733999	2.1846218 *	2.6543143 *
12 N	5.4082266	4.6583473	2.6749821 *	2.0969983 *
13 C	6.2270718	4.9826978	2.6194970 *	1.1084791 *
14 C	7.6600090	6.3219778	3.8566577	2.1763908 *
15 C	8.4925265	7.3873112	4.9742896	3.5324099
16 C	9.8734328	8.6572198	6.1953752	4.6744440
17 C	10.5048167	9.0144456	6.5128428	4.8544722
18 C	9.8844084	8.1965343	5.7307156	3.9983372
19 C	8.4996374	6.8445623	4.3878926	2.5825758 *

20	O	8.0964400	7.3939514	5.2025122	4.1399001
21	N	6.0568633	6.4742327	5.2555966	4.7516799
22	H	2.3944943 *	4.7755112	5.9608770	7.1730713
23	H	4.7776346	6.8506141	7.3389598	8.0266998
24	H	5.9760719	7.3502365	6.9594351	7.0241460
25	H	0.0000000	2.5315839 *	4.3481552	5.9896353
26	H	2.5315839 *	0.0000000	2.5016634 *	4.4542425
27	H	4.3481552	2.5016634 *	0.0000000	2.1430128 *
28	H	5.9896353	4.4542425	2.1430128 *	0.0000000
29	H	10.5751500	9.5064198	7.0907124	5.6718146
30	H	11.6019410	10.0791609	7.5795059	5.9346546
31	H	10.5840486	8.7426392	6.3508155	4.6575560
32	H	8.1733942	6.3481191	4.0236445	2.2670131 *
33	H	8.8987559	8.2597923	6.0976195	5.0984201
34	H	6.3273318	6.6168513	5.3331333	4.5248203
35	H	6.7646394	7.4019770	6.2663156	5.7582914

H H H H

1	CO	4.6142983	6.4193419	6.6801173	5.2857279
2	C	9.9425522	11.4194653	10.8788971	8.6414593
3	C	9.7936584	11.4798029	11.2000087	9.1128114
4	C	8.5793181	10.3495247	10.2536973	8.3314730
5	C	7.4027698	9.0432344	8.8596199	6.9305065
6	C	7.5370469	8.9020119	8.3866472	6.2376061
7	C	8.9316076	10.2312338	9.5528184	7.2739751
8	C	9.4874069	10.5243062	9.5643020	7.1787811
9	C	8.8419646	9.6194192	8.4740611	6.0732266
10	C	7.4431788	8.2082390	7.1516419	4.7997824
11	C	6.6957320	7.7841436	7.0737373	4.8688476
12	N	5.2653065	6.4005144	5.9182507	3.9719765
13	C	4.7945845	5.4480365	4.6573684	2.6413010 *
14	C	3.5029025	3.9868598	3.4935016	2.1974612 *
15	C	2.1945656 *	3.4396651	3.9295529	3.4508420
16	C	1.1065611 *	2.1913719 *	3.4742130	3.9511812
17	C	2.1996016 *	1.1051016 *	2.1971918 *	3.4570162
18	C	3.4729652	2.2011281 *	1.1041505 *	2.1858838 *
19	C	3.9520312	3.4612326	2.1882660 *	1.1056738 *
20	O	2.6878837 *	4.6498973	5.3951138	4.6923239
21	N	6.2744545	8.0132077	8.0944725	6.4587903
22	H	10.9704977	12.3910647	11.7444246	9.4400302
23	H	10.7166810	12.4837686	12.2721881	10.2054445
24	H	8.7060074	10.6132478	10.7263780	8.9606299
25	H	10.5751500	11.6019410	10.5840486	8.1733942
26	H	9.5064198	10.0791609	8.7426392	6.3481191
27	H	7.0907124	7.5795059	6.3508155	4.0236445

28 H	5.6718146	5.9346546	4.6575560	2.2670131 *
29 H	0.0000000	2.5185367 *	4.3856724	5.0577016
30 H	2.5185367 *	0.0000000	2.5408625 *	4.3747379
31 H	4.3856724	2.5408625 *	0.0000000	2.5155818 *
32 H	5.0577016	4.3747379	2.5155818 *	0.0000000
33 H	2.3127022 *	4.6326259	5.8161805	5.4654695
34 H	6.3525755	7.8683679	7.7895301	6.1312410
35 H	6.6131771	8.5315833	8.8446267	7.3667944

H H H

1 CO	2.6521111 *	2.5090891 *	2.6108036 *
2 C	7.9636230	4.7617699	4.7445450
3 C	7.7083355	4.3132389	3.9255359
4 C	6.5003697	3.0536740	2.4940621 *
5 C	5.4320439	2.1089908 *	2.0924991 *
6 C	5.7292288	2.9622239 *	3.4260276
7 C	7.1039107	4.2396644	4.5683081
8 C	7.8410666	5.3741458	5.8940006
9 C	7.4468893	5.5664057	6.3063457
10 C	6.1542030	4.7009259	5.5556183
11 C	5.1783653	3.3475858	4.1522637
12 N	3.8829413	3.0305523	3.8908210
13 C	4.0136258	3.8974335	4.9634780
14 C	3.3298312	4.6158952	5.5532602
15 C	2.0460016 *	4.7450230	5.3262954
16 C	2.5112975 *	5.9434882	6.4495300
17 C	3.9310199	6.8961588	7.6211296
18 C	4.7306628	6.8431712	7.8162449
19 C	4.4867719	5.8149049	6.8977259
20 O	0.9912078 *	4.0496655	4.2246516
21 N	4.3789277	1.0445260 *	1.0398117 *
22 H	9.0025148	5.8358143	5.8285537
23 H	8.5815772	5.1662694	4.5936589
24 H	6.6051814	3.2148863	2.2209793 *
25 H	8.8987559	6.3273318	6.7646394
26 H	8.2597923	6.6168513	7.4019770
27 H	6.0976195	5.3331333	6.2663156
28 H	5.0984201	4.5248203	5.7582914
29 H	2.3127022 *	6.3525755	6.6131771
30 H	4.6326259	7.8683679	8.5315833
31 H	5.8161805	7.7895301	8.8446267
32 H	5.4654695	6.1312410	7.3667944
33 H	0.0000000	4.7403120	4.6450535
34 H	4.7403120	0.0000000	1.6674986 *
35 H	4.6450535	1.6674986 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.68 , TOTAL = 6791.6 SECONDS (113.2 MIN)
WALL CLOCK TIME: STEP = 0.70 , TOTAL = 6276.7 SECONDS (104.6 MIN)

CPU UTILIZATION: STEP = 97.53%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.18 , TOTAL = 6792.8 SECONDS (113.2 MIN)
WALL CLOCK TIME: STEP = 1.17 , TOTAL = 6277.9 SECONDS (104.6 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636663746	-284.636663746	0.026993172	0.000668012	198071368
11333093						
2	1	-284.636730543	-0.000066797	0.003919440	0.000109235	159125380
14613778						
3	2	-284.636728488	0.000002055	0.002240398	0.000330525	144519033
15800708						
4	3	-284.636732183	-0.000003695	0.000931790	0.000126342	139230594
16246941						
5	4	-284.636731629	0.000000554	0.000675835	0.000211243	133858286
16648156						
6	5	-284.636732382	-0.000000753	0.000202886	0.000013060	129619552
16985453						
7	6	-284.636732403	-0.000000021	0.000121330	0.000018097	119527748
17658327						
8	7	-284.636732409	-0.000000006	0.000071420	0.000012283	113004612
18151001						
9	8	-284.636732391	0.000000018	0.000103677	0.000010876	107976588
18557601						
10	9	-284.636732409	-0.000000017	0.000467770	0.000011457	130383298
17069427						
11	10	-284.636732432	-0.000000023	0.000232030	0.000013841	162533658
14518302						

12 11	-284.636732442	-0.000000010	0.000189434	0.000016048	158615872
14833194					
13 12	-284.636732452	-0.000000010	0.000182623	0.000012239	158834336
14741592					
14 13	-284.636732462	-0.000000010	0.000227650	0.000005738	155109630
15094047					
-----DISABLING FDIFF OPTION-----					
15 14	-284.636732463	-0.000000001	0.000041543	0.000005324	198088241
11331472					
16 15	-284.636732465	-0.000000002	0.000024427	0.000004251	198088227
11331470					
17 16	-284.636732466	-0.000000001	0.000034093	0.000003564	198088209
11331471					
18 17	-284.636732467	-0.000000001	0.000045962	0.000002702	198088197
11331473					
19 18	-284.636732467	0.000000000	0.000042479	0.000001800	198088233
11331469					
20 19	-284.636732467	0.000000000	0.000015778	0.000001538	198088236
11331469					
21 20	-284.636732468	0.000000000	0.000033467	0.000001614	198088224
11331471					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 68.5 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 22.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 3.2 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6367324677 AFTER 21 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6037974327
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998784334

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 73.15 , TOTAL = 6865.9 SECONDS (114.4 MIN)
 WALL CLOCK TIME: STEP = 67.63 , TOTAL = 6345.6 SECONDS (105.8 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
 END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.62 , TOTAL = 6869.5 SECONDS (114.5 MIN)
 WALL CLOCK TIME: STEP = 3.60 , TOTAL = 6349.2 SECONDS (105.8 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
 USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84 , TOTAL = 6872.4 SECONDS (114.5 MIN)
 WALL CLOCK TIME: STEP = 2.69 , TOTAL = 6351.8 SECONDS (105.9 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 70 ENERGY= -284.6367325

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0002558	0.0000405	-0.0003640
2 C	6.0	-0.0003742	0.0000788	-0.0003844
3 C	6.0	-0.0000164	-0.0000135	-0.0002808
4 C	6.0	0.0004820	0.0001781	0.0001059
5 C	6.0	-0.0001497	0.0001480	0.0000640
6 C	6.0	0.0001485	-0.0000006	0.0000527
7 C	6.0	0.0000660	0.0001173	-0.0000054
8 C	6.0	-0.0004876	0.0000129	0.0003182
9 C	6.0	0.0000190	-0.0004647	0.0001158
10 C	6.0	0.0005146	-0.0003558	0.0000694
11 C	6.0	0.0003333	-0.0001400	0.0001178
12 N	7.0	0.0000290	0.0001654	-0.0000849
13 C	6.0	0.0001365	0.0000085	-0.0003111
14 C	6.0	0.0001190	0.0004231	-0.0000433
15 C	6.0	0.0003411	-0.0002487	0.0000276
16 C	6.0	-0.0001144	0.0001047	-0.0001698

17 C	6.0	-0.0001869	-0.0001056	0.0001262
18 C	6.0	-0.0000845	0.0003359	0.0007070
19 C	6.0	0.0003062	0.0003919	0.0004762
20 O	8.0	0.0001121	0.0000250	0.0006025
21 N	7.0	0.0000963	0.0000363	-0.0001036
22 H	1.0	-0.0000134	0.0004939	-0.0001073
23 H	1.0	-0.0003114	0.0000351	0.0003116
24 H	1.0	-0.0000867	-0.0004846	0.0004392
25 H	1.0	-0.0000277	-0.0000916	0.0000230
26 H	1.0	-0.0003219	0.0000172	-0.0002939
27 H	1.0	-0.0003507	-0.0005029	0.0001502
28 H	1.0	0.0000109	0.0000809	-0.0004347
29 H	1.0	-0.0000964	0.0001766	-0.0001354
30 H	1.0	0.0001007	-0.0001971	-0.0003729
31 H	1.0	-0.0000470	-0.0001070	-0.0000168
32 H	1.0	-0.0000549	-0.0001858	-0.0000707
33 H	1.0	0.0004003	0.0003218	-0.0002975
34 H	1.0	0.0002362	0.0001743	-0.0004891
35 H	1.0	-0.0004721	-0.0004681	0.0002581

MAXIMUM GRADIENT = 0.0007070 RMS GRADIENT = 0.0002646
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000447940
 PREDICTED ENERGY CHANGE WAS -0.0000292614 RATIO= 1.531
 GDIIS STEP HAS LENGTH = 0.053226
 RADIUS OF STEP TAKEN= 0.05278 CURRENT TRUST RADIUS= 0.05278

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 6872.4 SECONDS (114.5 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6351.9 SECONDS (105.9
 MIN)
 CPU UTILIZATION: STEP = 90.05% , TOTAL = 100.00%

INSERCH= 71

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1541498930	-1.7391711010	0.8480583399
C	6.0	4.9791448666	0.6391722233	0.5446248850
C	6.0	5.1895702437	-0.7070270609	0.2166060267
C	6.0	4.0584843544	-1.5410913401	-0.0638274596
C	6.0	2.7488335698	-1.0318645435	0.0046069466
C	6.0	2.4699640094	0.3379788148	0.4199077631
C	6.0	3.6454262437	1.1806719507	0.6614643812

C	6.0	3.4924737519	2.5661073700	1.0378637913
C	6.0	2.2229421189	3.1336929947	1.2118145818
C	6.0	1.0648698772	2.3150038609	1.0382690411
C	6.0	1.1623536355	0.9645384889	0.6289110525
N	7.0	-0.0507750132	0.1680853142	0.5721454126
C	6.0	-1.2448538071	0.6994383525	0.3141502143
C	6.0	-2.5503154694	0.0456820478	0.4415597687
C	6.0	-2.8216798871	-1.2827855332	0.9167713642
C	6.0	-4.1213566811	-1.8066017805	1.0339750828
C	6.0	-5.2306573958	-0.9809088996	0.6771045886
C	6.0	-5.0184236914	0.3466345130	0.2093590426
C	6.0	-3.6990655917	0.8462906295	0.0915155902
O	8.0	-1.6993963431	-2.1448306965	1.3008235778
N	7.0	1.6469435199	-1.9703031802	-0.4263072096
H	1.0	5.8345402390	1.3128902819	0.7305317981
H	1.0	6.2095081986	-1.1249531185	0.1528425432
H	1.0	4.2271497199	-2.5925706142	-0.3690050728
H	1.0	4.4041320197	3.1680357704	1.2064676901
H	1.0	2.1067697838	4.1879857766	1.5185820742
H	1.0	0.0775139083	2.7435455031	1.2828243505
H	1.0	-1.2860155544	1.7501473644	-0.0375257351
H	1.0	-4.2964511116	-2.8386197583	1.3948002588
H	1.0	-6.2549723820	-1.3871647996	0.7640104793
H	1.0	-5.8765801647	0.9842131539	-0.0636754808
H	1.0	-3.5337332598	1.8771011591	-0.2737377173
H	1.0	-2.0181430230	-2.9608154611	1.7647794698
H	1.0	1.3058747383	-1.7074312267	-1.3777573855
H	1.0	2.0377716837	-2.9299714557	-0.5096470541

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3878721	5.1787558	4.0142993
2 C	5.3878721	0.0000000	1.4014734 *	2.4436406 *
3 C	5.1787558	1.4014734 *	0.0000000	1.4330602 *
4 C	4.0142993	2.4436406 *	1.4330602 *	0.0000000
5 C	2.8185238 *	2.8387095 *	2.4713677 *	1.4068335 *
6 C	3.1402006	2.5302688 *	2.9205525 *	2.5076486 *
7 C	4.5551412	1.4441879 *	2.4790497 *	2.8468686 *
8 C	5.4512251	2.4832549 *	3.7773019	4.2898919
9 C	5.3063193	3.7768280	4.9540340	5.1817069
10 C	4.1595583	4.2864490	5.1788951	5.0045794
11 C	2.8938808 *	3.8315614	4.3797946	3.8917401
12 N	1.9379755 *	5.0520070	5.3247956	4.4957490

13	C	2.8616578 *	6.2285560	6.5870686	5.7695958
14	C	3.2657426	7.5535175	7.7796533	6.8153871
15	C	3.0114070	8.0427160	8.0623730	6.9544918
16	C	4.2800781	9.4361222	9.4111910	8.2574491
17	C	5.4406191	10.3383885	10.4339932	9.3354667
18	C	5.6137367	10.0074651	10.2622315	9.2751496
19	C	4.7015145	8.6924992	9.0242058	8.1180851
20	O	1.9506895 *	7.2749860	7.1204401	5.9481059
21	N	1.9763255 *	4.3423078	3.8156792	2.4761146 *
22	H	6.4494748	1.1046079 *	2.1817819 *	3.4540689
23	H	6.1260063	2.1861897 *	1.1040840 *	2.2015950 *
24	H	4.3357654	3.4415662	2.1964672 *	1.1077861 *
25	H	6.5016525	2.6765326 *	4.0758866	4.8896830
26	H	6.2764253	4.6683197	5.9295827	6.2558400
27	H	4.5044026	5.3851009	6.2591048	6.0016422
28	H	3.8773289	6.3894757	6.9307648	6.2766729
29	H	4.6168781	9.9425608	9.7936934	8.5799838
30	H	6.4193318	11.4175112	11.4777957	10.3477727
31	H	6.6796546	10.8782282	11.1981488	10.2509838
32	H	5.2854833	8.6412545	9.1112118	8.3288577
33	H	2.6554941 *	7.9630852	7.7089256	6.5026779
34	H	2.5063386 *	4.7639285	4.3157727	3.0546588
35	H	2.6094828 *	4.7436223	3.9246349	2.4921924 *

C C C C

1	CO	2.8185238 *	3.1402006	4.5551412	5.4512251
2	C	2.8387095 *	2.5302688 *	1.4441879 *	2.4832549 *
3	C	2.4713677 *	2.9205525 *	2.4790497 *	3.7773019
4	C	1.4068335 *	2.5076486 *	2.8468686 *	4.2898919
5	C	0.0000000	1.4583257 *	2.4760165 *	3.8165459
6	C	1.4583257 *	0.0000000	1.4663536 *	2.5282311 *
7	C	2.4760165 *	1.4663536 *	0.0000000	1.4437806 *
8	C	3.8165459	2.5282311 *	1.4437806 *	0.0000000
9	C	4.3687277	2.9161883 *	2.4780310 *	1.4014717 *
10	C	3.8866077	2.5030558 *	2.8439342 *	2.4405560 *
11	C	2.6253189 *	1.4649588 *	2.4926739 *	2.8568733 *
12	N	3.0983524	2.5310404 *	3.8334336	4.3037211
13	C	4.3638017	3.7338598	4.9261600	5.1430037
14	C	5.4252203	5.0288281	6.3026800	6.5744524
15	C	5.6502766	5.5565498	6.9251185	7.3957539
16	C	6.9899450	6.9585784	8.3297950	8.7801489
17	C	8.0079414	7.8169806	9.1355097	9.4236134
18	C	7.8912907	7.4913521	8.7156361	8.8344697
19	C	6.7164294	6.1986409	7.3741584	7.4546350
20	O	4.7650415	4.9319288	6.3273120	7.0155257

21 N	1.5101377 *	2.5926065 *	3.8866212	5.1116337
22 H	3.9428959	3.5167190	2.1941905 *	2.6740010 *
23 H	3.4650986	4.0243862	3.4855587	4.6679188
24 H	2.1819276 *	3.5068797	3.9544442	5.3973130
25 H	4.6715784	3.5169454	2.1959686 *	1.1053804 *
26 H	5.4727693	4.0201429	3.4851185	2.1867225 *
27 H	4.7982819	3.5007419	3.9444468	3.4283291
28 H	4.9011604	4.0386691	5.0131834	4.9655023
29 H	7.4049334	7.5382735	8.9311759	9.4871402
30 H	9.0427570	8.9005080	10.2284991	10.5221701
31 H	8.8581597	8.3854798	9.5515983	9.5652992
32 H	6.9289395	6.2365393	7.2732350	7.1807112
33 H	5.4353588	5.7300810	7.1024812	7.8385062
34 H	2.1093723 *	2.9614871 *	4.2394654	5.3739718
35 H	2.0911423 *	3.4249615	4.5665572	5.8921838

C C C N

1 CO	5.3063193	4.1595583	2.8938808 *	1.9379755 *
2 C	3.7768280	4.2864490	3.8315614	5.0520070
3 C	4.9540340	5.1788951	4.3797946	5.3247956
4 C	5.1817069	5.0045794	3.8917401	4.4957490
5 C	4.3687277	3.8866077	2.6253189 *	3.0983524
6 C	2.9161883 *	2.5030558 *	1.4649588 *	2.5310404 *
7 C	2.4780310 *	2.8439342 *	2.4926739 *	3.8334336
8 C	1.4014717 *	2.4405560 *	2.8568733 *	4.3037211
9 C	0.0000000	1.4288111 *	2.4839194 *	3.7912788
10 C	1.4288111 *	0.0000000	1.4145083 *	2.4639793 *
11 C	2.4839194 *	1.4145083 *	0.0000000	1.4523227 *
12 N	3.7912788	2.4639793 *	1.4523227 *	0.0000000
13 C	4.3309359	2.9101930 *	2.4421302 *	1.3321868 *
14 C	5.7369933	4.3099244	3.8292701	2.5059405 *
15 C	6.7112252	5.2975579	4.5832141	3.1466978
16 C	8.0429016	6.6245451	5.9800410	4.5477809
17 C	8.5306512	7.1152754	6.6826401	5.3068244
18 C	7.8236814	6.4473274	6.2257399	4.9840774
19 C	6.4465072	5.0743021	4.8924609	3.7417899
20 O	6.5768894	5.2535918	4.2789317	2.9323207 *
21 N	5.3912887	4.5659227	3.1562016	2.9072085 *
22 H	4.0731556	4.8835120	4.6862569	5.9977163
23 H	5.9287602	6.2517668	5.4832824	6.4061618
24 H	6.2694445	6.0053910	4.8001913	5.1776081
25 H	2.1814668 *	3.4505979	3.9620827	5.4081664
26 H	1.1041447 *	2.1964329 *	3.4747732	4.6594358
27 H	2.1817698 *	1.1037785 *	2.1838832 *	2.6747930 *
28 H	3.9733907	2.6463295 *	2.6562814 *	2.0977222 *

29 H	8.8433303	7.4451806	6.6969507	5.2671436
30 H	9.6184052	8.2073967	7.7823830	6.3990374
31 H	8.4764025	7.1532520	7.0729522	5.9169535
32 H	6.0766109	4.8021111	4.8683444	3.9707999
33 H	7.4455092	6.1536213	5.1782391	3.8836752
34 H	5.5662716	4.6984307	3.3446582	3.0265792
35 H	6.3060086	5.5544890	4.1508889	3.8897632

C C C C

1 CO	2.8616578 *	3.2657426	3.0114070	4.2800781
2 C	6.2285560	7.5535175	8.0427160	9.4361222
3 C	6.5870686	7.7796533	8.0623730	9.4111910
4 C	5.7695958	6.8153871	6.9544918	8.2574491
5 C	4.3638017	5.4252203	5.6502766	6.9899450
6 C	3.7338598	5.0288281	5.5565498	6.9585784
7 C	4.9261600	6.3026800	6.9251185	8.3297950
8 C	5.1430037	6.5744524	7.3957539	8.7801489
9 C	4.3309359	5.7369933	6.7112252	8.0429016
10 C	2.9101930 *	4.3099244	5.2975579	6.6245451
11 C	2.4421302 *	3.8292701	4.5832141	5.9800410
12 N	1.3321868 *	2.5059405 *	3.1466978	4.5477809
13 C	0.0000000	1.4655581 *	2.6036022 *	3.8823516
14 C	1.4655581 *	0.0000000	1.4367640 *	2.5000164 *
15 C	2.6036022 *	1.4367640 *	0.0000000	1.4061579 *
16 C	3.8823516	2.5000164 *	1.4061579 *	0.0000000
17 C	4.3407295	2.8798617 *	2.4396193 *	1.4281713 *
18 C	3.7914748	2.4972080 *	2.8250885 *	2.4740953 *
19 C	2.4686610 *	1.4433059 *	2.4461844 *	2.8468224 *
20 O	3.0446674	2.5021478 *	1.4663350 *	2.4599794 *
21 N	4.0047832	4.7364937	4.7164749	5.9525213
22 H	7.1181119	8.4849942	9.0389361	10.4375855
23 H	7.6760626	8.8424123	9.0648142	10.3907559
24 H	6.4223708	7.3178840	7.2838696	8.5019797
25 H	6.2290645	7.6614957	8.4915306	9.8722201
26 H	4.9853786	6.3251166	7.3879044	8.6579145
27 H	2.6201832 *	3.8589740	4.9750036	6.1964732
28 H	1.1087649 *	2.1755871 *	3.5309531	4.6730865
29 H	4.7956132	3.5038342	2.1963793 *	1.1072100 *
30 H	5.4458769	3.9851609	3.4382740	2.1911468 *
31 H	4.6558284	3.4928699	3.9284825	3.4748085
32 H	2.6403543 *	2.1983760 *	3.4509732	3.9528574
33 H	4.0124506	3.3276336	2.0446451 *	2.5079458 *
34 H	3.8938141	4.6101544	4.7415075	5.9397920
35 H	4.9625485	5.5506623	5.3256136	6.4482239

	C	C	C	O
1 CO	5.4406191	5.6137367	4.7015145	1.9506895 *
2 C	10.3383885	10.0074651	8.6924992	7.2749860
3 C	10.4339932	10.2622315	9.0242058	7.1204401
4 C	9.3354667	9.2751496	8.1180851	5.9481059
5 C	8.0079414	7.8912907	6.7164294	4.7650415
6 C	7.8169806	7.4913521	6.1986409	4.9319288
7 C	9.1355097	8.7156361	7.3741584	6.3273120
8 C	9.4236134	8.8344697	7.4546350	7.0155257
9 C	8.5306512	7.8236814	6.4465072	6.5768894
10 C	7.1152754	6.4473274	5.0743021	5.2535918
11 C	6.6826401	6.2257399	4.8924609	4.2789317
12 N	5.3068244	4.9840774	3.7417899	2.9323207 *
13 C	4.3407295	3.7914748	2.4686610 *	3.0446674
14 C	2.8798617 *	2.4972080 *	1.4433059 *	2.5021478 *
15 C	2.4396193 *	2.8250885 *	2.4461844 *	1.4663350 *
16 C	1.4281713 *	2.4740953 *	2.8468224 *	2.4599794 *
17 C	0.0000000	1.4234467 *	2.4550654 *	3.7700854
18 C	1.4234467 *	0.0000000	1.4157151 *	4.2912278
19 C	2.4550654 *	1.4157151 *	0.0000000	3.7957752
20 O	3.7700854	4.2912278	3.7957752	0.0000000
21 N	7.0354682	7.0851529	6.0647469	3.7698052
22 H	11.3005738	10.9083499	9.5663837	8.3091075
23 H	11.4530777	11.3240990	10.1029400	8.0565986
24 H	9.6510059	9.7187478	8.6523254	6.1735522
25 H	10.5034820	9.8863080	8.5026719	8.0924972
26 H	9.0146211	8.1999041	6.8491729	7.3918119
27 H	6.5126907	5.7328954	4.3910529	5.2013417
28 H	4.8507282	3.9952060	2.5800037 *	4.1391928
29 H	2.1997541 *	3.4745302	3.9539834	2.6897711 *
30 H	1.1053586 *	2.2006251 *	3.4602358	4.6492471
31 H	2.1971973 *	1.1033979 *	2.1873904 *	5.3945934
32 H	3.4571483	2.1863248 *	1.1060358 *	4.6925442
33 H	3.9272529	4.7286618	4.4854620	0.9913050 *
34 H	6.8903225	6.8362910	5.8077264	4.0494158
35 H	7.6182206	7.8130026	6.8944074	4.2261892

	N	H	H	H
1 CO	1.9763255 *	6.4494748	6.1260063	4.3357654
2 C	4.3423078	1.1046079 *	2.1861897 *	3.4415662
3 C	3.8156792	2.1817819 *	1.1040840 *	2.1964672 *
4 C	2.4761146 *	3.4540689	2.2015950 *	1.1077861 *
5 C	1.5101377 *	3.9428959	3.4650986	2.1819276 *
6 C	2.5926065 *	3.5167190	4.0243862	3.5068797

7 C	3.8866212	2.1941905 *	3.4855587	3.9544442
8 C	5.1116337	2.6740010 *	4.6679188	5.3973130
9 C	5.3912887	4.0731556	5.9287602	6.2694445
10 C	4.5659227	4.8835120	6.2517668	6.0053910
11 C	3.1562016	4.6862569	5.4832824	4.8001913
12 N	2.9072085 *	5.9977163	6.4061618	5.1776081
13 C	4.0047832	7.1181119	7.6760626	6.4223708
14 C	4.7364937	8.4849942	8.8424123	7.3178840
15 C	4.7164749	9.0389361	9.0648142	7.2838696
16 C	5.9525213	10.4375855	10.3907559	8.5019797
17 C	7.0354682	11.3005738	11.4530777	9.6510059
18 C	7.0851529	10.9083499	11.3240990	9.7187478
19 C	6.0647469	9.5663837	10.1029400	8.6523254
20 O	3.7698052	8.3091075	8.0565986	6.1735522
21 N	0.0000000	5.4455121	4.6762194	2.6548002 *
22 H	5.4455121	0.0000000	2.5332600 *	4.3640933
23 H	4.6762194	2.5332600 *	0.0000000	2.5211052 *
24 H	2.6548002 *	4.3640933	2.5211052 *	0.0000000
25 H	6.0556230	2.3904283 *	4.7748573	5.9747823
26 H	6.4744542	4.7732033	6.8501844	7.3508463
27 H	5.2540089	5.9577809	7.3378126	6.9586028
28 H	4.7534358	7.1751948	8.0302752	7.0259568
29 H	6.2764915	10.9687408	10.7170095	8.7076587
30 H	8.0123144	12.3874022	12.4822096	10.6118618
31 H	8.0909874	11.7426204	12.2706558	10.7224981
32 H	6.4548594	9.4388262	10.2041685	8.9564695
33 H	4.3834729	8.9999369	8.5827138	6.6100168
34 H	1.0443596 *	5.8374683	5.1698779	3.2147940
35 H	1.0395458 *	5.8271237	4.5935138	2.2196837 *

H H H H

1 CO	6.5016525	6.2764253	4.5044026	3.8773289
2 C	2.6765326 *	4.6683197	5.3851009	6.3894757
3 C	4.0758866	5.9295827	6.2591048	6.9307648
4 C	4.8896830	6.2558400	6.0016422	6.2766729
5 C	4.6715784	5.4727693	4.7982819	4.9011604
6 C	3.5169454	4.0201429	3.5007419	4.0386691
7 C	2.1959686 *	3.4851185	3.9444468	5.0131834
8 C	1.1053804 *	2.1867225 *	3.4283291	4.9655023
9 C	2.1814668 *	1.1041447 *	2.1817698 *	3.9733907
10 C	3.4505979	2.1964329 *	1.1037785 *	2.6463295 *
11 C	3.9620827	3.4747732	2.1838832 *	2.6562814 *
12 N	5.4081664	4.6594358	2.6747930 *	2.0977222 *
13 C	6.2290645	4.9853786	2.6201832 *	1.1087649 *
14 C	7.6614957	6.3251166	3.8589740	2.1755871 *

15 C	8.4915306	7.3879044	4.9750036	3.5309531
16 C	9.8722201	8.6579145	6.1964732	4.6730865
17 C	10.5034820	9.0146211	6.5126907	4.8507282
18 C	9.8863080	8.1999041	5.7328954	3.9952060
19 C	8.5026719	6.8491729	4.3910529	2.5800037 *
20 O	8.0924972	7.3918119	5.2013417	4.1391928
21 N	6.0556230	6.4744542	5.2540089	4.7534358
22 H	2.3904283 *	4.7732033	5.9577809	7.1751948
23 H	4.7748573	6.8501844	7.3378126	8.0302752
24 H	5.9747823	7.3508463	6.9586028	7.0259568
25 H	0.0000000	2.5329008 *	4.3480624	5.9946398
26 H	2.5329008 *	0.0000000	2.5019730 *	4.4581969
27 H	4.3480624	2.5019730 *	0.0000000	2.1422831 *
28 H	5.9946398	4.4581969	2.1422831 *	0.0000000
29 H	10.5742861	9.5073522	7.0925791	5.6719541
30 H	11.6000917	10.0782148	7.5784113	5.9309122
31 H	10.5865664	8.7465178	6.3529165	4.6540974
32 H	8.1772383	6.3535716	4.0267502	2.2636582 *
33 H	8.8949506	8.2571713	6.0962113	5.0968113
34 H	6.3283170	6.6171109	5.3290486	4.5242641
35 H	6.7624258	7.4016072	6.2645318	5.7596851

H H H H

1 CO	4.6168781	6.4193318	6.6796546	5.2854833
2 C	9.9425608	11.4175112	10.8782282	8.6412545
3 C	9.7936934	11.4777957	11.1981488	9.1112118
4 C	8.5799838	10.3477727	10.2509838	8.3288577
5 C	7.4049334	9.0427570	8.8581597	6.9289395
6 C	7.5382735	8.9005080	8.3854798	6.2365393
7 C	8.9311759	10.2284991	9.5515983	7.2732350
8 C	9.4871402	10.5221701	9.5652992	7.1807112
9 C	8.8433303	9.6184052	8.4764025	6.0766109
10 C	7.4451806	8.2073967	7.1532520	4.8021111
11 C	6.6969507	7.7823830	7.0729522	4.8683444
12 N	5.2671436	6.3990374	5.9169535	3.9707999
13 C	4.7956132	5.4458769	4.6558284	2.6403543 *
14 C	3.5038342	3.9851609	3.4928699	2.1983760 *
15 C	2.1963793 *	3.4382740	3.9284825	3.4509732
16 C	1.1072100 *	2.1911468 *	3.4748085	3.9528574
17 C	2.1997541 *	1.1053586 *	2.1971973 *	3.4571483
18 C	3.4745302	2.2006251 *	1.1033979 *	2.1863248 *
19 C	3.9539834	3.4602358	2.1873904 *	1.1060358 *
20 O	2.6897711 *	4.6492471	5.3945934	4.6925442
21 N	6.2764915	8.0123144	8.0909874	6.4548594
22 H	10.9687408	12.3874022	11.7426204	9.4388262

23 H	10.7170095	12.4822096	12.2706558	10.2041685
24 H	8.7076587	10.6118618	10.7224981	8.9564695
25 H	10.5742861	11.6000917	10.5865664	8.1772383
26 H	9.5073522	10.0782148	8.7465178	6.3535716
27 H	7.0925791	7.5784113	6.3529165	4.0267502
28 H	5.6719541	5.9309122	4.6540974	2.2636582 *
29 H	0.0000000	2.5180196 *	4.3861157	5.0600179
30 H	2.5180196 *	0.0000000	2.5400154 *	4.3746424
31 H	4.3861157	2.5400154 *	0.0000000	2.5160101 *
32 H	5.0600179	4.3746424	2.5160101 *	0.0000000
33 H	2.3113858 *	4.6291077	5.8132638	5.4642477
34 H	6.3523789	7.8648680	7.7819933	6.1228700
35 H	6.6149560	8.5306541	8.8406276	7.3624227

H H H

1 CO	2.6554941 *	2.5063386 *	2.6094828 *
2 C	7.9630852	4.7639285	4.7436223
3 C	7.7089256	4.3157727	3.9246349
4 C	6.5026779	3.0546588	2.4921924 *
5 C	5.4353588	2.1093723 *	2.0911423 *
6 C	5.7300810	2.9614871 *	3.4249615
7 C	7.1024812	4.2394654	4.5665572
8 C	7.8385062	5.3739718	5.8921838
9 C	7.4455092	5.5662716	6.3060086
10 C	6.1536213	4.6984307	5.5544890
11 C	5.1782391	3.3446582	4.1508889
12 N	3.8836752	3.0265792	3.8897632
13 C	4.0124506	3.8938141	4.9625485
14 C	3.3276336	4.6101544	5.5506623
15 C	2.0446451 *	4.7415075	5.3256136
16 C	2.5079458 *	5.9397920	6.4482239
17 C	3.9272529	6.8903225	7.6182206
18 C	4.7286618	6.8362910	7.8130026
19 C	4.4854620	5.8077264	6.8944074
20 O	0.9913050 *	4.0494158	4.2261892
21 N	4.3834729	1.0443596 *	1.0395458 *
22 H	8.9999369	5.8374683	5.8271237
23 H	8.5827138	5.1698779	4.5935138
24 H	6.6100168	3.2147940	2.2196837 *
25 H	8.8949506	6.3283170	6.7624258
26 H	8.2571713	6.6171109	7.4016072
27 H	6.0962113	5.3290486	6.2645318
28 H	5.0968113	4.5242641	5.7596851
29 H	2.3113858 *	6.3523789	6.6149560
30 H	4.6291077	7.8648680	8.5306541

31 H	5.8132638	7.7819933	8.8406276
32 H	5.4642477	6.1228700	7.3624227
33 H	0.0000000	4.7429531	4.6502055
34 H	4.7429531	0.0000000	1.6685003 *
35 H	4.6502055	1.6685003 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.81 , TOTAL = 6873.2 SECONDS (114.6 MIN)
WALL CLOCK TIME: STEP = 0.81 , TOTAL = 6352.7 SECONDS (105.9 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.88 , TOTAL = 6874.1 SECONDS (114.6 MIN)
WALL CLOCK TIME: STEP = 0.88 , TOTAL = 6353.5 SECONDS (105.9 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636689247	-284.636689247	0.008960700	0.000902292	198109212
11329872					
2 1	-284.636754558	-0.000065311	0.002427579	0.000092732	157230894
14763230					
3 2	-284.636753479	0.000001079	0.001830257	0.000142196	143411386
15869827					
4 3	-284.636756106	-0.000002628	0.000547010	0.000055630	138084768
16282844					
5 4	-284.636755869	0.000000237	0.000351635	0.000131885	130806482
16914425					
6 5	-284.636756209	-0.000000340	0.000244555	0.000022637	125367678
17346135					
7 6	-284.636756184	0.000000025	0.000178258	0.000025175	117680506
17854903					
8 7	-284.636756215	-0.000000030	0.000109760	0.000014375	136042241
16494999					

9 8	-284.636756221	-0.000000006	0.000134316	0.000009127	133857349
16681670					
10 9	-284.636756235	-0.000000013	0.000234302	0.000009476	152306676
15350611					
-----DISABLING FDIFF OPTION-----					
11 10	-284.636756239	-0.000000005	0.000228223	0.000011649	198109575
11329738					
12 11	-284.636756248	-0.000000009	0.000160894	0.000018563	198109791
11329733					
13 12	-284.636756259	-0.000000011	0.000474084	0.000016679	198109790
11329738					
14 13	-284.636756274	-0.000000015	0.000130035	0.000008190	198109963
11329743					
15 14	-284.636756278	-0.000000004	0.000047504	0.000008444	198109857
11329742					
16 15	-284.636756281	-0.000000003	0.000064021	0.000007031	198109805
11329742					
17 16	-284.636756284	-0.000000003	0.000102435	0.000004309	198109835
11329739					
18 17	-284.636756286	-0.000000002	0.000076922	0.000002063	198109852
11329745					
19 18	-284.636756286	-0.000000001	0.000018528	0.000001366	198109966
11329742					
20 19	-284.636756286	0.000000000	0.000017019	0.000001022	198109957
11329743					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 66.8 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 21.8 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6367562865 AFTER 20 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6043663577
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998743178

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 70.62 , TOTAL = 6944.7 SECONDS (115.7 MIN)
WALL CLOCK TIME: STEP = 64.56 , TOTAL = 6418.1 SECONDS (107.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.65 , TOTAL = 6948.3 SECONDS (115.8 MIN)
WALL CLOCK TIME: STEP = 3.63 , TOTAL = 6421.7 SECONDS (107.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.01 , TOTAL = 6951.3 SECONDS (115.9 MIN)
WALL CLOCK TIME: STEP = 2.84 , TOTAL = 6424.6 SECONDS (107.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 71 ENERGY= -284.6367563

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0002048	-0.0000151	-0.0006386
2 C	6.0	0.0005874	0.0004746	-0.0002840
3 C	6.0	-0.0001041	0.0003973	-0.0000267
4 C	6.0	-0.0004879	-0.0005793	-0.0000846
5 C	6.0	0.0007123	-0.0005135	-0.0000899
6 C	6.0	0.0003154	0.0006031	0.0001900
7 C	6.0	-0.0006572	0.0002141	-0.0000885
8 C	6.0	-0.0006186	-0.0006157	0.0000240
9 C	6.0	-0.0000238	0.0000997	0.0001698
10 C	6.0	0.0004834	-0.0002009	0.0000871
11 C	6.0	0.0000372	-0.0005621	0.0000396
12 N	7.0	0.0000550	0.0003129	-0.0001099

13	C	6.0	-0.0000026	-0.0002405	-0.0001900
14	C	6.0	0.0005272	-0.0005483	0.0003183
15	C	6.0	-0.0002469	0.0005476	-0.0002977
16	C	6.0	0.0003086	0.0000646	-0.0002300
17	C	6.0	0.0005652	-0.0000765	0.0000975
18	C	6.0	-0.0005047	0.0008086	0.0003628
19	C	6.0	-0.0002302	0.0003981	0.0003192
20	O	8.0	0.0002443	-0.0000185	0.0007870
21	N	7.0	0.0001344	0.0001128	-0.0001592
22	H	1.0	-0.0005337	0.0002745	-0.0001838
23	H	1.0	-0.0000734	0.0000001	0.0003242
24	H	1.0	-0.0002162	-0.0001542	0.0003591
25	H	1.0	0.0002554	-0.0000215	0.0001918
26	H	1.0	-0.0002978	-0.0000206	-0.0002038
27	H	1.0	-0.0000559	-0.0006703	0.0000619
28	H	1.0	-0.0001542	0.0002833	-0.0004175
29	H	1.0	-0.0003012	-0.0002539	-0.0000029
30	H	1.0	-0.0000587	-0.0001541	-0.0001975
31	H	1.0	0.0003870	-0.0003224	0.0001351
32	H	1.0	-0.0000009	0.0000637	-0.0001138
33	H	1.0	0.0000673	0.0003479	-0.0003188
34	H	1.0	0.0001013	0.0002422	-0.0003109
35	H	1.0	-0.0004182	-0.0002774	0.0004806

MAXIMUM GRADIENT = 0.0008086 RMS GRADIENT = 0.0003379
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000238187
 PREDICTED ENERGY CHANGE WAS -0.0000238657 RATIO= 0.998
 GDIIS STEP HAS LENGTH = 0.030332
 RADIUS OF STEP TAKEN= 0.03033 CURRENT TRUST RADIUS= 0.10556

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 6951.4 SECONDS (115.9 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6424.6 SECONDS (107.1 MIN)
 CPU UTILIZATION: STEP = 89.78%, TOTAL = 100.00%

INSERCH= 72

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1552426050	-1.7393956866	0.8499746659
C	6.0	4.9786236455	0.6383799205	0.5460399982
C	6.0	5.1897702831	-0.7078884915	0.2173901042

C	6.0	4.0588205078	-1.5404015339	-0.0652556132
C	6.0	2.7483998888	-1.0310550705	0.0037572483
C	6.0	2.4695037398	0.3378583629	0.4190512634
C	6.0	3.6457157697	1.1804976964	0.6611103930
C	6.0	3.4934016522	2.5661419825	1.0376462373
C	6.0	2.2240432404	3.1342476292	1.2111898192
C	6.0	1.0653529183	2.3161516573	1.0367410568
C	6.0	1.1621626638	0.9656018033	0.6281578244
N	7.0	-0.0510335915	0.1677874738	0.5721518844
C	6.0	-1.2457148155	0.6989258254	0.3157726985
C	6.0	-2.5510643527	0.0446601106	0.4404760490
C	6.0	-2.8218040176	-1.2841055547	0.9170753555
C	6.0	-4.1217467678	-1.8079087148	1.0351329742
C	6.0	-5.2302744073	-0.9812094552	0.6769491815
C	6.0	-5.0176846099	0.3445657466	0.2053016401
C	6.0	-3.6986593275	0.8444746496	0.0877767329
O	8.0	-1.6998485911	-2.1447463175	1.3015578031
N	7.0	1.6470921874	-1.9694796822	-0.4256774887
H	1.0	5.8342355203	1.3123216140	0.7327425244
H	1.0	6.2099029985	-1.1247714854	0.1529210330
H	1.0	4.2268231392	-2.5909356722	-0.3748636448
H	1.0	4.4052904609	3.1659084399	1.2086823918
H	1.0	2.1086594796	4.1883710154	1.5209547224
H	1.0	0.0787928783	2.7456611118	1.2808215910
H	1.0	-1.2882551966	1.7498388717	-0.0333120667
H	1.0	-4.2973460095	-2.8390226918	1.3975867520
H	1.0	-6.2543319139	-1.3847998183	0.7684457577
H	1.0	-5.8761803231	0.9833297007	-0.0665561879
H	1.0	-3.5328938836	1.8755926470	-0.2758462918
H	1.0	-2.0209953517	-2.9597166831	1.7657212981
H	1.0	1.3026801927	-1.7058082195	-1.3757401693
H	1.0	2.0393163879	-2.9279661812	-0.5109905381

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3862044	5.1778991	4.0143699
2 C	5.3862044	0.0000000	1.4017961 *	2.4427052 *
3 C	5.1778991	1.4017961 *	0.0000000	1.4324852 *
4 C	4.0143699	2.4427052 *	1.4324852 *	0.0000000
5 C	2.8182078 *	2.8381300 *	2.4719153 *	1.4076217 *
6 C	3.1395038	2.5302415 *	2.9213188 *	2.5076565 *
7 C	4.5546515	1.4435291 *	2.4793133 *	2.8463232 *
8 C	5.4512550	2.4827057 *	3.7775339	4.2894977

9 C	5.3068646	3.7761744	4.9543097	5.1815119
10 C	4.1606065	4.2859530	5.1794762	5.0048224
11 C	2.8948406 *	3.8313434	4.3807446	3.8924930
12 N	1.9383196 *	5.0516919	5.3252877	4.4961204
13 C	2.8624230 *	6.2288906	6.5881920	5.7704302
14 C	3.2672070	7.5537969	7.7805281	6.8160665
15 C	3.0124074	8.0424057	8.0626862	6.9551172
16 C	4.2815436	9.4361158	9.4118594	8.2585771
17 C	5.4413764	10.3373984	10.4337544	9.3354619
18 C	5.6140604	10.0064283	10.2615760	9.2741171
19 C	4.7021157	8.6918191	9.0239023	8.1172376
20 O	1.9518196 *	7.2745165	7.1208727	5.9494270
21 N	1.9763204 *	4.3409986	3.8151955	2.4759736 *
22 H	6.4480759	1.1050461 *	2.1822402 *	3.4535386
23 H	6.1255660	2.1861597 *	1.1039105 *	2.2017051 *
24 H	4.3362561	3.4411839	2.1963375 *	1.1080180 *
25 H	6.5002759	2.6751087 *	4.0748462	4.8879764
26 H	6.2772980	4.6679321	5.9300828	6.2560392
27 H	4.5063520	5.3841322	6.2593915	6.0019061
28 H	3.8779684	6.3909906	6.9331154	6.2783693
29 H	4.6189397	9.9428906	9.7948952	8.5820652
30 H	6.4198934	11.4158666	11.4773406	10.3479651
31 H	6.6806680	10.8775472	11.1980403	10.2505347
32 H	5.2856375	8.6401460	9.1105723	8.3275142
33 H	2.6577786 *	7.9642067	7.7112386	6.5062349
34 H	2.5043058 *	4.7645585	4.3177977	3.0563113
35 H	2.6104904 *	4.7408507	3.9223262	2.4904642 *

C C C C

1 CO	2.8182078 *	3.1395038	4.5546515	5.4512550
2 C	2.8381300 *	2.5302415 *	1.4435291 *	2.4827057 *
3 C	2.4719153 *	2.9213188 *	2.4793133 *	3.7775339
4 C	1.4076217 *	2.5076565 *	2.8463232 *	4.2894977
5 C	0.0000000	1.4574554 *	2.4755312 *	3.8162522
6 C	1.4574554 *	0.0000000	1.4670066 *	2.5290857 *
7 C	2.4755312 *	1.4670066 *	0.0000000	1.4439491 *
8 C	3.8162522	2.5290857 *	1.4439491 *	0.0000000
9 C	4.3683624	2.9167666 *	2.4780797 *	1.4014750 *
10 C	3.8863216	2.5033627 *	2.8441309 *	2.4408844 *
11 C	2.6253882 *	1.4652399 *	2.4930508 *	2.8572863 *
12 N	3.0979225	2.5309035 *	3.8339864	4.3048589
13 C	4.3638446	3.7341512	4.9271962	5.1445916
14 C	5.4251459	5.0291677	6.3038790	6.5764772
15 C	5.6502527	5.5566836	6.9259367	7.3973486
16 C	6.9904329	6.9590557	8.3309027	8.7819594

17 C	8.0071790	7.8162033	9.1354491	9.4242415
18 C	7.8895514	7.4902419	8.7155637	8.8355412
19 C	6.7148525	6.1977930	7.3743792	7.4560131
20 O	4.7656593	4.9321033	6.3279127	7.0165494
21 N	1.5092825 *	2.5910879 *	3.8856096	5.1109724
22 H	3.9427421	3.5170159	2.1936562 *	2.6729263 *
23 H	3.4659827	4.0250091	3.4853377	4.6674362
24 H	2.1822733 *	3.5066090	3.9540660	5.3970864
25 H	4.6702927	3.5169098	2.1951411 *	1.1047689 *
26 H	5.4729850	4.0212992	3.4855668	2.1869442 *
27 H	4.7980496	3.5008086	3.9442005	3.4279607
28 H	4.9019720	4.0396873	5.0150216	4.9676498
29 H	7.4063515	7.5392546	8.9325904	9.4889995
30 H	9.0420719	8.8991537	10.2275714	10.5214410
31 H	8.8569788	8.3846819	9.5516951	9.5662754
32 H	6.9268630	6.2350851	7.2727905	7.1812917
33 H	5.4379577	5.7316754	7.1044462	7.8405218
34 H	2.1091255 *	2.9596160 *	4.2390256	5.3733838
35 H	2.0895063 *	3.4228130	4.5644074	5.8904893

C C C N

1 CO	5.3068646	4.1606065	2.8948406 *	1.9383196 *
2 C	3.7761744	4.2859530	3.8313434	5.0516919
3 C	4.9543097	5.1794762	4.3807446	5.3252877
4 C	5.1815119	5.0048224	3.8924930	4.4961204
5 C	4.3683624	3.8863216	2.6253882 *	3.0979225
6 C	2.9167666 *	2.5033627 *	1.4652399 *	2.5309035 *
7 C	2.4780797 *	2.8441309 *	2.4930508 *	3.8339864
8 C	1.4014750 *	2.4408844 *	2.8572863 *	4.3048589
9 C	0.0000000	1.4290825 *	2.4840574 *	3.7926547
10 C	1.4290825 *	0.0000000	1.4143187 *	2.4652851 *
11 C	2.4840574 *	1.4143187 *	0.0000000	1.4530965 *
12 N	3.7926547	2.4652851 *	1.4530965 *	0.0000000
13 C	4.3326418	2.9113998 *	2.4426573 *	1.3323293 *
14 C	5.7394428	4.3120389	3.8303280	2.5065220 *
15 C	6.7133392	5.2996378	4.5843917	3.1470835
16 C	8.0451822	6.6267548	5.9814453	4.5484539
17 C	8.5316617	7.1159654	6.6824925	5.3061956
18 C	7.8253919	6.4483942	6.2253518	4.9833174
19 C	6.4485287	5.0756457	4.8922667	3.7413498
20 O	6.5782118	5.2551002	4.2800516	2.9323091 *
21 N	5.3907550	4.5654928	3.1560147	2.9064077 *
22 H	4.0720774	4.8828610	4.6860876	5.9976779
23 H	5.9284277	6.2519985	5.4840854	6.4066988
24 H	6.2693235	6.0055831	4.8007452	5.1775911

25 H	2.1814784 *	3.4506279	3.9618475	5.4085788
26 H	1.1047370 *	2.1973067 *	3.4755120	4.6615012
27 H	2.1812719 *	1.1033378 *	2.1836372 *	2.6766584 *
28 H	3.9751243	2.6467329 *	2.6565236 *	2.0976631 *
29 H	8.8455198	7.4474541	6.6987628	5.2681514
30 H	9.6177262	8.2065102	7.7812891	6.3976534
31 H	8.4777771	7.1539194	7.0725677	5.9165354
32 H	6.0776487	4.8021715	4.8671206	3.9697671
33 H	7.4474330	6.1556271	5.1802192	3.8841524
34 H	5.5648232	4.6960144	3.3424219	3.0227777
35 H	6.3047970	5.5538140	4.1505336	3.8892739

C C C C

1 CO	2.8624230 *	3.2672070	3.0124074	4.2815436
2 C	6.2288906	7.5537969	8.0424057	9.4361158
3 C	6.5881920	7.7805281	8.0626862	9.4118594
4 C	5.7704302	6.8160665	6.9551172	8.2585771
5 C	4.3638446	5.4251459	5.6502527	6.9904329
6 C	3.7341512	5.0291677	5.5566836	6.9590557
7 C	4.9271962	6.3038790	6.9259367	8.3309027
8 C	5.1445916	6.5764772	7.3973486	8.7819594
9 C	4.3326418	5.7394428	6.7133392	8.0451822
10 C	2.9113998 *	4.3120389	5.2996378	6.6267548
11 C	2.4426573 *	3.8303280	4.5843917	5.9814453
12 N	1.3323293 *	2.5065220 *	3.1470835	4.5484539
13 C	0.0000000	1.4654528 *	2.6034661 *	3.8824294
14 C	1.4654528 *	0.0000000	1.4373813 *	2.5005342 *
15 C	2.6034661 *	1.4373813 *	0.0000000	1.4064702 *
16 C	3.8824294	2.5005342 *	1.4064702 *	0.0000000
17 C	4.3393569	2.8786272 *	2.4392901 *	1.4284820 *
18 C	3.7901888	2.4958898 *	2.8250812 *	2.4747669 *
19 C	2.4678135 *	1.4425929 *	2.4469297 *	2.8480914 *
20 O	3.0437610	2.5019054 *	1.4653714 *	2.4596814 *
21 N	4.0048057	4.7361904	4.7163287	5.9531148
22 H	7.1186948	8.4856137	9.0389398	10.4378571
23 H	7.6771498	8.8433482	9.0653765	10.3917256
24 H	6.4225259	7.3178482	7.2842334	8.5029313
25 H	6.2303412	7.6631067	8.4922644	9.8731626
26 H	4.9880375	6.3285702	7.3906793	8.6607942
27 H	2.6219774 *	3.8623485	4.9784328	6.1999915
28 H	1.1081914 *	2.1741198 *	3.5298480	4.6720250
29 H	4.7958163	3.5044525	2.1967892 *	1.1069796 *
30 H	5.4436266	3.9831031	3.4372195	2.1904480 *
31 H	4.6549191	3.4920737	3.9291231	3.4760276
32 H	2.6392700 *	2.1975943 *	3.4514350	3.9539343

33 H	4.0111190	3.3261882	2.0418538 *	2.5047110 *
34 H	3.8907941	4.6058797	4.7377427	5.9369303
35 H	4.9627929	5.5509811	5.3265506	6.4500950

C C C O

1 CO	5.4413764	5.6140604	4.7021157	1.9518196 *
2 C	10.3373984	10.0064283	8.6918191	7.2745165
3 C	10.4337544	10.2615760	9.0239023	7.1208727
4 C	9.3354619	9.2741171	8.1172376	5.9494270
5 C	8.0071790	7.8895514	6.7148525	4.7656593
6 C	7.8162033	7.4902419	6.1977930	4.9321033
7 C	9.1354491	8.7155637	7.3743792	6.3279127
8 C	9.4242415	8.8355412	7.4560131	7.0165494
9 C	8.5316617	7.8253919	6.4485287	6.5782118
10 C	7.1159654	6.4483942	5.0756457	5.2551002
11 C	6.6824925	6.2253518	4.8922667	4.2800516
12 N	5.3061956	4.9833174	3.7413498	2.9323091 *
13 C	4.3393569	3.7901888	2.4678135 *	3.0437610
14 C	2.8786272 *	2.4958898 *	1.4425929 *	2.5019054 *
15 C	2.4392901 *	2.8250812 *	2.4469297 *	1.4653714 *
16 C	1.4284820 *	2.4747669 *	2.8480914 *	2.4596814 *
17 C	0.0000000	1.4231394 *	2.4548098 *	3.7693316
18 C	1.4231394 *	0.0000000	1.4154677 *	4.2902783
19 C	2.4548098 *	1.4154677 *	0.0000000	3.7952537
20 O	3.7693316	4.2902783	3.7952537	0.0000000
21 N	7.0349581	7.0832331	6.0629228	3.7704208
22 H	11.2998574	10.9077457	9.5661354	8.3088683
23 H	11.4530727	11.3234456	10.1025631	8.0575359
24 H	9.6506074	9.7167219	8.6503961	6.1753471
25 H	10.5035916	9.8873256	8.5040865	8.0922434
26 H	9.0164770	8.2030825	6.8527800	7.3933243
27 H	6.5146313	5.7355109	4.3939744	5.2038524
28 H	4.8479492	3.9925396	2.5776724 *	4.1375211
29 H	2.2002600 *	3.4750060	3.9550197	2.6903966 *
30 H	1.1045137 *	2.1993483 *	3.4589648	4.6481228
31 H	2.1975916 *	1.1040566 *	2.1873950 *	5.3942879
32 H	3.4569116	2.1863555 *	1.1058500 *	4.6916292
33 H	3.9242054	4.7258162	4.4835172	0.9913424 *
34 H	6.8860782	6.8301345	5.8016568	4.0466987
35 H	7.6189247	7.8117733	6.8930543	4.2284890

N H H H

1 CO	1.9763204 *	6.4480759	6.1255660	4.3362561
2 C	4.3409986	1.1050461 *	2.1861597 *	3.4411839

3 C	3.8151955	2.1822402 *	1.1039105 *	2.1963375 *
4 C	2.4759736 *	3.4535386	2.2017051 *	1.1080180 *
5 C	1.5092825 *	3.9427421	3.4659827	2.1822733 *
6 C	2.5910879 *	3.5170159	4.0250091	3.5066090
7 C	3.8856096	2.1936562 *	3.4853377	3.9540660
8 C	5.1109724	2.6729263 *	4.6674362	5.3970864
9 C	5.3907550	4.0720774	5.9284277	6.2693235
10 C	4.5654928	4.8828610	6.2519985	6.0055831
11 C	3.1560147	4.6860876	5.4840854	4.8007452
12 N	2.9064077 *	5.9976779	6.4066988	5.1775911
13 C	4.0048057	7.1186948	7.6771498	6.4225259
14 C	4.7361904	8.4856137	8.8433482	7.3178482
15 C	4.7163287	9.0389398	9.0653765	7.2842334
16 C	5.9531148	10.4378571	10.3917256	8.5029313
17 C	7.0349581	11.2998574	11.4530727	9.6506074
18 C	7.0832331	10.9077457	11.3234456	9.7167219
19 C	6.0629228	9.5661354	10.1025631	8.6503961
20 O	3.7704208	8.3088683	8.0575359	6.1753471
21 N	0.0000000	5.4446603	4.6762753	2.6540161 *
22 H	5.4446603	0.0000000	2.5331289 *	4.3641704
23 H	4.6762753	2.5331289 *	0.0000000	2.5220626 *
24 H	2.6540161 *	4.3641704	2.5220626 *	0.0000000
25 H	6.0540070	2.3883440 *	4.7729648	5.9733343
26 H	6.4746851	4.7720913	6.8499049	7.3511729
27 H	5.2539751	5.9565068	7.3377735	6.9589305
28 H	4.7543186	7.1769168	8.0324619	7.0267397
29 H	6.2782755	10.9692580	10.7186814	8.7100280
30 H	8.0125080	12.3858468	12.4821327	10.6120936
31 H	8.0899741	11.7422721	12.2705204	10.7210590
32 H	6.4528510	9.4380951	10.2033385	8.9539314
33 H	4.3860762	9.0012226	8.5857927	6.6146307
34 H	1.0443952 *	5.8386472	5.1725472	3.2149365
35 H	1.0391412 *	5.8248025	4.5919584	2.2174999 *

H H H H

1 CO	6.5002759	6.2772980	4.5063520	3.8779684
2 C	2.6751087 *	4.6679321	5.3841322	6.3909906
3 C	4.0748462	5.9300828	6.2593915	6.9331154
4 C	4.8879764	6.2560392	6.0019061	6.2783693
5 C	4.6702927	5.4729850	4.7980496	4.9019720
6 C	3.5169098	4.0212992	3.5008086	4.0396873
7 C	2.1951411 *	3.4855668	3.9442005	5.0150216
8 C	1.1047689 *	2.1869442 *	3.4279607	4.9676498
9 C	2.1814784 *	1.1047370 *	2.1812719 *	3.9751243
10 C	3.4506279	2.1973067 *	1.1033378 *	2.6467329 *

11 C	3.9618475	3.4755120	2.1836372 *	2.6565236 *
12 N	5.4085788	4.6615012	2.6766584 *	2.0976631 *
13 C	6.2303412	4.9880375	2.6219774 *	1.1081914 *
14 C	7.6631067	6.3285702	3.8623485	2.1741198 *
15 C	8.4922644	7.3906793	4.9784328	3.5298480
16 C	9.8731626	8.6607942	6.1999915	4.6720250
17 C	10.5035916	9.0164770	6.5146313	4.8479492
18 C	9.8873256	8.2030825	5.7355109	3.9925396
19 C	8.5040865	6.8527800	4.3939744	2.5776724 *
20 O	8.0922434	7.3933243	5.2038524	4.1375211
21 N	6.0540070	6.4746851	5.2539751	4.7543186
22 H	2.3883440 *	4.7720913	5.9565068	7.1769168
23 H	4.7729648	6.8499049	7.3377735	8.0324619
24 H	5.9733343	7.3511729	6.9589305	7.0267397
25 H	0.0000000	2.5332701 *	4.3474582	5.9970214
26 H	2.5332701 *	0.0000000	2.5018861 *	4.4610776
27 H	4.3474582	2.5018861 *	0.0000000	2.1418286 *
28 H	5.9970214	4.4610776	2.1418286 *	0.0000000
29 H	10.5750066	9.5098049	7.0959791	5.6709567
30 H	11.5987199	10.0780022	7.5783709	5.9271151
31 H	10.5876591	8.7492941	6.3547576	4.6516340
32 H	8.1782340	6.3564583	4.0279666	2.2612032 *
33 H	8.8955452	8.2588811	6.0988174	5.0944423
34 H	6.3276420	6.6167811	5.3264247	4.5228925
35 H	6.7594686	7.4010719	6.2645263	5.7604487

H H H H

1 CO	4.6189397	6.4198934	6.6806680	5.2856375
2 C	9.9428906	11.4158666	10.8775472	8.6401460
3 C	9.7948952	11.4773406	11.1980403	9.1105723
4 C	8.5820652	10.3479651	10.2505347	8.3275142
5 C	7.4063515	9.0420719	8.8569788	6.9268630
6 C	7.5392546	8.8991537	8.3846819	6.2350851
7 C	8.9325904	10.2275714	9.5516951	7.2727905
8 C	9.4889995	10.5214410	9.5662754	7.1812917
9 C	8.8455198	9.6177262	8.4777771	6.0776487
10 C	7.4474541	8.2065102	7.1539194	4.8021715
11 C	6.6987628	7.7812891	7.0725677	4.8671206
12 N	5.2681514	6.3976534	5.9165354	3.9697671
13 C	4.7958163	5.4436266	4.6549191	2.6392700 *
14 C	3.5044525	3.9831031	3.4920737	2.1975943 *
15 C	2.1967892 *	3.4372195	3.9291231	3.4514350
16 C	1.1069796 *	2.1904480 *	3.4760276	3.9539343
17 C	2.2002600 *	1.1045137 *	2.1975916 *	3.4569116
18 C	3.4750060	2.1993483 *	1.1040566 *	2.1863555 *

19 C	3.9550197	3.4589648	2.1873950 *	1.1058500 *
20 O	2.6903966 *	4.6481228	5.3942879	4.6916292
21 N	6.2782755	8.0125080	8.0899741	6.4528510
22 H	10.9692580	12.3858468	11.7422721	9.4380951
23 H	10.7186814	12.4821327	12.2705204	10.2033385
24 H	8.7100280	10.6120936	10.7210590	8.9539314
25 H	10.5750066	11.5987199	10.5876591	8.1782340
26 H	9.5098049	10.0780022	8.7492941	6.3564583
27 H	7.0959791	7.5783709	6.3547576	4.0279666
28 H	5.6709567	5.9271151	4.6516340	2.2612032 *
29 H	0.0000000	2.5180104 *	4.3871187	5.0608658
30 H	2.5180104 *	0.0000000	2.5393433 *	4.3734346
31 H	4.3871187	2.5393433 *	0.0000000	2.5161333 *
32 H	5.0608658	4.3734346	2.5161333 *	0.0000000
33 H	2.3090826 *	4.6255875	5.8109644	5.4620556
34 H	6.3510480	7.8618707	7.7769829	6.1171051
35 H	6.6184491	8.5324628	8.8402967	7.3606384

H H H

1 CO	2.6577786 *	2.5043058 *	2.6104904 *
2 C	7.9642067	4.7645585	4.7408507
3 C	7.7112386	4.3177977	3.9223262
4 C	6.5062349	3.0563113	2.4904642 *
5 C	5.4379577	2.1091255 *	2.0895063 *
6 C	5.7316754	2.9596160 *	3.4228130
7 C	7.1044462	4.2390256	4.5644074
8 C	7.8405218	5.3733838	5.8904893
9 C	7.4474330	5.5648232	6.3047970
10 C	6.1556271	4.6960144	5.5538140
11 C	5.1802192	3.3424219	4.1505336
12 N	3.8841524	3.0227777	3.8892739
13 C	4.0111190	3.8907941	4.9627929
14 C	3.3261882	4.6058797	5.5509811
15 C	2.0418538 *	4.7377427	5.3265506
16 C	2.5047110 *	5.9369303	6.4500950
17 C	3.9242054	6.8860782	7.6189247
18 C	4.7258162	6.8301345	7.8117733
19 C	4.4835172	5.8016568	6.8930543
20 O	0.9913424 *	4.0466987	4.2284890
21 N	4.3860762	1.0443952 *	1.0391412 *
22 H	9.0012226	5.8386472	5.8248025
23 H	8.5857927	5.1725472	4.5919584
24 H	6.6146307	3.2149365	2.2174999 *
25 H	8.8955452	6.3276420	6.7594686
26 H	8.2588811	6.6167811	7.4010719

27 H	6.0988174	5.3264247	6.2645263
28 H	5.0944423	4.5228925	5.7604487
29 H	2.3090826 *	6.3510480	6.6184491
30 H	4.6255875	7.8618707	8.5324628
31 H	5.8109644	7.7769829	8.8402967
32 H	5.4620556	6.1171051	7.3606384
33 H	0.0000000	4.7421394	4.6551645
34 H	4.7421394	0.0000000	1.6685607 *
35 H	4.6551645	1.6685607 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80 , TOTAL = 6952.2 SECONDS (115.9 MIN)
WALL CLOCK TIME: STEP = 0.81 , TOTAL = 6425.4 SECONDS (107.1 MIN)
CPU UTILIZATION: STEP = 99.34%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.11 , TOTAL = 6953.3 SECONDS (115.9 MIN)
WALL CLOCK TIME: STEP = 1.11 , TOTAL = 6426.5 SECONDS (107.1 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636752399	-284.636752399	0.012024206	0.000481166	198096654
11330640						
2	1	-284.636782718	-0.000030320	0.002204608	0.000105455	154471610
14971309						
3	2	-284.636781659	0.000001059	0.001553693	0.000211492	141536321
16031364						
4	3	-284.636783566	-0.000001907	0.000329726	0.000028934	135844430
16456380						
5	4	-284.636783454	0.000000113	0.000282930	0.000074907	126408403
17210160						
6	5	-284.636783600	-0.000000146	0.000088741	0.000016919	120895514
17646643						

7 6	-284.636783588	0.000000011	0.000054961	0.000024314	115116534
18031706					
8 7	-284.636783606	-0.000000018	0.000091958	0.000007279	134245861
16625041					
9 8	-284.636783606	0.000000000	0.000053580	0.000008890	153546923
15118754					
10 9	-284.636783610	-0.000000003	0.000083437	0.000006856	148458504
15576927					

-----DISABLING FDIFF OPTION-----

11 10	-284.636783616	-0.000000006	0.000123754	0.000005983	198099567
11330281					
12 11	-284.636783618	-0.000000002	0.000069719	0.000008772	198099465
11330289					
13 12	-284.636783621	-0.000000003	0.000099621	0.000006942	198099345
11330300					
14 13	-284.636783623	-0.000000002	0.000048982	0.000005247	198099457
11330291					
15 14	-284.636783624	-0.000000001	0.000033429	0.000003705	198099468
11330282					
16 15	-284.636783624	0.000000000	0.000023732	0.000002028	198099426
11330288					
17 16	-284.636783624	0.000000000	0.000013786	0.000001653	198099423
11330290					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 56.9 SECONDS (3.3 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 18.5 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
 TIME TO SOLVE SCF EQUATIONS= 1.5 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6367836245 AFTER 17 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6048342050
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998715280

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
 PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 59.81 , TOTAL = 7013.1 SECONDS (116.9 MIN)
 WALL CLOCK TIME: STEP = 55.38 , TOTAL = 6481.9 SECONDS (108.0 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
 END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.63 , TOTAL = 7016.7 SECONDS (116.9 MIN)
 WALL CLOCK TIME: STEP = 3.59 , TOTAL = 6485.5 SECONDS (108.1 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
 USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.96 , TOTAL = 7019.7 SECONDS (117.0 MIN)
 WALL CLOCK TIME: STEP = 2.79 , TOTAL = 6488.3 SECONDS (108.1 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 72 ENERGY= -284.6367836

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0003874	-0.0000523	-0.0006829
2 C	6.0	-0.0000974	0.0004153	-0.0002359
3 C	6.0	-0.0000153	-0.0001078	0.0000530
4 C	6.0	0.0001432	-0.0003303	0.0001064
5 C	6.0	0.0000480	-0.0002403	-0.0001116
6 C	6.0	0.0000643	-0.0001986	-0.0000782
7 C	6.0	-0.0000681	0.0002608	-0.0001336
8 C	6.0	-0.0002332	-0.0001788	-0.0000469
9 C	6.0	-0.0000229	-0.0001622	-0.0000205
10 C	6.0	0.0001733	-0.0002058	0.0000750
11 C	6.0	0.0001193	-0.0000403	0.0001160
12 N	7.0	0.0000411	-0.0000641	-0.0001484
13 C	6.0	-0.0001491	0.0001058	-0.0001769
14 C	6.0	0.0000729	0.0001320	0.0000277

15 C	6.0	0.0001895	-0.0000300	0.0000773
16 C	6.0	0.0000809	-0.0005812	0.0000179
17 C	6.0	0.0001326	0.0001071	-0.0000690
18 C	6.0	0.0000296	0.0002433	0.0002407
19 C	6.0	-0.0000791	0.0002977	0.0001306
20 O	8.0	0.0001091	0.0002363	0.0006188
21 N	7.0	0.0004019	0.0000441	0.0000353
22 H	1.0	-0.0003355	0.0004767	-0.0001592
23 H	1.0	-0.0001387	0.0001134	0.0002824
24 H	1.0	-0.0002082	-0.0002416	0.0001587
25 H	1.0	-0.0000315	-0.0003438	0.0001994
26 H	1.0	-0.0002810	0.0003308	0.0000420
27 H	1.0	0.0002385	-0.0007428	-0.0000001
28 H	1.0	-0.0002791	-0.0000707	-0.0002534
29 H	1.0	-0.0002488	-0.0001280	-0.0000747
30 H	1.0	0.0004773	0.0001262	-0.0000808
31 H	1.0	0.0000738	0.0000384	0.0001439
32 H	1.0	0.0000265	-0.0000031	0.0000553
33 H	1.0	-0.0002486	0.0004665	-0.0003485
34 H	1.0	0.0000165	0.0002807	-0.0002780
35 H	1.0	-0.0003892	0.0000468	0.0005183

MAXIMUM GRADIENT = 0.0007428 RMS GRADIENT = 0.0002367
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000273380
 PREDICTED ENERGY CHANGE WAS -0.0000181419 RATIO= 1.507
 GDIIS STEP HAS LENGTH = 0.054820
 RADIUS OF STEP TAKEN= 0.05000 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 7019.7 SECONDS (117.0 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6488.3 SECONDS (108.1 MIN)
 CPU UTILIZATION: STEP = 88.57% , TOTAL = 100.00%

INSERCH= 73

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1556590966	-1.7393568983	0.8531317711
C	6.0	4.9791386971	0.6364037691	0.5491364715
C	6.0	5.1905206004	-0.7087707343	0.2172271181
C	6.0	4.0586404176	-1.5389851364	-0.0682272555
C	6.0	2.7479745160	-1.0299463429	0.0020664876

C	6.0	2.4689696037	0.3383618520	0.4188029808
C	6.0	3.6460085008	1.1792573087	0.6630198707
C	6.0	3.4943240313	2.5654039233	1.0404374503
C	6.0	2.2250945134	3.1345297945	1.2120067162
C	6.0	1.0655841097	2.3177350764	1.0347470516
C	6.0	1.1615180705	0.9665282180	0.6266826754
N	7.0	-0.0513951118	0.1676681837	0.5715384602
C	6.0	-1.2466584767	0.6980971928	0.3168844734
C	6.0	-2.5517126884	0.0432004242	0.4396551041
C	6.0	-2.8224539113	-1.2840046778	0.9198005687
C	6.0	-4.1224062302	-1.8070923857	1.0398977360
C	6.0	-5.2304857845	-0.9819039324	0.6771534015
C	6.0	-5.0177167802	0.3413455582	0.1979404447
C	6.0	-3.6988127278	0.8415418797	0.0821134685
O	8.0	-1.7002548471	-2.1440234236	1.3042480786
N	7.0	1.6462100578	-1.9685032473	-0.4270944739
H	1.0	5.8352168580	1.3095893030	0.7362157040
H	1.0	6.2108362880	-1.1247619948	0.1501513523
H	1.0	4.2278263842	-2.5880388152	-0.3823536941
H	1.0	4.4063485284	3.1640113925	1.2147478550
H	1.0	2.1108270151	4.1872921598	1.5239866309
H	1.0	0.0787041764	2.7501970349	1.2768349701
H	1.0	-1.2891017271	1.7495240181	-0.0303043779
H	1.0	-4.2974174982	-2.8369419819	1.4069220875
H	1.0	-6.2548368664	-1.3834415012	0.7729968647
H	1.0	-5.8759750214	0.9807734699	-0.0743567384
H	1.0	-3.5328128455	1.8732683374	-0.2796230867
H	1.0	-2.0217983012	-2.9587167155	1.7691561115
H	1.0	1.2994068884	-1.7035157186	-1.3753233355
H	1.0	2.0410274644	-2.9256203903	-0.5173319431

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3854069	5.1784470	4.0152602
2 C	5.3854069	0.0000000	1.4015493 *	2.4414692 *
3 C	5.1784470	1.4015493 *	0.0000000	1.4324430 *
4 C	4.0152602	2.4414692 *	1.4324430 *	0.0000000
5 C	2.8191621 *	2.8379750 *	2.4729495 *	1.4078021 *
6 C	3.1395799	2.5311588 *	2.9230052 *	2.5077248 *
7 C	4.5537886	1.4439167 *	2.4796973 *	2.8449656 *
8 C	5.4509387	2.4833632 *	3.7782242	4.2887760
9 C	5.3071768	3.7768757	4.9552293	5.1809875
10 C	4.1618437	4.2870272	5.1810402	5.0049205

11 C	2.8956598 *	3.8326522	4.3825953	3.8927901
12 N	1.9387911 *	5.0523742	5.3264775	4.4960380
13 C	2.8627326 *	6.2304332	6.5898773	5.7705324
14 C	3.2677723	7.5549718	7.7818450	6.8160123
15 C	3.0134610	8.0430223	8.0642584	6.9563405
16 C	4.2826759	9.4366117	9.4134852	8.2601057
17 C	5.4419905	10.3378789	10.4347261	9.3356198
18 C	5.6144827	10.0073732	10.2621258	9.2729040
19 C	4.7023888	8.6929301	9.0245206	8.1158851
20 O	1.9523518 *	7.2742881	7.1221030	5.9510196
21 N	1.9781884 *	4.3413109	3.8163089	2.4765080 *
22 H	6.4472567	1.1050101 *	2.1814581 *	3.4522063
23 H	6.1267511	2.1858575 *	1.1038985 *	2.2025479 *
24 H	4.3392663	3.4393566	2.1949774 *	1.1080672 *
25 H	6.4993959	2.6758041 *	4.0753423	4.8872387
26 H	6.2767744	4.6675854	5.9298874	6.2545482
27 H	4.5101598	5.3862720	6.2624192	6.0038461
28 H	3.8781546	6.3926228	6.9346947	6.2780631
29 H	4.6196610	9.9425561	9.7961960	8.5839654
30 H	6.4208688	11.4163083	11.4786876	10.3488968
31 H	6.6813138	10.8784571	11.1985225	10.2491856
32 H	5.2857374	8.6411802	9.1110006	8.3257627
33 H	2.6584318 *	7.9640730	7.7128649	6.5087134
34 H	2.5050860 *	4.7664657	4.3204746	3.0576037
35 H	2.6153405 *	4.7389734	3.9208808	2.4890188 *

C C C C

1 CO	2.8191621 *	3.1395799	4.5537886	5.4509387
2 C	2.8379750 *	2.5311588 *	1.4439167 *	2.4833632 *
3 C	2.4729495 *	2.9230052 *	2.4796973 *	3.7782242
4 C	1.4078021 *	2.5077248 *	2.8449656 *	4.2887760
5 C	0.0000000	1.4573196 *	2.4746525 *	3.8159921
6 C	1.4573196 *	0.0000000	1.4670268 *	2.5293275 *
7 C	2.4746525 *	1.4670268 *	0.0000000	1.4445950 *
8 C	3.8159921	2.5293275 *	1.4445950 *	0.0000000
9 C	4.3680912	2.9167109 *	2.4786032 *	1.4015291 *
10 C	3.8863656	2.5033570 *	2.8448028 *	2.4413418 *
11 C	2.6254333 *	1.4653452 *	2.4938458 *	2.8582477 *
12 N	3.0975876	2.5307514 *	3.8343806	4.3059409
13 C	4.3637527	3.7343927	4.9284394	5.1465793
14 C	5.4249251	5.0293942	6.3049397	6.5785264
15 C	5.6512348	5.5571787	6.9263700	7.3982554
16 C	6.9916508	6.9595235	8.3311817	8.7825568
17 C	8.0071143	7.8161026	9.1358069	9.4253740
18 C	7.8882678	7.4899441	8.7165665	8.8380470

19	C	6.7134150	6.1974260	7.3754934	7.4586394
20	O	4.7669266	4.9324114	6.3275509	7.0165484
21	N	1.5096202 *	2.5911585 *	3.8853494	5.1113100
22	H	3.9425204	3.5179048	2.1943057 *	2.6738363 *
23	H	3.4673233	4.0267197	3.4856679	4.6679088
24	H	2.1829779 *	3.5070287	3.9527001	5.3963258
25	H	4.6701265	3.5172803	2.1958528 *	1.1047641 *
26	H	5.4719078	4.0204430	3.4851570	2.1859564 *
27	H	4.7999503	3.5023616	3.9459195	3.4287740
28	H	4.9014781	4.0393287	5.0160957	4.9692364
29	H	7.4078608	7.5394249	8.9320358	9.4884608
30	H	9.0426714	8.8991494	10.2277201	10.5219315
31	H	8.8555824	8.3841517	9.5525541	9.5685069
32	H	6.9250483	6.2341904	7.2736307	7.1834716
33	H	5.4399902	5.7324669	7.1042523	7.8405705
34	H	2.1093237 *	2.9590590 *	4.2393116	5.3737544
35	H	2.0888104 *	3.4224353	4.5628078	5.8898272

C C C N

1	CO	5.3071768	4.1618437	2.8956598 *	1.9387911 *
2	C	3.7768757	4.2870272	3.8326522	5.0523742
3	C	4.9552293	5.1810402	4.3825953	5.3264775
4	C	5.1809875	5.0049205	3.8927901	4.4960380
5	C	4.3680912	3.8863656	2.6254333 *	3.0975876
6	C	2.9167109 *	2.5033570 *	1.4653452 *	2.5307514 *
7	C	2.4786032 *	2.8448028 *	2.4938458 *	3.8343806
8	C	1.4015291 *	2.4413418 *	2.8582477 *	4.3059409
9	C	0.0000000	1.4293491 *	2.4847595 *	3.7940575
10	C	1.4293491 *	0.0000000	1.4147367 *	2.4667777 *
11	C	2.4847595 *	1.4147367 *	0.0000000	1.4534017 *
12	N	3.7940575	2.4667777 *	1.4534017 *	0.0000000
13	C	4.3348029	2.9129057 *	2.4428149 *	1.3322380 *
14	C	5.7420146	4.3142182	3.8308741	2.5068852 *
15	C	6.7146539	5.3011868	4.5850681	3.1476034
16	C	8.0461181	6.6279312	5.9819373	4.5488648
17	C	8.5332744	7.1173019	6.6825630	5.3061899
18	C	7.8286987	6.4508070	6.2255615	4.9833814
19	C	6.4519090	5.0780050	4.8923402	3.7412963
20	O	6.5787537	5.2564042	4.2806974	2.9324938 *
21	N	5.3909838	4.5657361	3.1559123	2.9055739 *
22	H	4.0730539	4.8841453	4.6875525	5.9986084
23	H	5.9291855	6.2535522	5.4859996	6.4080797
24	H	6.2690280	6.0062108	4.8015985	5.1783750
25	H	2.1814550 *	3.4509840	3.9627866	5.4095535
26	H	1.1039462 *	2.1970735 *	3.4755808	4.6625893

27 H	2.1814917 *	1.1043378 *	2.1855568 *	2.6802657 *
28 H	3.9763241	2.6460808 *	2.6552310 *	2.0967595 *
29 H	8.8453168	7.4478853	6.6988907	5.2682306
30 H	9.6184214	8.2070570	7.7811366	6.3975946
31 H	8.4806088	7.1556146	7.0723382	5.9164222
32 H	6.0802333	4.8031629	4.8662419	3.9691079
33 H	7.4480982	6.1572908	5.1813412	3.8847213
34 H	5.5639787	4.6939930	3.3400862	3.0193155
35 H	6.3047532	5.5545671	4.1510393	3.8900264

C C C C

1 CO	2.8627326 *	3.2677723	3.0134610	4.2826759
2 C	6.2304332	7.5549718	8.0430223	9.4366117
3 C	6.5898773	7.7818450	8.0642584	9.4134852
4 C	5.7705324	6.8160123	6.9563405	8.2601057
5 C	4.3637527	5.4249251	5.6512348	6.9916508
6 C	3.7343927	5.0293942	5.5571787	6.9595235
7 C	4.9284394	6.3049397	6.9263700	8.3311817
8 C	5.1465793	6.5785264	7.3982554	8.7825568
9 C	4.3348029	5.7420146	6.7146539	8.0461181
10 C	2.9129057 *	4.3142182	5.3011868	6.6279312
11 C	2.4428149 *	3.8308741	4.5850681	5.9819373
12 N	1.3322380 *	2.5068852 *	3.1476034	4.5488648
13 C	0.0000000	1.4653085 *	2.6029535 *	3.8818357
14 C	1.4653085 *	0.0000000	1.4371200 *	2.5001906 *
15 C	2.6029535 *	1.4371200 *	0.0000000	1.4063855 *
16 C	3.8818357	2.5001906 *	1.4063855 *	0.0000000
17 C	4.3385571	2.8780323 *	2.4390080 *	1.4284116 *
18 C	3.7897625	2.4956948 *	2.8252477 *	2.4751280 *
19 C	2.4675401 *	1.4425753 *	2.4469721 *	2.8481653 *
20 O	3.0427432	2.5012896 *	1.4651836 *	2.4597197 *
21 N	4.0041167	4.7350567	4.7171625	5.9544146
22 H	7.1205842	8.4871831	9.0396735	10.4383995
23 H	7.6788569	8.8447845	9.0674169	10.3938984
24 H	6.4232086	7.3185564	7.2871505	8.5064129
25 H	6.2324457	7.6651710	8.4927867	9.8733025
26 H	4.9904194	6.3315518	7.3917109	8.6614193
27 H	2.6247295 *	3.8662377	4.9818646	6.2027699
28 H	1.1080794 *	2.1740719 *	3.5293292	4.6714524
29 H	4.7949781	3.5040421	2.1964561 *	1.1072154 *
30 H	5.4426733	3.9824054	3.4369597	2.1904284 *
31 H	4.6544116	3.4919867	3.9295750	3.4768898
32 H	2.6388161 *	2.1975139 *	3.4513186	3.9539614
33 H	4.0102647	3.3256411	2.0413512 *	2.5041186 *
34 H	3.8876420	4.6017699	4.7363826	5.9363354

35 H	4.9634791	5.5518450	5.3304506	6.4547644
	C	C	C	O
1 CO	5.4419905	5.6144827	4.7023888	1.9523518 *
2 C	10.3378789	10.0073732	8.6929301	7.2742881
3 C	10.4347261	10.2621258	9.0245206	7.1221030
4 C	9.3356198	9.2729040	8.1158851	5.9510196
5 C	8.0071143	7.8882678	6.7134150	4.7669266
6 C	7.8161026	7.4899441	6.1974260	4.9324114
7 C	9.1358069	8.7165665	7.3754934	6.3275509
8 C	9.4253740	8.8380470	7.4586394	7.0165484
9 C	8.5332744	7.8286987	6.4519090	6.5787537
10 C	7.1173019	6.4508070	5.0780050	5.2564042
11 C	6.6825630	6.2255615	4.8923402	4.2806974
12 N	5.3061899	4.9833814	3.7412963	2.9324938 *
13 C	4.3385571	3.7897625	2.4675401 *	3.0427432
14 C	2.8780323 *	2.4956948 *	1.4425753 *	2.5012896 *
15 C	2.4390080 *	2.8252477 *	2.4469721 *	1.4651836 *
16 C	1.4284116 *	2.4751280 *	2.8481653 *	2.4597197 *
17 C	0.0000000	1.4233429 *	2.4545976 *	3.7691246
18 C	1.4233429 *	0.0000000	1.4153163 *	4.2902831
19 C	2.4545976 *	1.4153163 *	0.0000000	3.7949238
20 O	3.7691246	4.2902831	3.7949238	0.0000000
21 N	7.0343221	7.0805361	6.0601085	3.7718937
22 H	11.3006285	10.9093265	9.5678962	8.3086362
23 H	11.4543437	11.3239639	10.1030750	8.0595407
24 H	9.6520409	9.7158686	8.6492405	6.1793141
25 H	10.5045798	9.8901136	8.5070773	8.0915912
26 H	9.0184582	8.2076696	6.8574745	7.3931175
27 H	6.5173379	5.7393454	4.3977219	5.2075753
28 H	4.8472367	3.9921964	2.5775524 *	4.1363980
29 H	2.2009873 *	3.4759142	3.9553368	2.6899688 *
30 H	1.1044064 *	2.1991013 *	3.4584867	4.6481104
31 H	2.1985282 *	1.1043645 *	2.1872138 *	5.3945849
32 H	3.4568083	2.1862740 *	1.1058340 *	4.6910073
33 H	3.9237653	4.7259557	4.4833532	0.9915921 *
34 H	6.8827961	6.8236843	5.7951393	4.0462477
35 H	7.6210061	7.8109251	6.8917786	4.2339392
	N	H	H	H
1 CO	1.9781884 *	6.4472567	6.1267511	4.3392663
2 C	4.3413109	1.1050101 *	2.1858575 *	3.4393566
3 C	3.8163089	2.1814581 *	1.1038985 *	2.1949774 *
4 C	2.4765080 *	3.4522063	2.2025479 *	1.1080672 *

5 C	1.5096202 *	3.9425204	3.4673233	2.1829779 *
6 C	2.5911585 *	3.5179048	4.0267197	3.5070287
7 C	3.8853494	2.1943057 *	3.4856679	3.9527001
8 C	5.1113100	2.6738363 *	4.6679088	5.3963258
9 C	5.3909838	4.0730539	5.9291855	6.2690280
10 C	4.5657361	4.8841453	6.2535522	6.0062108
11 C	3.1559123	4.6875525	5.4859996	4.8015985
12 N	2.9055739 *	5.9986084	6.4080797	5.1783750
13 C	4.0041167	7.1205842	7.6788569	6.4232086
14 C	4.7350567	8.4871831	8.8447845	7.3185564
15 C	4.7171625	9.0396735	9.0674169	7.2871505
16 C	5.9544146	10.4383995	10.3938984	8.5064129
17 C	7.0343221	11.3006285	11.4543437	9.6520409
18 C	7.0805361	10.9093265	11.3239639	9.7158686
19 C	6.0601085	9.5678962	10.1030750	8.6492405
20 O	3.7718937	8.3086362	8.0595407	6.1793141
21 N	0.0000000	5.4449021	4.6777051	2.6552907 *
22 H	5.4449021	0.0000000	2.5319217 *	4.3619269
23 H	4.6777051	2.5319217 *	0.0000000	2.5213229 *
24 H	2.6552907 *	4.3619269	2.5213229 *	0.0000000
25 H	6.0544791	2.3894642 *	4.7731666	5.9723266
26 H	6.4742879	4.7720893	6.8494831	7.3498932
27 H	5.2560996	5.9586121	7.3408288	6.9616725
28 H	4.7536538	7.1789283	8.0338754	7.0267265
29 H	6.2804865	10.9687669	10.7207477	8.7145421
30 H	8.0130555	12.3864106	12.4839040	10.6147124
31 H	8.0873930	11.7438138	12.2708880	10.7199854
32 H	6.4500570	9.4397904	10.2035087	8.9521694
33 H	4.3884308	9.0010049	8.5884130	6.6199853
34 H	1.0438529 *	5.8404598	5.1753423	3.2162106
35 H	1.0392771 *	5.8227361	4.5908529	2.2168153 *

H H H H

1 CO	6.4993959	6.2767744	4.5101598	3.8781546
2 C	2.6758041 *	4.6675854	5.3862720	6.3926228
3 C	4.0753423	5.9298874	6.2624192	6.9346947
4 C	4.8872387	6.2545482	6.0038461	6.2780631
5 C	4.6701265	5.4719078	4.7999503	4.9014781
6 C	3.5172803	4.0204430	3.5023616	4.0393287
7 C	2.1958528 *	3.4851570	3.9459195	5.0160957
8 C	1.1047641 *	2.1859564 *	3.4287740	4.9692364
9 C	2.1814550 *	1.1039462 *	2.1814917 *	3.9763241
10 C	3.4509840	2.1970735 *	1.1043378 *	2.6460808 *
11 C	3.9627866	3.4755808	2.1855568 *	2.6552310 *
12 N	5.4095535	4.6625893	2.6802657 *	2.0967595 *

13 C	6.2324457	4.9904194	2.6247295 *	1.1080794 *
14 C	7.6651710	6.3315518	3.8662377	2.1740719 *
15 C	8.4927867	7.3917109	4.9818646	3.5293292
16 C	9.8733025	8.6614193	6.2027699	4.6714524
17 C	10.5045798	9.0184582	6.5173379	4.8472367
18 C	9.8901136	8.2076696	5.7393454	3.9921964
19 C	8.5070773	6.8574745	4.3977219	2.5775524 *
20 O	8.0915912	7.3931175	5.2075753	4.1363980
21 N	6.0544791	6.4742879	5.2560996	4.7536538
22 H	2.3894642 *	4.7720893	5.9586121	7.1789283
23 H	4.7731666	6.8494831	7.3408288	8.0338754
24 H	5.9723266	7.3498932	6.9616725	7.0267265
25 H	0.0000000	2.5322226 *	4.3478274	5.9990902
26 H	2.5322226 *	0.0000000	2.5011696 *	4.4629642
27 H	4.3478274	2.5011696 *	0.0000000	2.1402927 *
28 H	5.9990902	4.4629642	2.1402927 *	0.0000000
29 H	10.5737371	9.5088994	7.0981326	5.6702076
30 H	11.5989373	10.0787594	7.5798788	5.9261532
31 H	10.5903020	8.7535976	6.3572622	4.6510563
32 H	8.1810418	6.3606906	4.0292209	2.2609096 *
33 H	8.8947310	8.2585800	6.1029654	5.0933715
34 H	6.3288526	6.6155890	5.3253747	4.5202806
35 H	6.7585841	7.4003634	6.2677469	5.7605496

H H H H

1 CO	4.6196610	6.4208688	6.6813138	5.2857374
2 C	9.9425561	11.4163083	10.8784571	8.6411802
3 C	9.7961960	11.4786876	11.1985225	9.1110006
4 C	8.5839654	10.3488968	10.2491856	8.3257627
5 C	7.4078608	9.0426714	8.8555824	6.9250483
6 C	7.5394249	8.8991494	8.3841517	6.2341904
7 C	8.9320358	10.2277201	9.5525541	7.2736307
8 C	9.4884608	10.5219315	9.5685069	7.1834716
9 C	8.8453168	9.6184214	8.4806088	6.0802333
10 C	7.4478853	8.2070570	7.1556146	4.8031629
11 C	6.6988907	7.7811366	7.0723382	4.8662419
12 N	5.2682306	6.3975946	5.9164222	3.9691079
13 C	4.7949781	5.4426733	4.6544116	2.6388161 *
14 C	3.5040421	3.9824054	3.4919867	2.1975139 *
15 C	2.1964561 *	3.4369597	3.9295750	3.4513186
16 C	1.1072154 *	2.1904284 *	3.4768898	3.9539614
17 C	2.2009873 *	1.1044064 *	2.1985282 *	3.4568083
18 C	3.4759142	2.1991013 *	1.1043645 *	2.1862740 *
19 C	3.9553368	3.4584867	2.1872138 *	1.1058340 *
20 O	2.6899688 *	4.6481104	5.3945849	4.6910073

21 N	6.2804865	8.0130555	8.0873930	6.4500570
22 H	10.9687669	12.3864106	11.7438138	9.4397904
23 H	10.7207477	12.4839040	12.2708880	10.2035087
24 H	8.7145421	10.6147124	10.7199854	8.9521694
25 H	10.5737371	11.5989373	10.5903020	8.1810418
26 H	9.5088994	10.0787594	8.7535976	6.3606906
27 H	7.0981326	7.5798788	6.3572622	4.0292209
28 H	5.6702076	5.9261532	4.6510563	2.2609096 *
29 H	0.0000000	2.5191299 *	4.3887335	5.0611398
30 H	2.5191299 *	0.0000000	2.5398931 *	4.3730519
31 H	4.3887335	2.5398931 *	0.0000000	2.5157683 *
32 H	5.0611398	4.3730519	2.5157683 *	0.0000000
33 H	2.3074846 *	4.6251963	5.8114371	5.4615694
34 H	6.3521640	7.8603006	7.7707161	6.1109975
35 H	6.6246888	8.5360781	8.8394043	7.3589085

H H H

1 CO	2.6584318 *	2.5050860 *	2.6153405 *
2 C	7.9640730	4.7664657	4.7389734
3 C	7.7128649	4.3204746	3.9208808
4 C	6.5087134	3.0576037	2.4890188 *
5 C	5.4399902	2.1093237 *	2.0888104 *
6 C	5.7324669	2.9590590 *	3.4224353
7 C	7.1042523	4.2393116	4.5628078
8 C	7.8405705	5.3737544	5.8898272
9 C	7.4480982	5.5639787	6.3047532
10 C	6.1572908	4.6939930	5.5545671
11 C	5.1813412	3.3400862	4.1510393
12 N	3.8847213	3.0193155	3.8900264
13 C	4.0102647	3.8876420	4.9634791
14 C	3.3256411	4.6017699	5.5518450
15 C	2.0413512 *	4.7363826	5.3304506
16 C	2.5041186 *	5.9363354	6.4547644
17 C	3.9237653	6.8827961	7.6210061
18 C	4.7259557	6.8236843	7.8109251
19 C	4.4833532	5.7951393	6.8917786
20 O	0.9915921 *	4.0462477	4.2339392
21 N	4.3884308	1.0438529 *	1.0392771 *
22 H	9.0010049	5.8404598	5.8227361
23 H	8.5884130	5.1753423	4.5908529
24 H	6.6199853	3.2162106	2.2168153 *
25 H	8.8947310	6.3288526	6.7585841
26 H	8.2585800	6.6155890	7.4003634
27 H	6.1029654	5.3253747	6.2677469
28 H	5.0933715	4.5202806	5.7605496

29 H	2.3074846 *	6.3521640	6.6246888
30 H	4.6251963	7.8603006	8.5360781
31 H	5.8114371	7.7707161	8.8394043
32 H	5.4615694	6.1109975	7.3589085
33 H	0.0000000	4.7427507	4.6621536
34 H	4.7427507	0.0000000	1.6672403 *
35 H	4.6621536	1.6672403 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.65 , TOTAL = 7020.3 SECONDS (117.0 MIN)
WALL CLOCK TIME: STEP = 0.65 , TOTAL = 6488.9 SECONDS (108.1 MIN)

CPU UTILIZATION: STEP = 99.53%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.86 , TOTAL = 7021.2 SECONDS (117.0 MIN)
WALL CLOCK TIME: STEP = 0.87 , TOTAL = 6489.8 SECONDS (108.2 MIN)

CPU UTILIZATION: STEP = 98.92%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636748224	-284.636748224	0.006905956	0.001072917	198072145
11332722					
2 1	-284.636814543	-0.000066320	0.001117097	0.000114110	156033576
14913771					
3 2	-284.636813838	0.000000706	0.000746525	0.000279967	139573181
16233204					
4 3	-284.636815589	-0.000001752	0.000644397	0.000098661	134277935
16681353					
5 4	-284.636815303	0.000000287	0.000422402	0.000122531	131836541
16839132					
6 5	-284.636815782	-0.000000479	0.000255325	0.000013064	127096047
17167306					
7 6	-284.636815759	0.000000023	0.000142418	0.000015196	117772093
17829168					

8 7	-284.636815785	-0.000000026	0.000054053	0.000010598	135968077
16466378					
9 8	-284.636815790	-0.000000005	0.000102731	0.000009108	127222667
17200390					
10 9	-284.636815795	-0.000000005	0.000079969	0.000005401	152575866
15326933					
11 10	-284.636815797	-0.000000002	0.000075841	0.000005167	151364545
15371056					
12 11	-284.636815799	-0.000000001	0.000039450	0.000005816	150269280
15462314					
13 12	-284.636815801	-0.000000002	0.000089440	0.000004984	145579657
15851632					

-----DISABLING FDIFF OPTION-----

14 13	-284.636815780	0.000000021	0.000070025	0.000004087	198069219
11332925					
15 14	-284.636815780	-0.000000001	0.000036110	0.000005081	198069230
11332923					
16 15	-284.636815781	-0.000000001	0.000064329	0.000004332	198069232
11332920					
17 16	-284.636815783	-0.000000001	0.000078475	0.000002198	198069250
11332920					
18 17	-284.636815784	-0.000000001	0.000058003	0.000002219	198069250
11332920					
19 18	-284.636815784	0.000000000	0.000011923	0.000001782	198069227
11332923					
20 19	-284.636815784	0.000000000	0.000012616	0.000001386	198069227
11332923					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 65.8 SECONDS (3.3 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 21.8 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
 TIME TO SOLVE SCF EQUATIONS= 2.8 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6368157842 AFTER 20 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6038251989
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998670708

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 69.62 , TOTAL = 7090.8 SECONDS (118.2 MIN)
WALL CLOCK TIME: STEP = 64.20 , TOTAL = 6554.0 SECONDS (109.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.98 , TOTAL = 7094.8 SECONDS (118.2 MIN)
WALL CLOCK TIME: STEP = 3.96 , TOTAL = 6558.0 SECONDS (109.3 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.85 , TOTAL = 7097.7 SECONDS (118.3 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 6560.7 SECONDS (109.3 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 73 ENERGY= -284.6368158

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0001249	-0.0000674	-0.0002811
2 C	6.0	0.0000555	0.0000415	-0.0000991
3 C	6.0	0.0002938	-0.0002687	0.0001838
4 C	6.0	0.0000665	0.0000152	0.0002032
5 C	6.0	0.0000588	-0.0000639	-0.0000704
6 C	6.0	-0.0001150	-0.0001675	-0.0001439
7 C	6.0	-0.0002019	-0.0002930	-0.0002645
8 C	6.0	-0.0002098	0.0003380	-0.0000536
9 C	6.0	-0.0000691	0.0005304	0.0001066
10 C	6.0	0.0006383	-0.0002966	-0.0000191

11	C	6.0	0.0000549	-0.0002690	-0.0000902
12	N	7.0	-0.0000621	-0.0000808	-0.0002994
13	C	6.0	-0.0002802	-0.0000183	-0.0000038
14	C	6.0	0.0000024	0.0000011	0.0000546
15	C	6.0	0.0000957	-0.0000021	0.0003037
16	C	6.0	0.0000473	-0.0003631	0.0000765
17	C	6.0	0.0002514	-0.0000544	-0.0000552
18	C	6.0	0.0001715	0.0000862	-0.0002434
19	C	6.0	-0.0001380	0.0001613	-0.0001414
20	O	8.0	0.0001628	0.0004704	0.0003385
21	N	7.0	0.0000850	0.0001559	-0.0003475
22	H	1.0	-0.0002754	0.0003805	-0.0002821
23	H	1.0	-0.0000758	0.0002285	0.0002091
24	H	1.0	-0.0000004	-0.0001838	0.0000739
25	H	1.0	-0.0000500	-0.0003378	0.0002482
26	H	1.0	-0.0001542	-0.0002107	0.0000085
27	H	1.0	-0.0003019	-0.0003552	0.0001188
28	H	1.0	-0.0001786	-0.0001156	-0.0001573
29	H	1.0	-0.0001613	-0.0002943	-0.0000284
30	H	1.0	0.0005318	0.0002402	0.0000328
31	H	1.0	-0.0000430	0.0003032	0.0002526
32	H	1.0	0.0000155	0.0000686	0.0002793
33	H	1.0	-0.0003853	0.0003283	-0.0002661
34	H	1.0	0.0002134	0.0000349	0.0000706
35	H	1.0	-0.0001677	0.0000583	0.0002859

MAXIMUM GRADIENT = 0.0006383 RMS GRADIENT = 0.0002183
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000321597
 PREDICTED ENERGY CHANGE WAS -0.0000313386 RATIO= 1.026
 GDIIS STEP HAS LENGTH = 0.061451
 RADIUS OF STEP TAKEN= 0.06145 CURRENT TRUST RADIUS= 0.10000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 7097.7 SECONDS (118.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6560.7 SECONDS (109.3
 MIN)
 CPU UTILIZATION: STEP = 86.83% , TOTAL = 100.00%

1NSERCH= 74

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1559165947	-1.7383324306	0.8550557395

C	6.0	4.9795662135	0.6343467416	0.5527993864
C	6.0	5.1906027592	-0.7095896426	0.2160149010
C	6.0	4.0581141243	-1.5378493414	-0.0724948658
C	6.0	2.7473527454	-1.0287812574	-0.0007351006
C	6.0	2.4685658388	0.3390291838	0.4182109529
C	6.0	3.6469831307	1.1781180064	0.6661343530
C	6.0	3.4957930252	2.5635976234	1.0455455836
C	6.0	2.2260358497	3.1334153172	1.2141024464
C	6.0	1.0647739138	2.3196791096	1.0326807759
C	6.0	1.1607826413	0.9684236888	0.6245228220
N	7.0	-0.0517227518	0.1682844896	0.5700061302
C	6.0	-1.2473095776	0.6981593606	0.3161414052
C	6.0	-2.5523407060	0.0426940219	0.4385087944
C	6.0	-2.8226736829	-1.2827830351	0.9232752690
C	6.0	-4.1225710433	-1.8050356130	1.0458346302
C	6.0	-5.2314106509	-0.9830424036	0.6780546056
C	6.0	-5.0185564583	0.3373882630	0.1915127000
C	6.0	-3.6996683351	0.8383689994	0.0762354814
O	8.0	-1.7001729211	-2.1423604542	1.3086676251
N	7.0	1.6449563855	-1.9675756316	-0.4294880676
H	1.0	5.8370163448	1.3053809757	0.7412439841
H	1.0	6.2116099853	-1.1256678074	0.1463895543
H	1.0	4.2286829387	-2.5851683704	-0.3901601611
H	1.0	4.4074445092	3.1620533084	1.2238256595
H	1.0	2.1132086952	4.1860974079	1.5285717484
H	1.0	0.0788313314	2.7551520753	1.2720849080
H	1.0	-1.2894206835	1.7499457116	-0.0302080377
H	1.0	-4.2957222696	-2.8334437944	1.4176193988
H	1.0	-6.2558514227	-1.3842082421	0.7768658054
H	1.0	-5.8768743566	0.9762345720	-0.0828862191
H	1.0	-3.5343100235	1.8703120527	-0.2865390316
H	1.0	-2.0201942597	-2.9563311468	1.7771305007
H	1.0	1.2964160723	-1.7018415114	-1.3769610809
H	1.0	2.0421430439	-2.9235652269	-0.5246755965

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3841026	5.1782960	4.0159294
2 C	5.3841026	0.0000000	1.4014725 *	2.4410044 *
3 C	5.1782960	1.4014725 *	0.0000000	1.4324045 *
4 C	4.0159294	2.4410044 *	1.4324045 *	0.0000000
5 C	2.8198195 *	2.8381635 *	2.4735267 *	1.4079756 *
6 C	3.1392055	2.5318865 *	2.9240331 *	2.5080129 *

7 C	4.5529024	1.4437138 *	2.4796793 *	2.8444825 *
8 C	5.4495562	2.4832218 *	3.7781286	4.2881332
9 C	5.3054910	3.7768499	4.9551511	5.1800152
10 C	4.1623347	4.2890827	5.1832303	5.0061986
11 C	2.8964513 *	3.8340396	4.3842967	3.8938115
12 N	1.9389573 *	5.0528585	5.3270958	4.4960493
13 C	2.8628595 *	6.2316981	6.5907889	5.7704674
14 C	3.2680612	7.5559736	7.7825836	6.8159633
15 C	3.0139972	8.0428593	8.0648228	6.9571444
16 C	4.2832584	9.4362372	9.4140219	8.2610931
17 C	5.4428933	10.3390369	10.4358335	9.3362951
18 C	5.6146306	10.0090544	10.2627333	9.2721176
19 C	4.7022852	8.6947024	9.0251113	8.1149075
20 O	1.9529646 *	7.2732630	7.1224653	5.9523872
21 N	1.9798598 *	4.3421782	3.8171732	2.4769819 *
22 H	6.4460871	1.1049973 *	2.1803263 *	3.4511770
23 H	6.1277229	2.1864931 *	1.1047282 *	2.2034855 *
24 H	4.3422482	3.4377719	2.1932928 *	1.1076471 *
25 H	6.4980967	2.6771066 *	4.0765964	4.8878997
26 H	6.2756263	4.6672336	5.9296637	6.2537699
27 H	4.5134531	5.3881712	6.2649762	6.0060343
28 H	3.8782440	6.3941110	6.9354628	6.2775404
29 H	4.6187482	9.9400433	9.7951505	8.5840310
30 H	6.4220158	11.4175032	11.4800251	10.3500195
31 H	6.6815549	10.8804083	11.1991247	10.2481570
32 H	5.2861447	8.6439683	9.1122202	8.3250395
33 H	2.6587969 *	7.9616959	7.7123617	6.5099184
34 H	2.5067847 *	4.7694178	4.3228262	3.0586765
35 H	2.6203598 *	4.7379473	3.9195802	2.4877330 *

C C C C

1 CO	2.8198195 *	3.1392055	4.5529024	5.4495562
2 C	2.8381635 *	2.5318865 *	1.4437138 *	2.4832218 *
3 C	2.4735267 *	2.9240331 *	2.4796793 *	3.7781286
4 C	1.4079756 *	2.5080129 *	2.8444825 *	4.2881332
5 C	0.0000000	1.4574441 *	2.4747634 *	3.8157636
6 C	1.4574441 *	0.0000000	1.4677205 *	2.5293179 *
7 C	2.4747634 *	1.4677205 *	0.0000000	1.4444255 *
8 C	3.8157636	2.5293179 *	1.4444255 *	0.0000000
9 C	4.3670908	2.9156231 *	2.4784164 *	1.4019226 *
10 C	3.8873136	2.5042322 *	2.8469848 *	2.4432592 *
11 C	2.6262102 *	1.4659464 *	2.4953749 *	2.8590407 *
12 N	3.0973433	2.5306225 *	3.8352874	4.3068005
13 C	4.3634919	3.7345847	4.9302086	5.1486807
14 C	5.4247346	5.0296848	6.3065535	6.5805296

15 C	5.6518587	5.5572098	6.9266597	7.3981495
16 C	6.9924053	6.9594548	8.3312274	8.7820514
17 C	8.0077158	7.8169706	9.1376492	9.4275017
18 C	7.8875043	7.4905537	8.7191553	8.8419188
19 C	6.7123957	6.1978545	7.3781229	7.4626162
20 O	4.7681316	4.9324021	6.3269664	7.0152218
21 N	1.5101131 *	2.5917855 *	3.8863721	5.1120301
22 H	3.9426980	3.5191824	2.1950132 *	2.6752636 *
23 H	3.4687333	4.0285982	3.4863842	4.6684926
24 H	2.1836510 *	3.5074788	3.9517663	5.3951988
25 H	4.6710329	3.5181999	2.1966612 *	1.1050074 *
26 H	5.4713689	4.0198400	3.4848533	2.1857171 *
27 H	4.8020026	3.5039380	3.9479007	3.4298164
28 H	4.9007889	4.0390875	5.0179640	4.9716743
29 H	7.4076610	7.5378376	8.9299455	9.4854734
30 H	9.0437092	8.9002043	10.2295606	10.5238743
31 H	8.8546107	8.3847183	9.5553990	9.5728770
32 H	6.9242843	6.2350636	7.2772035	7.1887025
33 H	5.4411175	5.7319307	7.1024560	7.8377896
34 H	2.1100297 *	2.9600221 *	4.2418830	5.3758505
35 H	2.0885499 *	3.4227757	4.5626029	5.8896221

C C C N

1 CO	5.3054910	4.1623347	2.8964513 *	1.9389573 *
2 C	3.7768499	4.2890827	3.8340396	5.0528585
3 C	4.9551511	5.1832303	4.3842967	5.3270958
4 C	5.1800152	5.0061986	3.8938115	4.4960493
5 C	4.3670908	3.8873136	2.6262102 *	3.0973433
6 C	2.9156231 *	2.5042322 *	1.4659464 *	2.5306225 *
7 C	2.4784164 *	2.8469848 *	2.4953749 *	3.8352874
8 C	1.4019226 *	2.4432592 *	2.8590407 *	4.3068005
9 C	0.0000000	1.4295488 *	2.4838594 *	3.7940803
10 C	1.4295488 *	0.0000000	1.4148151 *	2.4676166 *
11 C	2.4838594 *	1.4148151 *	0.0000000	1.4537414 *
12 N	3.7940803	2.4676166 *	1.4537414 *	0.0000000
13 C	4.3360044	2.9135005 *	2.4427546 *	1.3321571 *
14 C	5.7434298	4.3152311	3.8313003	2.5072205 *
15 C	6.7139300	5.3011274	4.5853145	3.1477873
16 C	8.0449625	6.6273669	5.9819233	4.5488692
17 C	8.5349915	7.1186845	6.6836532	5.3072022
18 C	7.8324693	6.4532123	6.2265508	4.9841038
19 C	6.4556912	5.0802537	4.8930069	3.7417014
20 O	6.5770714	5.2565099	4.2813665	2.9329318 *
21 N	5.3906541	4.5667387	3.1568109	2.9051002 *
22 H	4.0748601	4.8875386	4.6898108	5.9999632

23 H	5.9299748	6.2566644	5.4885961	6.4096100
24 H	6.2678907	6.0076889	4.8030834	5.1793141
25 H	2.1816183 *	3.4524741	3.9638350	5.4105734
26 H	1.1044277 *	2.1974168 *	3.4753193	4.6635391
27 H	2.1810393 *	1.1040986 *	2.1868593 *	2.6836250 *
28 H	3.9775283	2.6451013 *	2.6538548 *	2.0961406 *
29 H	8.8418412	7.4456546	6.6975103	5.2669111
30 H	9.6199018	8.2082750	7.7823227	6.3987684
31 H	8.4848549	7.1579196	7.0731255	5.9170468
32 H	6.0851409	4.8056056	4.8669633	3.9697584
33 H	7.4452994	6.1569082	5.1817776	3.8852609
34 H	5.5639475	4.6938960	3.3398579	3.0175372
35 H	6.3042985	5.5562776	4.1527137	3.8912899

C C C C

1 CO	2.8628595 *	3.2680612	3.0139972	4.2832584
2 C	6.2316981	7.5559736	8.0428593	9.4362372
3 C	6.5907889	7.7825836	8.0648228	9.4140219
4 C	5.7704674	6.8159633	6.9571444	8.2610931
5 C	4.3634919	5.4247346	5.6518587	6.9924053
6 C	3.7345847	5.0296848	5.5572098	6.9594548
7 C	4.9302086	6.3065535	6.9266597	8.3312274
8 C	5.1486807	6.5805296	7.3981495	8.7820514
9 C	4.3360044	5.7434298	6.7139300	8.0449625
10 C	2.9135005 *	4.3152311	5.3011274	6.6273669
11 C	2.4427546 *	3.8313003	4.5853145	5.9819233
12 N	1.3321571 *	2.5072205 *	3.1477873	4.5488692
13 C	0.0000000	1.4655084 *	2.6027901 *	3.8814386
14 C	1.4655084 *	0.0000000	1.4369996 *	2.4997145 *
15 C	2.6027901 *	1.4369996 *	0.0000000	1.4062367 *
16 C	3.8814386	2.4997145 *	1.4062367 *	0.0000000
17 C	4.3394103	2.8787034 *	2.4396703 *	1.4284468 *
18 C	3.7905133	2.4960112 *	2.8253022 *	2.4743961 *
19 C	2.4680513 *	1.4424636 *	2.4466062 *	2.8472016 *
20 O	3.0428188	2.5015654 *	1.4654039 *	2.4598540 *
21 N	4.0034121	4.7341214	4.7179050	5.9554487
22 H	7.1229982	8.4892484	9.0400199	10.4384313
23 H	7.6805366	8.8463119	9.0689866	10.3954721
24 H	6.4238304	7.3194696	7.2899212	8.5096493
25 H	6.2346538	7.6671856	8.4924384	9.8724272
26 H	4.9928731	6.3343019	7.3917503	8.6609271
27 H	2.6274887 *	3.8697990	4.9845079	6.2046984
28 H	1.1081452 *	2.1747117 *	3.5295097	4.6714560
29 H	4.7935680	3.5028853	2.1951759 *	1.1071715 *
30 H	5.4437132	3.9832810	3.4377947	2.1909644 *

31 H	4.6550423	3.4922593	3.9298426	3.4766442
32 H	2.6396092 *	2.1977593 *	3.4513889	3.9534101
33 H	4.0108778	3.3270467	2.0429893 *	2.5060453 *
34 H	3.8855039	4.5991590	4.7364119	5.9368350
35 H	4.9643087	5.5529901	5.3343387	6.4592036

C C C O

1 CO	5.4428933	5.6146306	4.7022852	1.9529646 *
2 C	10.3390369	10.0090544	8.6947024	7.2732630
3 C	10.4358335	10.2627333	9.0251113	7.1224653
4 C	9.3362951	9.2721176	8.1149075	5.9523872
5 C	8.0077158	7.8875043	6.7123957	4.7681316
6 C	7.8169706	7.4905537	6.1978545	4.9324021
7 C	9.1376492	8.7191553	7.3781229	6.3269664
8 C	9.4275017	8.8419188	7.4626162	7.0152218
9 C	8.5349915	7.8324693	6.4556912	6.5770714
10 C	7.1186845	6.4532123	5.0802537	5.2565099
11 C	6.6836532	6.2265508	4.8930069	4.2813665
12 N	5.3072022	4.9841038	3.7417014	2.9329318 *
13 C	4.3394103	3.7905133	2.4680513 *	3.0428188
14 C	2.8787034 *	2.4960112 *	1.4424636 *	2.5015654 *
15 C	2.4396703 *	2.8253022 *	2.4466062 *	1.4654039 *
16 C	1.4284468 *	2.4743961 *	2.8472016 *	2.4598540 *
17 C	0.0000000	1.4232242 *	2.4547831 *	3.7697919
18 C	1.4232242 *	0.0000000	1.4155340 *	4.2905545
19 C	2.4547831 *	1.4155340 *	0.0000000	3.7949465
20 O	3.7697919	4.2905545	3.7949465	0.0000000
21 N	7.0342292	7.0781992	6.0575651	3.7738078
22 H	11.3026966	10.9125009	9.5712429	8.3077140
23 H	11.4562529	11.3251582	10.1042466	8.0610708
24 H	9.6540800	9.7155091	8.6485193	6.1833184
25 H	10.5065319	9.8941345	8.5112720	8.0899317
26 H	9.0214644	8.2135475	6.8633888	7.3918615
27 H	6.5211686	5.7442650	4.4024054	5.2107412
28 H	4.8487261	3.9938618	2.5790688 *	4.1365871
29 H	2.2014664 *	3.4756298	3.9543394	2.6881858 *
30 H	1.1046160 *	2.1994162 *	3.4590178	4.6488509
31 H	2.1987316 *	1.1045945 *	2.1873620 *	5.3950803
32 H	3.4571987	2.1866358 *	1.1062799 *	4.6915119
33 H	3.9260345	4.7278904	4.4847995	0.9921791 *
34 H	6.8812995	6.8189036	5.7901044	4.0479877
35 H	7.6234357	7.8102638	6.8906924	4.2398534

N H H H

1 CO	1.9798598 *	6.4460871	6.1277229	4.3422482
2 C	4.3421782	1.1049973 *	2.1864931 *	3.4377719
3 C	3.8171732	2.1803263 *	1.1047282 *	2.1932928 *
4 C	2.4769819 *	3.4511770	2.2034855 *	1.1076471 *
5 C	1.5101131 *	3.9426980	3.4687333	2.1836510 *
6 C	2.5917855 *	3.5191824	4.0285982	3.5074788
7 C	3.8863721	2.1950132 *	3.4863842	3.9517663
8 C	5.1120301	2.6752636 *	4.6684926	5.3951988
9 C	5.3906541	4.0748601	5.9299748	6.2678907
10 C	4.5667387	4.8875386	6.2566644	6.0076889
11 C	3.1568109	4.6898108	5.4885961	4.8030834
12 N	2.9051002 *	5.9999632	6.4096100	5.1793141
13 C	4.0034121	7.1229982	7.6805366	6.4238304
14 C	4.7341214	8.4892484	8.8463119	7.3194696
15 C	4.7179050	9.0400199	9.0689866	7.2899212
16 C	5.9554487	10.4384313	10.3954721	8.5096493
17 C	7.0342292	11.3026966	11.4562529	9.6540800
18 C	7.0781992	10.9125009	11.3251582	9.7155091
19 C	6.0575651	9.5712429	10.1042466	8.6485193
20 O	3.7738078	8.3077140	8.0610708	6.1833184
21 N	0.0000000	5.4457529	4.6791846	2.6568045 *
22 H	5.4457529	0.0000000	2.5306462 *	4.3592644
23 H	4.6791846	2.5306462 *	0.0000000	2.5199260 *
24 H	2.6568045 *	4.3592644	2.5199260 *	0.0000000
25 H	6.0562265	2.3924450 *	4.7749800	5.9722243
26 H	6.4746390	4.7733799	6.8499759	7.3489321
27 H	5.2585412	5.9615705	7.3443126	6.9644346
28 H	4.7528895	7.1818438	8.0352847	7.0265388
29 H	6.2811780	10.9663005	10.7208468	8.7175221
30 H	8.0136366	12.3884063	12.4860697	10.6174251
31 H	8.0848061	11.7474577	12.2720012	10.7191556
32 H	6.4478382	9.4444292	10.2052084	8.9513185
33 H	4.3909147	8.9983893	8.5891353	6.6244529
34 H	1.0439349 *	5.8435632	5.1780020	3.2174884
35 H	1.0395836 *	5.8213058	4.5899039	2.2166559 *

H H H H

1 CO	6.4980967	6.2756263	4.5134531	3.8782440
2 C	2.6771066 *	4.6672336	5.3881712	6.3941110
3 C	4.0765964	5.9296637	6.2649762	6.9354628
4 C	4.8878997	6.2537699	6.0060343	6.2775404
5 C	4.6710329	5.4713689	4.8020026	4.9007889
6 C	3.5181999	4.0198400	3.5039380	4.0390875
7 C	2.1966612 *	3.4848533	3.9479007	5.0179640
8 C	1.1050074 *	2.1857171 *	3.4298164	4.9716743

9 C	2.1816183 *	1.1044277 *	2.1810393 *	3.9775283
10 C	3.4524741	2.1974168 *	1.1040986 *	2.6451013 *
11 C	3.9638350	3.4753193	2.1868593 *	2.6538548 *
12 N	5.4105734	4.6635391	2.6836250 *	2.0961406 *
13 C	6.2346538	4.9928731	2.6274887 *	1.1081452 *
14 C	7.6671856	6.3343019	3.8697990	2.1747117 *
15 C	8.4924384	7.3917503	4.9845079	3.5295097
16 C	9.8724272	8.6609271	6.2046984	4.6714560
17 C	10.5065319	9.0214644	6.5211686	4.8487261
18 C	9.8941345	8.2135475	5.7442650	3.9938618
19 C	8.5112720	6.8633888	4.4024054	2.5790688 *
20 O	8.0899317	7.3918615	5.2107412	4.1365871
21 N	6.0562265	6.4746390	5.2585412	4.7528895
22 H	2.3924450 *	4.7733799	5.9615705	7.1818438
23 H	4.7749800	6.8499759	7.3443126	8.0352847
24 H	5.9722243	7.3489321	6.9644346	7.0265388
25 H	0.0000000	2.5308209 *	4.3479638	6.0017432
26 H	2.5308209 *	0.0000000	2.5004162 *	4.4657044
27 H	4.3479638	2.5004162 *	0.0000000	2.1397477 *
28 H	6.0017432	4.4657044	2.1397477 *	0.0000000
29 H	10.5701776	9.5058227	7.0986128	5.6693485
30 H	11.6006098	10.0813954	7.5833865	5.9278768
31 H	10.5949287	8.7602194	6.3616762	4.6525407
32 H	8.1866515	6.3680418	4.0332420	2.2626802 *
33 H	8.8913056	8.2559728	6.1059004	5.0940695
34 H	6.3324610	6.6164262	5.3258567	4.5183106
35 H	6.7591908	7.4005525	6.2714250	5.7606874

H H H H

1 CO	4.6187482	6.4220158	6.6815549	5.2861447
2 C	9.9400433	11.4175032	10.8804083	8.6439683
3 C	9.7951505	11.4800251	11.1991247	9.1122202
4 C	8.5840310	10.3500195	10.2481570	8.3250395
5 C	7.4076610	9.0437092	8.8546107	6.9242843
6 C	7.5378376	8.9002043	8.3847183	6.2350636
7 C	8.9299455	10.2295606	9.5553990	7.2772035
8 C	9.4854734	10.5238743	9.5728770	7.1887025
9 C	8.8418412	9.6199018	8.4848549	6.0851409
10 C	7.4456546	8.2082750	7.1579196	4.8056056
11 C	6.6975103	7.7823227	7.0731255	4.8669633
12 N	5.2669111	6.3987684	5.9170468	3.9697584
13 C	4.7935680	5.4437132	4.6550423	2.6396092 *
14 C	3.5028853	3.9832810	3.4922593	2.1977593 *
15 C	2.1951759 *	3.4377947	3.9298426	3.4513889
16 C	1.1071715 *	2.1909644 *	3.4766442	3.9534101

17 C	2.2014664 *	1.1046160 *	2.1987316 *	3.4571987
18 C	3.4756298	2.1994162 *	1.1045945 *	2.1866358 *
19 C	3.9543394	3.4590178	2.1873620 *	1.1062799 *
20 O	2.6881858 *	4.6488509	5.3950803	4.6915119
21 N	6.2811780	8.0136366	8.0848061	6.4478382
22 H	10.9663005	12.3884063	11.7474577	9.4444292
23 H	10.7208468	12.4860697	12.2720012	10.2052084
24 H	8.7175221	10.6174251	10.7191556	8.9513185
25 H	10.5701776	11.6006098	10.5949287	8.1866515
26 H	9.5058227	10.0813954	8.7602194	6.3680418
27 H	7.0986128	7.5833865	6.3616762	4.0332420
28 H	5.6693485	5.9278768	4.6525407	2.2626802 *
29 H	0.0000000	2.5205069 *	4.3892150	5.0605557
30 H	2.5205069 *	0.0000000	2.5405683 *	4.3737306
31 H	4.3892150	2.5405683 *	0.0000000	2.5156424 *
32 H	5.0605557	4.3737306	2.5156424 *	0.0000000
33 H	2.3070278 *	4.6274066	5.8136664	5.4633106
34 H	6.3531264	7.8598095	7.7654888	6.1061621
35 H	6.6294169	8.5393408	8.8382381	7.3576353

H H H

1 CO	2.6587969 *	2.5067847 *	2.6203598 *
2 C	7.9616959	4.7694178	4.7379473
3 C	7.7123617	4.3228262	3.9195802
4 C	6.5099184	3.0586765	2.4877330 *
5 C	5.4411175	2.1100297 *	2.0885499 *
6 C	5.7319307	2.9600221 *	3.4227757
7 C	7.1024560	4.2418830	4.5626029
8 C	7.8377896	5.3758505	5.8896221
9 C	7.4452994	5.5639475	6.3042985
10 C	6.1569082	4.6938960	5.5562776
11 C	5.1817776	3.3398579	4.1527137
12 N	3.8852609	3.0175372	3.8912899
13 C	4.0108778	3.8855039	4.9643087
14 C	3.3270467	4.5991590	5.5529901
15 C	2.0429893 *	4.7364119	5.3343387
16 C	2.5060453 *	5.9368350	6.4592036
17 C	3.9260345	6.8812995	7.6234357
18 C	4.7278904	6.8189036	7.8102638
19 C	4.4847995	5.7901044	6.8906924
20 O	0.9921791 *	4.0479877	4.2398534
21 N	4.3909147	1.0439349 *	1.0395836 *
22 H	8.9983893	5.8435632	5.8213058
23 H	8.5891353	5.1780020	4.5899039
24 H	6.6244529	3.2174884	2.2166559 *

25 H	8.8913056	6.3324610	6.7591908
26 H	8.2559728	6.6164262	7.4005525
27 H	6.1059004	5.3258567	6.2714250
28 H	5.0940695	4.5183106	5.7606874
29 H	2.3070278 *	6.3531264	6.6294169
30 H	4.6274066	7.8598095	8.5393408
31 H	5.8136664	7.7654888	8.8382381
32 H	5.4633106	6.1061621	7.3576353
33 H	0.0000000	4.7457288	4.6692579
34 H	4.7457288	0.0000000	1.6658656 *
35 H	4.6692579	1.6658656 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.69 , TOTAL = 7098.4 SECONDS (118.3 MIN)
WALL CLOCK TIME: STEP = 0.69 , TOTAL = 6561.4 SECONDS (109.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.09 , TOTAL = 7099.5 SECONDS (118.3 MIN)
WALL CLOCK TIME: STEP = 1.08 , TOTAL = 6562.5 SECONDS (109.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636746746	-284.636746746	0.009886943	0.001216903	198045501
11335600						
2	1	-284.636834832	-0.000088086	0.001123569	0.000105858	156756377
14836873						
3	2	-284.636833977	0.000000855	0.000919354	0.000272562	140440291
16152775						
4	3	-284.636836249	-0.000002272	0.000404780	0.000114058	134574602
16636531						
5	4	-284.636835825	0.000000424	0.000307953	0.000155562	131408795
16870997						

6 5	-284.636836439	-0.000000614	0.000293333	0.000019426	126870890
17207001					
7 6	-284.636836429	0.000000010	0.000200589	0.000037128	119037190
17758124					
8 7	-284.636836468	-0.000000038	0.000088321	0.000016453	138332311
16306434					
9 8	-284.636836476	-0.000000009	0.000126804	0.000014111	131120510
16889563					
10 9	-284.636836490	-0.000000013	0.000456983	0.000010517	151242138
15463656					

-----DISABLING FDIFF OPTION-----

11 10	-284.636836476	0.000000014	0.000202408	0.000012549	198038850
11336179					
12 11	-284.636836484	-0.000000008	0.000069630	0.000013551	198038809
11336188					
13 12	-284.636836492	-0.000000008	0.000196693	0.000010860	198038797
11336191					
14 13	-284.636836503	-0.000000011	0.000180483	0.000006909	198038811
11336192					
15 14	-284.636836507	-0.000000004	0.000114607	0.000008253	198038706
11336189					
16 15	-284.636836510	-0.000000003	0.000069131	0.000007787	198038787
11336194					
17 16	-284.636836512	-0.000000002	0.000097613	0.000005274	198038760
11336194					
18 17	-284.636836514	-0.000000002	0.000041935	0.000002987	198038945
11336188					
19 18	-284.636836514	0.000000000	0.000023003	0.000001935	198038912
11336191					
20 19	-284.636836514	0.000000000	0.000010014	0.000001767	198038921
11336190					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 67.1 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 21.8 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6368365144 AFTER 20 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6017616906
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998613022

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 70.57 , TOTAL = 7170.0 SECONDS (119.5 MIN)
WALL CLOCK TIME: STEP = 64.67 , TOTAL = 6627.1 SECONDS (110.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.81 , TOTAL = 7173.8 SECONDS (119.6 MIN)
WALL CLOCK TIME: STEP = 3.79 , TOTAL = 6630.9 SECONDS (110.5 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84 , TOTAL = 7176.7 SECONDS (119.6 MIN)
WALL CLOCK TIME: STEP = 2.68 , TOTAL = 6633.6 SECONDS (110.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 74 ENERGY= -284.6368365

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000942	0.0000111	0.0000611
2 C	6.0	-0.0002368	0.0000669	0.0000973
3 C	6.0	0.0000203	-0.0001500	0.0002709
4 C	6.0	0.0000056	-0.0001187	0.0001189
5 C	6.0	0.0001698	0.0000097	-0.0000802
6 C	6.0	-0.0002865	-0.0003884	-0.0002851

7 C	6.0	0.0001951	-0.0002207	-0.0001631
8 C	6.0	0.0002090	0.0001605	-0.0001356
9 C	6.0	-0.0002446	0.0000746	-0.0000552
10 C	6.0	-0.0000781	-0.0001557	0.0000273
11 C	6.0	-0.0001090	0.0001365	-0.0002044
12 N	7.0	-0.0000891	-0.0002139	-0.0003244
13 C	6.0	-0.0001728	-0.0001157	0.0000983
14 C	6.0	-0.0002305	-0.0000505	0.0000794
15 C	6.0	0.0000548	0.0001335	0.0003722
16 C	6.0	0.0000518	-0.0000083	0.0001381
17 C	6.0	0.0002018	-0.0000057	-0.0001311
18 C	6.0	0.0002017	-0.0002720	-0.0004545
19 C	6.0	-0.0000440	-0.0002304	-0.0002101
20 O	8.0	0.0001511	0.0007020	0.0000507
21 N	7.0	-0.0001537	0.0002153	-0.0002053
22 H	1.0	-0.0001539	0.0002289	-0.0003930
23 H	1.0	0.0004774	0.0000576	0.0001139
24 H	1.0	0.0001827	0.0001392	0.0001302
25 H	1.0	0.0000555	-0.0001836	0.0002900
26 H	1.0	-0.0001200	0.0000565	0.0001776
27 H	1.0	-0.0001212	-0.0002647	0.0000706
28 H	1.0	-0.0000629	-0.0000530	-0.0000972
29 H	1.0	-0.0000086	-0.0002776	-0.0000509
30 H	1.0	0.0003761	0.0002226	0.0001007
31 H	1.0	-0.0001612	0.0004444	0.0003284
32 H	1.0	0.0000422	0.0003944	0.0003128
33 H	1.0	-0.0003992	-0.0001468	0.0000069
34 H	1.0	0.0003102	-0.0001581	-0.0000188
35 H	1.0	0.0000611	-0.0000397	-0.0000366

MAXIMUM GRADIENT = 0.0007020 RMS GRADIENT = 0.0002068
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000207302
 PREDICTED ENERGY CHANGE WAS -0.0000156764 RATIO= 1.322
 GDIIS STEP HAS LENGTH = 0.035600
 RADIUS OF STEP TAKEN= 0.03560 CURRENT TRUST RADIUS= 0.08691

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 7176.7 SECONDS (119.6 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6633.6 SECONDS (110.6 MIN)
 CPU UTILIZATION: STEP = 86.51% , TOTAL = 100.00%

INSERCH= 75

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1562199372	-1.7373960200	0.8561541387
C	6.0	4.9799775801	0.6328938227	0.5546267252
C	6.0	5.1906270587	-0.7097806639	0.2146393755
C	6.0	4.0576411177	-1.5368883211	-0.0752272906
C	6.0	2.7466275822	-1.0281319420	-0.0019867711
C	6.0	2.4686465970	0.3398614243	0.4183901786
C	6.0	3.6471789810	1.1774774735	0.6681346976
C	6.0	3.4964282022	2.5625638322	1.0488980126
C	6.0	2.2269176528	3.1331652677	1.2153323535
C	6.0	1.0646470440	2.3210583367	1.0309611464
C	6.0	1.1605274509	0.9694176019	0.6235356357
N	7.0	-0.0516707554	0.1692818115	0.5696219672
C	6.0	-1.2473832679	0.6987576635	0.3158277537
C	6.0	-2.5522958147	0.0425560390	0.4377728265
C	6.0	-2.8225217553	-1.2824726316	0.9242909463
C	6.0	-4.1225733961	-1.8038942058	1.0487306307
C	6.0	-5.2321492861	-0.9837656754	0.6787943480
C	6.0	-5.0189108321	0.3354448077	0.1888028540
C	6.0	-3.7000614475	0.8367905567	0.0736266213
O	8.0	-1.6999798062	-2.1419956495	1.3100887240
N	7.0	1.6442944382	-1.9673012050	-0.4302435577
H	1.0	5.8379983775	1.3027657276	0.7448981810
H	1.0	6.2109888273	-1.1262125547	0.1438814873
H	1.0	4.2285158123	-2.5838859427	-0.3953072318
H	1.0	4.4079460684	3.1606162343	1.2288813718
H	1.0	2.1148350808	4.1851445105	1.5305345083
H	1.0	0.0789165741	2.7586923371	1.2684497016
H	1.0	-1.2898784771	1.7506991292	-0.0291023958
H	1.0	-4.2943832658	-2.8311737160	1.4234476221
H	1.0	-6.2568369337	-1.3851442210	0.7787355069
H	1.0	-5.8772089649	0.9729095930	-0.0884438869
H	1.0	-3.5350013571	1.8679365769	-0.2904708033
H	1.0	-2.0184903906	-2.9550956948	1.7815516387
H	1.0	1.2941919620	-1.7010212113	-1.3773129440
H	1.0	2.0422164062	-2.9227680911	-0.5276270718

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3831060	5.1781068	4.0160630
2 C	5.3831060	0.0000000	1.4009780 *	2.4403637 *

3 C	5.1781068	1.4009780 *	0.0000000	1.4324060 *
4 C	4.0160630	2.4403637 *	1.4324060 *	0.0000000
5 C	2.8195165 *	2.8384287 *	2.4741479 *	1.4081739 *
6 C	3.1391006	2.5320371 *	2.9244556 *	2.5081370 *
7 C	4.5517726	1.4442325 *	2.4798454 *	2.8440900 *
8 C	5.4482838	2.4837168 *	3.7781657	4.2876713
9 C	5.3046362	3.7771985	4.9551179	5.1794298
10 C	4.1625532	4.2902922	5.1842142	5.0065376
11 C	2.8964780 *	3.8348658	4.3850434	3.8939834
12 N	1.9392626 *	5.0529839	5.3273305	4.4959194
13 C	2.8630228 *	6.2322858	6.5910694	5.7701231
14 C	3.2679244	7.5562753	7.7825866	6.8153562
15 C	3.0140504	8.0426536	8.0648704	6.9570400
16 C	4.2836410	9.4360219	9.4142708	8.2613851
17 C	5.4437063	10.3400455	10.4367032	9.3367392
18 C	5.6146242	10.0099986	10.2629347	9.2714151
19 C	4.7020944	8.6957468	9.0253038	8.1140901
20 O	1.9532626 *	7.2727275	7.1226197	5.9527686
21 N	1.9804144 *	4.3425529	3.8175525	2.4770010 *
22 H	6.4449645	1.1050481 *	2.1795887 *	3.4504946
23 H	6.1270796	2.1859908 *	1.1043371 *	2.2030818 *
24 H	4.3435348	3.4372578	2.1931629 *	1.1080854 *
25 H	6.4966626	2.6779134 *	4.0769165	4.8877359
26 H	6.2743485	4.6668965	5.9289433	6.2525696
27 H	4.5156145	5.3897089	6.2666103	6.0073064
28 H	3.8783614	6.3954142	6.9361605	6.2774457
29 H	4.6180126	9.9382284	9.7942303	8.5835606
30 H	6.4231903	11.4187873	11.4812348	10.3508809
31 H	6.6813387	10.8815279	11.1991205	10.2469755
32 H	5.2856680	8.6454836	9.1124285	8.3239043
33 H	2.6586685 *	7.9597467	7.7115516	6.5098628
34 H	2.5069261 *	4.7712227	4.3242429	3.0592512
35 H	2.6223921 *	4.7375569	3.9192809	2.4874214 *

C C C C

1 CO	2.8195165 *	3.1391006	4.5517726	5.4482838
2 C	2.8384287 *	2.5320371 *	1.4442325 *	2.4837168 *
3 C	2.4741479 *	2.9244556 *	2.4798454 *	3.7781657
4 C	1.4081739 *	2.5081370 *	2.8440900 *	4.2876713
5 C	0.0000000	1.4578738 *	2.4748270 *	3.8157117
6 C	1.4578738 *	0.0000000	1.4672803 *	2.5286916 *
7 C	2.4748270 *	1.4672803 *	0.0000000	1.4443582 *
8 C	3.8157117	2.5286916 *	1.4443582 *	0.0000000
9 C	4.3667332	2.9148064 *	2.4781611 *	1.4017644 *
10 C	3.8875591	2.5043161 *	2.8476115 *	2.4438098 *

11 C	2.6262513 *	1.4661519 *	2.4957391 *	2.8592797 *
12 N	3.0969356	2.5306063 *	3.8350558	4.3065660
13 C	4.3629436	3.7347294	4.9305205	5.1492633
14 C	5.4238686	5.0297742	6.3067108	6.5811075
15 C	5.6513807	5.5573704	6.9263265	7.3979025
16 C	6.9922626	6.9596838	8.3308152	8.7815227
17 C	8.0078906	7.8180596	9.1385752	9.4287589
18 C	7.8866551	7.4910778	8.7200855	8.8436882
19 C	6.7114419	6.1982868	7.3791225	7.4645101
20 O	4.7680763	4.9327667	6.3263824	7.0145390
21 N	1.5101593 *	2.5928238 *	3.8868515	5.1125274
22 H	3.9430311	3.5194209	2.1957412 *	2.6762769 *
23 H	3.4688177	4.0286292	3.4863950	4.6685078
24 H	2.1842766 *	3.5082106	3.9517991	5.3951484
25 H	4.6712554	3.5177317	2.1968256 *	1.1049550 *
26 H	5.4704693	4.0184885	3.4839449	2.1848435 *
27 H	4.8031999	3.5048757	3.9488119	3.4301684
28 H	4.9006141	4.0394583	5.0188902	4.9729208
29 H	7.4066630	7.5368546	8.9279445	9.4831132
30 H	9.0442998	8.9016603	10.2307768	10.5253773
31 H	8.8533722	8.3851616	9.5565802	9.5752609
32 H	6.9230989	6.2354861	7.2786931	7.1914823
33 H	5.4406386	5.7314352	7.1005400	7.8355392
34 H	2.1104197 *	2.9612658 *	4.2433664	5.3772206
35 H	2.0885734 *	3.4236739	4.5626489	5.8897393

C C C N

1 CO	5.3046362	4.1625532	2.8964780 *	1.9392626 *
2 C	3.7771985	4.2902922	3.8348658	5.0529839
3 C	4.9551179	5.1842142	4.3850434	5.3273305
4 C	5.1794298	5.0065376	3.8939834	4.4959194
5 C	4.3667332	3.8875591	2.6262513 *	3.0969356
6 C	2.9148064 *	2.5043161 *	1.4661519 *	2.5306063 *
7 C	2.4781611 *	2.8476115 *	2.4957391 *	3.8350558
8 C	1.4017644 *	2.4438098 *	2.8592797 *	4.3065660
9 C	0.0000000	1.4298194 *	2.4837905 *	3.7938783
10 C	1.4298194 *	0.0000000	1.4149633 *	2.4676186 *
11 C	2.4837905 *	1.4149633 *	0.0000000	1.4534609 *
12 N	3.7938783	2.4676186 *	1.4534609 *	0.0000000
13 C	4.3366134	2.9135476 *	2.4425345 *	1.3320978 *
14 C	5.7443316	4.3157526	3.8312709	2.5073032 *
15 C	6.7141196	5.3015937	4.5854274	3.1481735
16 C	8.0447715	6.6274282	5.9819064	4.5491996
17 C	8.5366664	7.1200792	6.6846312	5.3083703
18 C	7.8347325	6.4545773	6.2270677	4.9845870

19	C	6.4580113	5.0815339	4.8933950	3.7419693
20	O	6.5769921	5.2573686	4.2819095	2.9338059 *
21	N	5.3909302	4.5673995	3.1573404	2.9053427 *
22	H	4.0757300	4.8891344	4.6909044	6.0003092
23	H	5.9298507	6.2574292	5.4889793	6.4094045
24	H	6.2677930	6.0085593	4.8038068	5.1798666
25	H	2.1812432 *	3.4527783	3.9640286	5.4102576
26	H	1.1038909 *	2.1971085 *	3.4748021	4.6630734
27	H	2.1810456 *	1.1043500 *	2.1879900 *	2.6852300 *
28	H	3.9784024	2.6443969 *	2.6534556 *	2.0958316 *
29	H	8.8399105	7.4443768	6.6962978	5.2661524
30	H	9.6218413	8.2099746	7.7836587	6.4003169
31	H	8.4878387	7.1596046	7.0736597	5.9174119
32	H	6.0883460	4.8071059	4.8673129	3.9697329
33	H	7.4438576	6.1568599	5.1815982	3.8857287
34	H	5.5642741	4.6935699	3.3395366	3.0166099
35	H	6.3044707	5.5572075	4.1535118	3.8921834

C C C C

1	CO	2.8630228 *	3.2679244	3.0140504	4.2836410
2	C	6.2322858	7.5562753	8.0426536	9.4360219
3	C	6.5910694	7.7825866	8.0648704	9.4142708
4	C	5.7701231	6.8153562	6.9570400	8.2613851
5	C	4.3629436	5.4238686	5.6513807	6.9922626
6	C	3.7347294	5.0297742	5.5573704	6.9596838
7	C	4.9305205	6.3067108	6.9263265	8.3308152
8	C	5.1492633	6.5811075	7.3979025	8.7815227
9	C	4.3366134	5.7443316	6.7141196	8.0447715
10	C	2.9135476 *	4.3157526	5.3015937	6.6274282
11	C	2.4425345 *	3.8312709	4.5854274	5.9819064
12	N	1.3320978 *	2.5073032 *	3.1481735	4.5491996
13	C	0.0000000	1.4656971 *	2.6031831 *	3.8816403
14	C	1.4656971 *	0.0000000	1.4371579 *	2.4996839 *
15	C	2.6031831 *	1.4371579 *	0.0000000	1.4062361 *
16	C	3.8816403	2.4996839 *	1.4062361 *	0.0000000
17	C	4.3406209	2.8797643 *	2.4404506 *	1.4285035 *
18	C	3.7911148	2.4963893 *	2.8253716 *	2.4737963 *
19	C	2.4684701 *	1.4424898 *	2.4464223 *	2.8464996 *
20	O	3.0435634	2.5019280 *	1.4655102 *	2.4599960 *
21	N	4.0032852	4.7333232	4.7176478	5.9557393
22	H	7.1240129	8.4899641	9.0399252	10.4382297
23	H	7.6803253	8.8457645	9.0685043	10.3952159
24	H	6.4239344	7.3192640	7.2905519	8.5108356
25	H	6.2351555	7.6676671	8.4919656	9.8716048
26	H	4.9934876	6.3353988	7.3918780	8.6605995

27 H	2.6286671 *	3.8717824	4.9867629	6.2062864
28 H	1.1078644 *	2.1747236 *	3.5296013	4.6712973
29 H	4.7928537	3.5021060	2.1940849 *	1.1069032 *
30 H	5.4453243	3.9847470	3.4389313	2.1916500 *
31 H	4.6555215	3.4924933	3.9298212	3.4759964
32 H	2.6396541 *	2.1972854 *	3.4508479	3.9523465
33 H	4.0116826	3.3281535	2.0442677 *	2.5078789 *
34 H	3.8839759	4.5967452	4.7349652	5.9361281
35 H	4.9647085	5.5528989	5.3351956	6.4607597

C C C O

1 CO	5.4437063	5.6146242	4.7020944	1.9532626 *
2 C	10.3400455	10.0099986	8.6957468	7.2727275
3 C	10.4367032	10.2629347	9.0253038	7.1226197
4 C	9.3367392	9.2714151	8.1140901	5.9527686
5 C	8.0078906	7.8866551	6.7114419	4.7680763
6 C	7.8180596	7.4910778	6.1982868	4.9327667
7 C	9.1385752	8.7200855	7.3791225	6.3263824
8 C	9.4287589	8.8436882	7.4645101	7.0145390
9 C	8.5366664	7.8347325	6.4580113	6.5769921
10 C	7.1200792	6.4545773	5.0815339	5.2573686
11 C	6.6846312	6.2270677	4.8933950	4.2819095
12 N	5.3083703	4.9845870	3.7419693	2.9338059 *
13 C	4.3406209	3.7911148	2.4684701 *	3.0435634
14 C	2.8797643 *	2.4963893 *	1.4424898 *	2.5019280 *
15 C	2.4404506 *	2.8253716 *	2.4464223 *	1.4655102 *
16 C	1.4285035 *	2.4737963 *	2.8464996 *	2.4599960 *
17 C	0.0000000	1.4233336 *	2.4551876 *	3.7704443
18 C	1.4233336 *	0.0000000	1.4156189 *	4.2907221
19 C	2.4551876 *	1.4156189 *	0.0000000	3.7950405
20 O	3.7704443	4.2907221	3.7950405	0.0000000
21 N	7.0344002	7.0770165	6.0563153	3.7740489
22 H	11.3040154	10.9140932	9.5729997	8.3070414
23 H	11.4565192	11.3247122	10.1038228	8.0607245
24 H	9.6549605	9.7148637	8.6477317	6.1847152
25 H	10.5076132	9.8959076	8.5131995	8.0889459
26 H	9.0233737	8.2164933	6.8663729	7.3914891
27 H	6.5238873	5.7467913	4.4047683	5.2137270
28 H	4.8497335	3.9945100	2.5796829 *	4.1369903
29 H	2.2015517 *	3.4751634	3.9533779	2.6867724 *
30 H	1.1050239 *	2.2002064 *	3.4599528	4.6497427
31 H	2.1984846 *	1.1044921 *	2.1874109 *	5.3951619
32 H	3.4571653	2.1863718 *	1.1059267 *	4.6913379
33 H	3.9280809	4.7293793	4.4858768	0.9924001 *
34 H	6.8800554	6.8158037	5.7869060	4.0474252

35 H	7.6244068	7.8095289	6.8898144	4.2415607
	N	H	H	H
1 CO	1.9804144 *	6.4449645	6.1270796	4.3435348
2 C	4.3425529	1.1050481 *	2.1859908 *	3.4372578
3 C	3.8175525	2.1795887 *	1.1043371 *	2.1931629 *
4 C	2.4770010 *	3.4504946	2.2030818 *	1.1080854 *
5 C	1.5101593 *	3.9430311	3.4688177	2.1842766 *
6 C	2.5928238 *	3.5194209	4.0286292	3.5082106
7 C	3.8868515	2.1957412 *	3.4863950	3.9517991
8 C	5.1125274	2.6762769 *	4.6685078	5.3951484
9 C	5.3909302	4.0757300	5.9298507	6.2677930
10 C	4.5673995	4.8891344	6.2574292	6.0085593
11 C	3.1573404	4.6909044	5.4889793	4.8038068
12 N	2.9053427 *	6.0003092	6.4094045	5.1798666
13 C	4.0032852	7.1240129	7.6803253	6.4239344
14 C	4.7333232	8.4899641	8.8457645	7.3192640
15 C	4.7176478	9.0399252	9.0685043	7.2905519
16 C	5.9557393	10.4382297	10.3952159	8.5108356
17 C	7.0344002	11.3040154	11.4565192	9.6549605
18 C	7.0770165	10.9140932	11.3247122	9.7148637
19 C	6.0563153	9.5729997	10.1038228	8.6477317
20 O	3.7740489	8.3070414	8.0607245	6.1847152
21 N	0.0000000	5.4462325	4.6788618	2.6569903 *
22 H	5.4462325	0.0000000	2.5298772 *	4.3585048
23 H	4.6788618	2.5298772 *	0.0000000	2.5190743 *
24 H	2.6569903 *	4.3585048	2.5190743 *	0.0000000
25 H	6.0568972	2.3939294 *	4.7754674	5.9723939
26 H	6.4744612	4.7736021	6.8492186	7.3482165
27 H	5.2603214	5.9632920	7.3457096	6.9663767
28 H	4.7532948	7.1837560	8.0355183	7.0267638
29 H	6.2809505	10.9642621	10.7194694	8.7183043
30 H	8.0142632	12.3899575	12.4866635	10.6187561
31 H	8.0829871	11.7494403	12.2713004	10.7177718
32 H	6.4462152	9.4469324	10.2047987	8.9499672
33 H	4.3913288	8.9960241	8.5878464	6.6258281
34 H	1.0442304 *	5.8457414	5.1787382	3.2177697
35 H	1.0395876 *	5.8208605	4.5888124	2.2163607 *

H H H H

1 CO	6.4966626	6.2743485	4.5156145	3.8783614
2 C	2.6779134 *	4.6668965	5.3897089	6.3954142
3 C	4.0769165	5.9289433	6.2666103	6.9361605
4 C	4.8877359	6.2525696	6.0073064	6.2774457

5 C	4.6712554	5.4704693	4.8031999	4.9006141
6 C	3.5177317	4.0184885	3.5048757	4.0394583
7 C	2.1968256 *	3.4839449	3.9488119	5.0188902
8 C	1.1049550 *	2.1848435 *	3.4301684	4.9729208
9 C	2.1812432 *	1.1038909 *	2.1810456 *	3.9784024
10 C	3.4527783	2.1971085 *	1.1043500 *	2.6443969 *
11 C	3.9640286	3.4748021	2.1879900 *	2.6534556 *
12 N	5.4102576	4.6630734	2.6852300 *	2.0958316 *
13 C	6.2351555	4.9934876	2.6286671 *	1.1078644 *
14 C	7.6676671	6.3353988	3.8717824	2.1747236 *
15 C	8.4919656	7.3918780	4.9867629	3.5296013
16 C	9.8716048	8.6605995	6.2062864	4.6712973
17 C	10.5076132	9.0233737	6.5238873	4.8497335
18 C	9.8959076	8.2164933	5.7467913	3.9945100
19 C	8.5131995	6.8663729	4.4047683	2.5796829 *
20 O	8.0889459	7.3914891	5.2137270	4.1369903
21 N	6.0568972	6.4744612	5.2603214	4.7532948
22 H	2.3939294 *	4.7736021	5.9632920	7.1837560
23 H	4.7754674	6.8492186	7.3457096	8.0355183
24 H	5.9723939	7.3482165	6.9663767	7.0267638
25 H	0.0000000	2.5296266 *	4.3478276	6.0029654
26 H	2.5296266 *	0.0000000	2.4996837 *	4.4666616
27 H	4.3478276	2.4996837 *	0.0000000	2.1385256 *
28 H	6.0029654	4.4666616	2.1385256 *	0.0000000
29 H	10.5673998	9.5035924	7.0990407	5.6683780
30 H	11.6019035	10.0835614	7.5863676	5.9293163
31 H	10.5974440	8.7642634	6.3644019	4.6531794
32 H	8.1896194	6.3722967	4.0353540	2.2633238 *
33 H	8.8885579	8.2541153	6.1081718	5.0944920
34 H	6.3342902	6.6163418	5.3259740	4.5176836
35 H	6.7594056	7.4002516	6.2737095	5.7613088

H H H H

1 CO	4.6180126	6.4231903	6.6813387	5.2856680
2 C	9.9382284	11.4187873	10.8815279	8.6454836
3 C	9.7942303	11.4812348	11.1991205	9.1124285
4 C	8.5835606	10.3508809	10.2469755	8.3239043
5 C	7.4066630	9.0442998	8.8533722	6.9230989
6 C	7.5368546	8.9016603	8.3851616	6.2354861
7 C	8.9279445	10.2307768	9.5565802	7.2786931
8 C	9.4831132	10.5253773	9.5752609	7.1914823
9 C	8.8399105	9.6218413	8.4878387	6.0883460
10 C	7.4443768	8.2099746	7.1596046	4.8071059
11 C	6.6962978	7.7836587	7.0736597	4.8673129
12 N	5.2661524	6.4003169	5.9174119	3.9697329

13 C	4.7928537	5.4453243	4.6555215	2.6396541 *
14 C	3.5021060	3.9847470	3.4924933	2.1972854 *
15 C	2.1940849 *	3.4389313	3.9298212	3.4508479
16 C	1.1069032 *	2.1916500 *	3.4759964	3.9523465
17 C	2.2015517 *	1.1050239 *	2.1984846 *	3.4571653
18 C	3.4751634	2.2002064 *	1.1044921 *	2.1863718 *
19 C	3.9533779	3.4599528	2.1874109 *	1.1059267 *
20 O	2.6867724 *	4.6497427	5.3951619	4.6913379
21 N	6.2809505	8.0142632	8.0829871	6.4462152
22 H	10.9642621	12.3899575	11.7494403	9.4469324
23 H	10.7194694	12.4866635	12.2713004	10.2047987
24 H	8.7183043	10.6187561	10.7177718	8.9499672
25 H	10.5673998	11.6019035	10.5974440	8.1896194
26 H	9.5035924	10.0835614	8.7642634	6.3722967
27 H	7.0990407	7.5863676	6.3644019	4.0353540
28 H	5.6683780	5.9293163	4.6531794	2.2633238 *
29 H	0.0000000	2.5214836 *	4.3888726	5.0592307
30 H	2.5214836 *	0.0000000	2.5409713 *	4.3742572
31 H	4.3888726	2.5409713 *	0.0000000	2.5155168 *
32 H	5.0592307	4.3742572	2.5155168 *	0.0000000
33 H	2.3072242 *	4.6296835	5.8151370	5.4639475
34 H	6.3524544	7.8591578	7.7614484	6.1024416
35 H	6.6308052	8.5407937	8.8366557	7.3561167

H H H

1 CO	2.6586685 *	2.5069261 *	2.6223921 *
2 C	7.9597467	4.7712227	4.7375569
3 C	7.7115516	4.3242429	3.9192809
4 C	6.5098628	3.0592512	2.4874214 *
5 C	5.4406386	2.1104197 *	2.0885734 *
6 C	5.7314352	2.9612658 *	3.4236739
7 C	7.1005400	4.2433664	4.5626489
8 C	7.8355392	5.3772206	5.8897393
9 C	7.4438576	5.5642741	6.3044707
10 C	6.1568599	4.6935699	5.5572075
11 C	5.1815982	3.3395366	4.1535118
12 N	3.8857287	3.0166099	3.8921834
13 C	4.0116826	3.8839759	4.9647085
14 C	3.3281535	4.5967452	5.5528989
15 C	2.0442677 *	4.7349652	5.3351956
16 C	2.5078789 *	5.9361281	6.4607597
17 C	3.9280809	6.8800554	7.6244068
18 C	4.7293793	6.8158037	7.8095289
19 C	4.4858768	5.7869060	6.8898144
20 O	0.9924001 *	4.0474252	4.2415607

21 N	4.3913288	1.0442304 *	1.0395876 *
22 H	8.9960241	5.8457414	5.8208605
23 H	8.5878464	5.1787382	4.5888124
24 H	6.6258281	3.2177697	2.2163607 *
25 H	8.8885579	6.3342902	6.7594056
26 H	8.2541153	6.6163418	7.4002516
27 H	6.1081718	5.3259740	6.2737095
28 H	5.0944920	4.5176836	5.7613088
29 H	2.3072242 *	6.3524544	6.6308052
30 H	4.6296835	7.8591578	8.5407937
31 H	5.8151370	7.7614484	8.8366557
32 H	5.4639475	6.1024416	7.3561167
33 H	0.0000000	4.7460502	4.6714763
34 H	4.7460502	0.0000000	1.6655846 *
35 H	4.6714763	1.6655846 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.67, TOTAL = 7177.4 SECONDS (119.6 MIN)
WALL CLOCK TIME: STEP = 0.69, TOTAL = 6634.3 SECONDS (110.6 MIN)

CPU UTILIZATION: STEP = 97.46%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.90, TOTAL = 7178.3 SECONDS (119.6 MIN)
WALL CLOCK TIME: STEP = 0.97, TOTAL = 6635.3 SECONDS (110.6 MIN)

CPU UTILIZATION: STEP = 92.38%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636819371	-284.636819371	0.004730216	0.000575832	198032141
11337034					
2 1	-284.636849013	-0.000029642	0.001860441	0.000073552	151973024
15210713					
3 2	-284.636848802	0.000000211	0.000794307	0.000130640	137404116
16351646					

4 3	-284.636849525	-0.000000722	0.000349148	0.000045198	131308976
16826129					
5 4	-284.636849426	0.000000099	0.000241707	0.000087773	124225251
17403823					
6 5	-284.636849553	-0.000000127	0.000126510	0.000009231	119271395
17778287					
7 6	-284.636849543	0.000000009	0.000095326	0.000019878	111837485
18252515					
8 7	-284.636849557	-0.000000014	0.000050467	0.000008109	130837312
16852664					
9 8	-284.636849565	-0.000000008	0.000116468	0.000007226	126894422
17218880					
10 9	-284.636849572	-0.000000007	0.000307161	0.000006708	153742965
15201732					

-----DISABLING FDIFF OPTION-----

11 10	-284.636849568	0.000000003	0.000186539	0.000007281	198030861
11337140					
12 11	-284.636849572	-0.000000003	0.000045909	0.000008410	198030859
11337139					
13 12	-284.636849576	-0.000000004	0.000077063	0.000006821	198030841
11337134					
14 13	-284.636849579	-0.000000003	0.000116716	0.000004354	198030846
11337140					
15 14	-284.636849582	-0.000000003	0.000135551	0.000004297	198030979
11337135					
16 15	-284.636849583	-0.000000001	0.000049942	0.000004060	198030976
11337136					
17 16	-284.636849584	-0.000000001	0.000022724	0.000002711	198030924
11337135					
18 17	-284.636849585	0.000000000	0.000021084	0.000001708	198031004
11337135					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 59.7 SECONDS (3.3 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 19.6 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.1
 TIME TO SOLVE SCF EQUATIONS= 1.9 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6368495845 AFTER 18 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6013126578
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998591283

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 63.02 , TOTAL = 7241.3 SECONDS (120.7 MIN)
WALL CLOCK TIME: STEP = 57.84 , TOTAL = 6693.1 SECONDS (111.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.89 , TOTAL = 7245.2 SECONDS (120.8 MIN)
WALL CLOCK TIME: STEP = 3.87 , TOTAL = 6697.0 SECONDS (111.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.02 , TOTAL = 7248.2 SECONDS (120.8 MIN)
WALL CLOCK TIME: STEP = 2.85 , TOTAL = 6699.9 SECONDS (111.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 75 ENERGY= -284.6368496

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0001366	0.0000272	0.0001875
2 C	6.0	-0.0000230	-0.0004580	0.0000049
3 C	6.0	0.0003318	0.0000672	0.0002947
4 C	6.0	0.0001389	0.0002372	0.0002208
5 C	6.0	-0.0001568	-0.0000721	-0.0001190
6 C	6.0	0.0000722	0.0000648	-0.0001906

7 C	6.0	-0.0002429	-0.0002325	-0.0001286
8 C	6.0	0.0001559	0.0002134	-0.0000630
9 C	6.0	-0.0000036	0.0003715	0.0000420
10 C	6.0	-0.0002922	-0.0002114	-0.0000839
11 C	6.0	-0.0002900	-0.0001193	-0.0003563
12 N	7.0	0.0000009	-0.0000525	-0.0002187
13 C	6.0	-0.0000198	0.0000887	0.0000052
14 C	6.0	-0.0002467	0.0000600	0.0000365
15 C	6.0	0.0000918	0.0000183	0.0003438
16 C	6.0	0.0000070	0.0000830	0.0001793
17 C	6.0	0.0001342	-0.0000360	-0.0001450
18 C	6.0	0.0002299	-0.0001674	-0.0004683
19 C	6.0	-0.0000278	-0.0000444	-0.0002949
20 O	8.0	0.0000510	0.0007167	-0.0000895
21 N	7.0	-0.0000303	0.0000005	0.0000238
22 H	1.0	-0.0000729	0.0001738	-0.0003972
23 H	1.0	0.0002304	0.0001384	0.0001262
24 H	1.0	0.0002894	-0.0001028	0.0000285
25 H	1.0	0.0000073	-0.0001618	0.0002567
26 H	1.0	-0.0000552	-0.0003094	0.0001120
27 H	1.0	-0.0002437	-0.0001058	0.0000979
28 H	1.0	-0.0000372	-0.0001988	0.0000353
29 H	1.0	0.0001105	-0.0000983	-0.0000814
30 H	1.0	0.0001020	0.0001171	0.0001348
31 H	1.0	-0.0001289	0.0003481	0.0003119
32 H	1.0	0.0000275	0.0001686	0.0004088
33 H	1.0	-0.0003198	-0.0003431	0.0001532
34 H	1.0	0.0002560	-0.0001580	-0.0002094
35 H	1.0	0.0000907	-0.0000225	-0.0001580

MAXIMUM GRADIENT = 0.0007167 RMS GRADIENT = 0.0002012
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000130701
 PREDICTED ENERGY CHANGE WAS -0.0000092796 RATIO= 1.408
 GDIIS STEP HAS LENGTH = 0.047315
 RADIUS OF STEP TAKEN= 0.04731 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 7248.2 SECONDS (120.8 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6699.9 SECONDS (111.7
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 76

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1566472871	-1.7364981371	0.8584225682
C	6.0	4.9803985341	0.6319117394	0.5567985282
C	6.0	5.1897445891	-0.7099755249	0.2120589343
C	6.0	4.0566694413	-1.5358425881	-0.0792506739
C	6.0	2.7462166912	-1.0267890189	-0.0026275223
C	6.0	2.4684041796	0.3406426965	0.4191741461
C	6.0	3.6481532534	1.1772204866	0.6705585187
C	6.0	3.4973921731	2.5610599038	1.0525794901
C	6.0	2.2281527982	3.1326418120	1.2159052943
C	6.0	1.0649109716	2.3234969769	1.0282970267
C	6.0	1.1609474348	0.9711558056	0.6233622878
N	7.0	-0.0513437644	0.1704987729	0.5708665077
C	6.0	-1.2473281616	0.6989992526	0.3169402218
C	6.0	-2.5518273997	0.0418818914	0.4373811500
C	6.0	-2.8226731168	-1.2828045983	0.9244015762
C	6.0	-4.1230210707	-1.8025579697	1.0517469122
C	6.0	-5.2336015513	-0.9844820370	0.6803084275
C	6.0	-5.0193204697	0.3332038892	0.1867010252
C	6.0	-3.6999530451	0.8346729315	0.0715694058
O	8.0	-1.6999483064	-2.1432164281	1.3097880432
N	7.0	1.6434032609	-1.9667906748	-0.4302473922
H	1.0	5.8391978559	1.2991571831	0.7507351312
H	1.0	6.2099274968	-1.1271262503	0.1403609104
H	1.0	4.2273128990	-2.5816952245	-0.4026803571
H	1.0	4.4087529976	3.1589025186	1.2340388712
H	1.0	2.1173388296	4.1845467561	1.5319008751
H	1.0	0.0798082512	2.7640425357	1.2629762069
H	1.0	-1.2905763847	1.7521712837	-0.0254710603
H	1.0	-4.2931718875	-2.8286041878	1.4306482554
H	1.0	-6.2586791870	-1.3860643248	0.7805684344
H	1.0	-5.8771675227	0.9682907712	-0.0970162976
H	1.0	-3.5351183112	1.8646059784	-0.2967351955
H	1.0	-2.0163573457	-2.9545937704	1.7852571962
H	1.0	1.2900316235	-1.6992414704	-1.3758758698
H	1.0	2.0426739563	-2.9217159800	-0.5305545756

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3822782	5.1772196	4.0161756
2 C	5.3822782	0.0000000	1.4011897 *	2.4406952 *

3 C	5.1772196	1.4011897 *	0.0000000	1.4320534 *
4 C	4.0161756	2.4406952 *	1.4320534 *	0.0000000
5 C	2.8197454 *	2.8382766 *	2.4733155 *	1.4079393 *
6 C	3.1387375	2.5325666 *	2.9244468 *	2.5084280 *
7 C	4.5514463	1.4440154 *	2.4795634 *	2.8442592 *
8 C	5.4467677	2.4832880 *	3.7775924	4.2870084
9 C	5.3035321	3.7766293	4.9542347	5.1783828
10 C	4.1638156	4.2912486	5.1848291	5.0071731
11 C	2.8974579 *	3.8350651	4.3848124	3.8940868
12 N	1.9397386 *	5.0528735	5.3266298	4.4955562
13 C	2.8628653 *	6.2327051	6.5903047	5.7692180
14 C	3.2673761	7.5562440	7.7812593	6.8138354
15 C	3.0143890	8.0429595	8.0643910	6.9567737
16 C	4.2845419	9.4363057	9.4141604	8.2618176
17 C	5.4453683	10.3418461	10.4374689	9.3375620
18 C	5.6147590	10.0110229	10.2622549	9.2702566
19 C	4.7014279	8.6962672	9.0239903	8.1121688
20 O	1.9534835 *	7.2729199	7.1222930	5.9528967
21 N	1.9809463 *	4.3431614	3.8168938	2.4764427 *
22 H	6.4434603	1.1047009 *	2.1791227 *	3.4501460
23 H	6.1261038	2.1861785 *	1.1045037 *	2.2026799 *
24 H	4.3445434	3.4372965	2.1926043 *	1.1079412 *
25 H	6.4951088	2.6778939 *	4.0770833	4.8876706
26 H	6.2734884	4.6657423	5.9277321	6.2513732
27 H	4.5193400	5.3907749	6.2677490	6.0088277
28 H	3.8789868	6.3968075	6.9363641	6.2774967
29 H	4.6174699	9.9366942	9.7928164	8.5831741
30 H	6.4253622	11.4209968	11.4824521	10.3522046
31 H	6.6809930	10.8824338	11.1977073	10.2446140
32 H	5.2850235	8.6465069	9.1110139	8.3213936
33 H	2.6579557 *	7.9578091	7.7098099	6.5092933
34 H	2.5056012 *	4.7737107	4.3252682	3.0597746
35 H	2.6250896 *	4.7371756	3.9175661	2.4860608 *

C C C C

1 CO	2.8197454 *	3.1387375	4.5514463	5.4467677
2 C	2.8382766 *	2.5325666 *	1.4440154 *	2.4832880 *
3 C	2.4733155 *	2.9244468 *	2.4795634 *	3.7775924
4 C	1.4079393 *	2.5084280 *	2.8442592 *	4.2870084
5 C	0.0000000	1.4577263 *	2.4747377 *	3.8144969
6 C	1.4577263 *	0.0000000	1.4679456 *	2.5278986 *
7 C	2.4747377 *	1.4679456 *	0.0000000	1.4434959 *
8 C	3.8144969	2.5278986 *	1.4434959 *	0.0000000
9 C	4.3650976	2.9133761 *	2.4773932 *	1.4015526 *
10 C	3.8876742	2.5045029 *	2.8486957 *	2.4441748 *

11 C	2.6261617 *	1.4658386 *	2.4961737 *	2.8584955 *
12 N	3.0965687	2.5300374 *	3.8353234	4.3058514
13 C	4.3622092	3.7343725	4.9314785	5.1498355
14 C	5.4226319	5.0291465	6.3073866	6.5816247
15 C	5.6513238	5.5575476	6.9273194	7.3983072
16 C	6.9928499	6.9599098	8.3315986	8.7813359
17 C	8.0091005	7.8195293	9.1410405	9.4307850
18 C	7.8859998	7.4913363	8.7219025	8.8457607
19 C	6.7099665	6.1978646	7.3804331	7.4662287
20 O	4.7683569	4.9333469	6.3274091	7.0148927
21 N	1.5108472 *	2.5935289 *	3.8878789	5.1124829
22 H	3.9426024	3.5200757	2.1958992 *	2.6772304 *
23 H	3.4681127	4.0287814	3.4862316	4.6682660
24 H	2.1843584 *	3.5084560	3.9517989	5.3943022
25 H	4.6704801	3.5173209	2.1961525 *	1.1049533 *
26 H	5.4688468	4.0170893	3.4827166	2.1840343 *
27 H	4.8043616	3.5057466	3.9499429	3.4300654
28 H	4.9009020	4.0398091	5.0205653	4.9740463
29 H	7.4063357	7.5356563	8.9268703	9.4807333
30 H	9.0460281	8.9036008	10.2336631	10.5278064
31 H	8.8516670	8.3850439	9.5584810	9.5781446
32 H	6.9211151	6.2351642	7.2806282	7.1945745
33 H	5.4401355	5.7304321	7.0993748	7.8333062
34 H	2.1115109 *	2.9617383 *	4.2453109	5.3777322
35 H	2.0891212 *	3.4243561	4.5630600	5.8892572

C C C N

1 CO	5.3035321	4.1638156	2.8974579 *	1.9397386 *
2 C	3.7766293	4.2912486	3.8350651	5.0528735
3 C	4.9542347	5.1848291	4.3848124	5.3266298
4 C	5.1783828	5.0071731	3.8940868	4.4955562
5 C	4.3650976	3.8876742	2.6261617 *	3.0965687
6 C	2.9133761 *	2.5045029 *	1.4658386 *	2.5300374 *
7 C	2.4773932 *	2.8486957 *	2.4961737 *	3.8353234
8 C	1.4015526 *	2.4441748 *	2.8584955 *	4.3058514
9 C	0.0000000	1.4293508 *	2.4823489 *	3.7929502
10 C	1.4293508 *	0.0000000	1.4149282 *	2.4679280 *
11 C	2.4823489 *	1.4149282 *	0.0000000	1.4537735 *
12 N	3.7929502	2.4679280 *	1.4537735 *	0.0000000
13 C	4.3370177	2.9140129 *	2.4428989 *	1.3319797 *
14 C	5.7451812	4.3169139	3.8318189	2.5073450 *
15 C	6.7150565	5.3037266	4.5869592	3.1491815
16 C	8.0449086	6.6286890	5.9830865	4.5500280
17 C	8.5390486	7.1228563	6.6871533	5.3105324
18 C	7.8372178	6.4565798	6.2284322	4.9854637

19	C	6.4600777	5.0828982	4.8940225	3.7420281
20	O	6.5782576	5.2607236	4.2842991	2.9355034 *
21	N	5.3903583	4.5682134	3.1582252	2.9055813 *
22	H	4.0764808	4.8908208	4.6914641	6.0003919
23	H	5.9293296	6.2583086	5.4889232	6.4087974
24	H	6.2665867	6.0091091	4.8039683	5.1796977
25	H	2.1808337 *	3.4527542	3.9632566	5.4095118
26	H	1.1039189 *	2.1965262 *	3.4736160	4.6625479
27	H	2.1802443 *	1.1043469 *	2.1891575 *	2.6875055 *
28	H	3.9784632	2.6429455 *	2.6534768 *	2.0959494 *
29	H	8.8380000	7.4441309	6.6960663	5.2656385
30	H	9.6246839	8.2132325	7.7866591	6.4029584
31	H	8.4914307	7.1620785	7.0748863	5.9180032
32	H	6.0919036	4.8090083	4.8680454	3.9698132
33	H	7.4427458	6.1583638	5.1823523	3.8861583
34	H	5.5627778	4.6918175	3.3383585	3.0141371
35	H	6.3039490	5.5586237	4.1549268	3.8935627

C C C C

1	CO	2.8628653 *	3.2673761	3.0143890	4.2845419
2	C	6.2327051	7.5562440	8.0429595	9.4363057
3	C	6.5903047	7.7812593	8.0643910	9.4141604
4	C	5.7692180	6.8138354	6.9567737	8.2618176
5	C	4.3622092	5.4226319	5.6513238	6.9928499
6	C	3.7343725	5.0291465	5.5575476	6.9599098
7	C	4.9314785	6.3073866	6.9273194	8.3315986
8	C	5.1498355	6.5816247	7.3983072	8.7813359
9	C	4.3370177	5.7451812	6.7150565	8.0449086
10	C	2.9140129 *	4.3169139	5.3037266	6.6286890
11	C	2.4428989 *	3.8318189	4.5869592	5.9830865
12	N	1.3319797 *	2.5073450 *	3.1491815	4.5500280
13	C	0.0000000	1.4656151 *	2.6035106 *	3.8816671
14	C	1.4656151 *	0.0000000	1.4371293 *	2.4996106 *
15	C	2.6035106 *	1.4371293 *	0.0000000	1.4061526 *
16	C	3.8816671	2.4996106 *	1.4061526 *	0.0000000
17	C	4.3424096	2.8817268 *	2.4415474 *	1.4284970 *
18	C	3.7919249	2.4972447 *	2.8250567 *	2.4724756 *
19	C	2.4685994 *	1.4424037 *	2.4455375 *	2.8451224 *
20	O	3.0444707	2.5022882 *	1.4660635 *	2.4604705 *
21	N	4.0026308	4.7315436	4.7168580	5.9560834
22	H	7.1251118	8.4904792	9.0401712	10.4382494
23	H	7.6796209	8.8443852	9.0679010	10.3950305
24	H	6.4228113	7.3174861	7.2904435	8.5117854
25	H	6.2356594	7.6681263	8.4922412	9.8711949
26	H	4.9946126	6.3372517	7.3935583	8.6612968

27 H	2.6307183 *	3.8752125	4.9915932	6.2098496
28 H	1.1082812 *	2.1748738 *	3.5299656	4.6711071
29 H	4.7918155	3.5012213	2.1927491 *	1.1069274 *
30 H	5.4475756	3.9871742	3.4405651	2.1927244 *
31 H	4.6561025	3.4930933	3.9294606	3.4748078
32 H	2.6399281 *	2.1972963 *	3.4503545	3.9512182
33 H	4.0119948	3.3290185	2.0459952 *	2.5106286 *
34 H	3.8801262	4.5912190	4.7306486	5.9333942
35 H	4.9650720	5.5524098	5.3361531	6.4631252

C C C O

1 CO	5.4453683	5.6147590	4.7014279	1.9534835 *
2 C	10.3418461	10.0110229	8.6962672	7.2729199
3 C	10.4374689	10.2622549	9.0239903	7.1222930
4 C	9.3375620	9.2702566	8.1121688	5.9528967
5 C	8.0091005	7.8859998	6.7099665	4.7683569
6 C	7.8195293	7.4913363	6.1978646	4.9333469
7 C	9.1410405	8.7219025	7.3804331	6.3274091
8 C	9.4307850	8.8457607	7.4662287	7.0148927
9 C	8.5390486	7.8372178	6.4600777	6.5782576
10 C	7.1228563	6.4565798	5.0828982	5.2607236
11 C	6.6871533	6.2284322	4.8940225	4.2842991
12 N	5.3105324	4.9854637	3.7420281	2.9355034 *
13 C	4.3424096	3.7919249	2.4685994 *	3.0444707
14 C	2.8817268 *	2.4972447 *	1.4424037 *	2.5022882 *
15 C	2.4415474 *	2.8250567 *	2.4455375 *	1.4660635 *
16 C	1.4284970 *	2.4724756 *	2.8451224 *	2.4604705 *
17 C	0.0000000	1.4233274 *	2.4560061 *	3.7716860
18 C	1.4233274 *	0.0000000	1.4161416 *	4.2909455
19 C	2.4560061 *	1.4161416 *	0.0000000	3.7948688
20 O	3.7716860	4.2909455	3.7948688	0.0000000
21 N	7.0350167	7.0754850	6.0540462	3.7731749
22 H	11.3060539	10.9159801	9.5745711	8.3066962
23 H	11.4571483	11.3239005	10.1024314	8.0601572
24 H	9.6557163	9.7130961	8.6451159	6.1852435
25 H	10.5094840	9.8979826	8.5149570	8.0891554
26 H	9.0266490	8.2203595	6.8698695	7.3933485
27 H	6.5286493	5.7505181	4.4077787	5.2202409
28 H	4.8512724	3.9952494	2.5799837 *	4.1381817
29 H	2.2018638 *	3.4744391	3.9520378	2.6849902 *
30 H	1.1054884 *	2.2010388 *	3.4614207	4.6513847
31 H	2.1981202 *	1.1044150 *	2.1878157 *	5.3953439
32 H	3.4578551	2.1867233 *	1.1061559 *	4.6916315
33 H	3.9310192	4.7310446	4.4866204	0.9922292 *
34 H	6.8772498	6.8103160	5.7806372	4.0434990

35 H	7.6264835	7.8090156	6.8884524	4.2426576
	N	H	H	H
1 CO	1.9809463 *	6.4434603	6.1261038	4.3445434
2 C	4.3431614	1.1047009 *	2.1861785 *	3.4372965
3 C	3.8168938	2.1791227 *	1.1045037 *	2.1926043 *
4 C	2.4764427 *	3.4501460	2.2026799 *	1.1079412 *
5 C	1.5108472 *	3.9426024	3.4681127	2.1843584 *
6 C	2.5935289 *	3.5200757	4.0287814	3.5084560
7 C	3.8878789	2.1958992 *	3.4862316	3.9517989
8 C	5.1124829	2.6772304 *	4.6682660	5.3943022
9 C	5.3903583	4.0764808	5.9293296	6.2665867
10 C	4.5682134	4.8908208	6.2583086	6.0091091
11 C	3.1582252	4.6914641	5.4889232	4.8039683
12 N	2.9055813 *	6.0003919	6.4087974	5.1796977
13 C	4.0026308	7.1251118	7.6796209	6.4228113
14 C	4.7315436	8.4904792	8.8443852	7.3174861
15 C	4.7168580	9.0401712	9.0679010	7.2904435
16 C	5.9560834	10.4382494	10.3950305	8.5117854
17 C	7.0350167	11.3060539	11.4571483	9.6557163
18 C	7.0754850	10.9159801	11.3239005	9.7130961
19 C	6.0540462	9.5745711	10.1024314	8.6451159
20 O	3.7731749	8.3066962	8.0601572	6.1852435
21 N	0.0000000	5.4466345	4.6780096	2.6562109 *
22 H	5.4466345	0.0000000	2.5291992 *	4.3577007
23 H	4.6780096	2.5291992 *	0.0000000	2.5182187 *
24 H	2.6562109 *	4.3577007	2.5182187 *	0.0000000
25 H	6.0572055	2.3954974 *	4.7760238	5.9721213
26 H	6.4740708	4.7736702	6.8483236	7.3468786
27 H	5.2623776	5.9648008	7.3470961	6.9680068
28 H	4.7542358	7.1861950	8.0358828	7.0265061
29 H	6.2808104	10.9620077	10.7179739	8.7189861
30 H	8.0153743	12.3923337	12.4877167	10.6200584
31 H	8.0798967	11.7516540	12.2696775	10.7143061
32 H	6.4431756	9.4495889	10.2033050	8.9462929
33 H	4.3906791	8.9930184	8.5858653	6.6264276
34 H	1.0443502 *	5.8487419	5.1799291	3.2176786
35 H	1.0398851 *	5.8198855	4.5865763	2.2146361 *

H H H H

1 CO	6.4951088	6.2734884	4.5193400	3.8789868
2 C	2.6778939 *	4.6657423	5.3907749	6.3968075
3 C	4.0770833	5.9277321	6.2677490	6.9363641
4 C	4.8876706	6.2513732	6.0088277	6.2774967

5 C	4.6704801	5.4688468	4.8043616	4.9009020
6 C	3.5173209	4.0170893	3.5057466	4.0398091
7 C	2.1961525 *	3.4827166	3.9499429	5.0205653
8 C	1.1049533 *	2.1840343 *	3.4300654	4.9740463
9 C	2.1808337 *	1.1039189 *	2.1802443 *	3.9784632
10 C	3.4527542	2.1965262 *	1.1043469 *	2.6429455 *
11 C	3.9632566	3.4736160	2.1891575 *	2.6534768 *
12 N	5.4095118	4.6625479	2.6875055 *	2.0959494 *
13 C	6.2356594	4.9946126	2.6307183 *	1.1082812 *
14 C	7.6681263	6.3372517	3.8752125	2.1748738 *
15 C	8.4922412	7.3935583	4.9915932	3.5299656
16 C	9.8711949	8.6612968	6.2098496	4.6711071
17 C	10.5094840	9.0266490	6.5286493	4.8512724
18 C	9.8979826	8.2203595	5.7505181	3.9952494
19 C	8.5149570	6.8698695	4.4077787	2.5799837 *
20 O	8.0891554	7.3933485	5.2202409	4.1381817
21 N	6.0572055	6.4740708	5.2623776	4.7542358
22 H	2.3954974 *	4.7736702	5.9648008	7.1861950
23 H	4.7760238	6.8483236	7.3470961	8.0358828
24 H	5.9721213	7.3468786	6.9680068	7.0265061
25 H	0.0000000	2.5280915 *	4.3470121	6.0039665
26 H	2.5280915 *	0.0000000	2.4983362 *	4.4671852
27 H	4.3470121	2.4983362 *	0.0000000	2.1358684 *
28 H	6.0039665	4.4671852	2.1358684 *	0.0000000
29 H	10.5646765	9.5020622	7.1013215	5.6673951
30 H	11.6041574	10.0873131	7.5916090	5.9312956
31 H	10.6005023	8.7698236	6.3686627	4.6536443
32 H	8.1928972	6.3777980	4.0384873	2.2636683 *
33 H	8.8859846	8.2534212	6.1130589	5.0950105
34 H	6.3355853	6.6150258	5.3243859	4.5161245
35 H	6.7591450	7.3998829	6.2767384	5.7628890

H H H H

1 CO	4.6174699	6.4253622	6.6809930	5.2850235
2 C	9.9366942	11.4209968	10.8824338	8.6465069
3 C	9.7928164	11.4824521	11.1977073	9.1110139
4 C	8.5831741	10.3522046	10.2446140	8.3213936
5 C	7.4063357	9.0460281	8.8516670	6.9211151
6 C	7.5356563	8.9036008	8.3850439	6.2351642
7 C	8.9268703	10.2336631	9.5584810	7.2806282
8 C	9.4807333	10.5278064	9.5781446	7.1945745
9 C	8.8380000	9.6246839	8.4914307	6.0919036
10 C	7.4441309	8.2132325	7.1620785	4.8090083
11 C	6.6960663	7.7866591	7.0748863	4.8680454
12 N	5.2656385	6.4029584	5.9180032	3.9698132

13 C	4.7918155	5.4475756	4.6561025	2.6399281 *
14 C	3.5012213	3.9871742	3.4930933	2.1972963 *
15 C	2.1927491 *	3.4405651	3.9294606	3.4503545
16 C	1.1069274 *	2.1927244 *	3.4748078	3.9512182
17 C	2.2018638 *	1.1054884 *	2.1981202 *	3.4578551
18 C	3.4744391	2.2010388 *	1.1044150 *	2.1867233 *
19 C	3.9520378	3.4614207	2.1878157 *	1.1061559 *
20 O	2.6849902 *	4.6513847	5.3953439	4.6916315
21 N	6.2808104	8.0153743	8.0798967	6.4431756
22 H	10.9620077	12.3923337	11.7516540	9.4495889
23 H	10.7179739	12.4877167	12.2696775	10.2033050
24 H	8.7189861	10.6200584	10.7143061	8.9462929
25 H	10.5646765	11.6041574	10.6005023	8.1928972
26 H	9.5020622	10.0873131	8.7698236	6.3777980
27 H	7.1013215	7.5916090	6.3686627	4.0384873
28 H	5.6673951	5.9312956	4.6536443	2.2636683 *
29 H	0.0000000	2.5232408 *	4.3885319	5.0581341
30 H	2.5232408 *	0.0000000	2.5413961 *	4.3755256
31 H	4.3885319	2.5413961 *	0.0000000	2.5156437 *
32 H	5.0581341	4.3755256	2.5156437 *	0.0000000
33 H	2.3077056 *	4.6332471	5.8170295	5.4649806
34 H	6.3501338	7.8569311	7.7537058	6.0948852
35 H	6.6330935	8.5434029	8.8342514	7.3535920

H H H

1 CO	2.6579557 *	2.5056012 *	2.6250896 *
2 C	7.9578091	4.7737107	4.7371756
3 C	7.7098099	4.3252682	3.9175661
4 C	6.5092933	3.0597746	2.4860608 *
5 C	5.4401355	2.1115109 *	2.0891212 *
6 C	5.7304321	2.9617383 *	3.4243561
7 C	7.0993748	4.2453109	4.5630600
8 C	7.8333062	5.3777322	5.8892572
9 C	7.4427458	5.5627778	6.3039490
10 C	6.1583638	4.6918175	5.5586237
11 C	5.1823523	3.3383585	4.1549268
12 N	3.8861583	3.0141371	3.8935627
13 C	4.0119948	3.8801262	4.9650720
14 C	3.3290185	4.5912190	5.5524098
15 C	2.0459952 *	4.7306486	5.3361531
16 C	2.5106286 *	5.9333942	6.4631252
17 C	3.9310192	6.8772498	7.6264835
18 C	4.7310446	6.8103160	7.8090156
19 C	4.4866204	5.7806372	6.8884524
20 O	0.9922292 *	4.0434990	4.2426576

21 N	4.3906791	1.0443502 *	1.0398851 *
22 H	8.9930184	5.8487419	5.8198855
23 H	8.5858653	5.1799291	4.5865763
24 H	6.6264276	3.2176786	2.2146361 *
25 H	8.8859846	6.3355853	6.7591450
26 H	8.2534212	6.6150258	7.3998829
27 H	6.1130589	5.3243859	6.2767384
28 H	5.0950105	4.5161245	5.7628890
29 H	2.3077056 *	6.3501338	6.6330935
30 H	4.6332471	7.8569311	8.5434029
31 H	5.8170295	7.7537058	8.8342514
32 H	5.4649806	6.0948852	7.3535920
33 H	0.0000000	4.7435092	4.6733072
34 H	4.7435092	0.0000000	1.6659779 *
35 H	4.6733072	1.6659779 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.69, TOTAL = 7248.9 SECONDS (120.8 MIN)
WALL CLOCK TIME: STEP = 0.70, TOTAL = 6700.6 SECONDS (111.7 MIN)
CPU UTILIZATION: STEP = 98.31%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.97, TOTAL = 7249.9 SECONDS (120.8 MIN)
WALL CLOCK TIME: STEP = 0.96, TOTAL = 6701.5 SECONDS (111.7 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636811771	-284.636811771	0.010597162	0.000734160	198020534
11338184						
2	1	-284.636866365	-0.000054594	0.001201712	0.000058243	156152182
14863004						
3	2	-284.636866276	0.000000089	0.000728414	0.000115655	139109415
16242949						

4 3	-284.636867234	-0.000000958	0.000391237	0.000074232	132763182
16722777					
5 4	-284.636867023	0.000000210	0.000224827	0.000123597	129034163
17050844					
6 5	-284.636867306	-0.000000283	0.000184992	0.000012410	124253951
17413552					
7 6	-284.636867317	-0.000000011	0.000141757	0.000024957	117134636
17906912					
8 7	-284.636867338	-0.000000021	0.000043377	0.000006706	111623217
18297003					
9 8	-284.636867347	-0.000000009	0.000044736	0.000006708	102121415
18974772					
10 9	-284.636867348	-0.000000001	0.000149630	0.000005963	123641062
17508515					
11 10	-284.636867353	-0.000000005	0.000128807	0.000004378	154155468
15172446					
12 11	-284.636867356	-0.000000003	0.000081903	0.000005808	151034810
15434572					
13 12	-284.636867358	-0.000000002	0.000158296	0.000006404	149274341
15569092					

-----DISABLING FDIFF OPTION-----

14 13	-284.636867329	0.000000029	0.000082740	0.000006069	198023129
11337829					
15 14	-284.636867331	-0.000000002	0.000099389	0.000004357	198023111
11337829					
16 15	-284.636867333	-0.000000002	0.000059344	0.000002821	198023102
11337831					
17 16	-284.636867334	-0.000000001	0.000035765	0.000002816	198023105
11337829					
18 17	-284.636867334	0.000000000	0.000015716	0.000002295	198023093
11337832					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 59.7 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 19.6 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.5 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6368673340 AFTER 18 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6011111349
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998580299

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 62.44 , TOTAL = 7312.3 SECONDS (121.9 MIN)
WALL CLOCK TIME: STEP = 57.27 , TOTAL = 6758.8 SECONDS (112.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 4.05 , TOTAL = 7316.4 SECONDS (121.9 MIN)
WALL CLOCK TIME: STEP = 4.02 , TOTAL = 6762.8 SECONDS (112.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.86 , TOTAL = 7319.2 SECONDS (122.0 MIN)
WALL CLOCK TIME: STEP = 2.69 , TOTAL = 6765.5 SECONDS (112.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 76 ENERGY= -284.6368673

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0002133	0.0000339	0.0003302
2 C	6.0	0.0000452	0.0000414	0.0000911
3 C	6.0	-0.0000629	-0.0000956	0.0001044
4 C	6.0	0.0000889	0.0001432	0.0001579
5 C	6.0	0.0003466	0.0002845	0.0001580
6 C	6.0	-0.0004386	-0.0000756	-0.0002758

7 C	6.0	0.0001580	0.0003096	0.0000272
8 C	6.0	-0.0000426	-0.0002047	-0.0000268
9 C	6.0	-0.0000465	-0.0002110	-0.0001136
10 C	6.0	-0.0004036	0.0000244	-0.0002327
11 C	6.0	0.0001488	0.0000500	-0.0003938
12 N	7.0	-0.0000466	0.0000665	-0.0000435
13 C	6.0	-0.0000529	-0.0003005	0.0000580
14 C	6.0	-0.0000513	0.0001692	-0.0000060
15 C	6.0	-0.0000668	0.0000644	0.0000651
16 C	6.0	-0.0000255	0.0005834	0.0000004
17 C	6.0	-0.0000021	-0.0001087	-0.0000874
18 C	6.0	0.0000129	-0.0001856	-0.0001683
19 C	6.0	0.0003081	-0.0001424	-0.0000625
20 O	8.0	-0.0000331	0.0002947	-0.0001283
21 N	7.0	-0.0000740	-0.0001446	-0.0000040
22 H	1.0	-0.0001934	-0.0000568	-0.0003580
23 H	1.0	0.0003116	0.0000611	0.0001515
24 H	1.0	0.0003267	-0.0000125	0.0000098
25 H	1.0	0.0000097	-0.0001444	0.0001776
26 H	1.0	-0.0000285	-0.0003265	0.0001827
27 H	1.0	-0.0002181	0.0000316	0.0001032
28 H	1.0	-0.0000232	0.0001072	0.0000713
29 H	1.0	0.0002259	-0.0000705	0.0000231
30 H	1.0	-0.0002274	0.0000025	0.0001147
31 H	1.0	-0.0001167	0.0001790	0.0001324
32 H	1.0	0.0000681	0.0002609	0.0002417
33 H	1.0	-0.0000793	-0.0002520	0.0001922
34 H	1.0	0.0001292	-0.0001441	-0.0002423
35 H	1.0	0.0002669	-0.0002320	-0.0002493

MAXIMUM GRADIENT = 0.0005834 RMS GRADIENT = 0.0001843
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000177494
 PREDICTED ENERGY CHANGE WAS -0.0000148237 RATIO= 1.197
 GDIIS STEP HAS LENGTH = 0.020051
 RADIUS OF STEP TAKEN= 0.02005 CURRENT TRUST RADIUS= 0.06691

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 7319.3 SECONDS (122.0 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6765.5 SECONDS (112.8
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

1NSERCH= 77

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1570589984	-1.7363916648	0.8589602133
C	6.0	4.9802769432	0.6318081872	0.5568622984
C	6.0	5.1890863910	-0.7097286837	0.2108488581
C	6.0	4.0559798754	-1.5355581950	-0.0807704294
C	6.0	2.7456066802	-1.0266870489	-0.0023785420
C	6.0	2.4692439507	0.3411458583	0.4202123659
C	6.0	3.6482167641	1.1769105196	0.6706064296
C	6.0	3.4978545797	2.5611082278	1.0526755317
C	6.0	2.2291560878	3.1332317523	1.2155617817
C	6.0	1.0659244405	2.3243937312	1.0277657987
C	6.0	1.1610890122	0.9716971456	0.6246860190
N	7.0	-0.0508922608	0.1710262051	0.5723724162
C	6.0	-1.2470029214	0.6993083063	0.3180298508
C	6.0	-2.5514567906	0.0412110184	0.4372686322
C	6.0	-2.8226425265	-1.2839811877	0.9227403777
C	6.0	-4.1233954751	-1.8033324728	1.0512660958
C	6.0	-5.2340512379	-0.9845960819	0.6812869763
C	6.0	-5.0191990649	0.3332022996	0.1878237112
C	6.0	-3.6999792115	0.8342233572	0.0720672785
O	8.0	-1.6999792051	-2.1449556962	1.3077344316
N	7.0	1.6433305658	-1.9662943750	-0.4288985571
H	1.0	5.8397048363	1.2983705287	0.7538358662
H	1.0	6.2086799927	-1.1276526557	0.1395619426
H	1.0	4.2254396214	-2.5810612923	-0.4054092510
H	1.0	4.4093863074	3.1588358195	1.2334051218
H	1.0	2.1186172484	4.1853765545	1.5313398599
H	1.0	0.0811789655	2.7658024814	1.2611894123
H	1.0	-1.2911971079	1.7528549246	-0.0229433971
H	1.0	-4.2935613627	-2.8287048862	1.4310675522
H	1.0	-6.2591697579	-1.3860605570	0.7808446314
H	1.0	-5.8767371119	0.9666288303	-0.0995011763
H	1.0	-3.5347195421	1.8630531888	-0.2994479881
H	1.0	-2.0161030481	-2.9548572409	1.7851776110
H	1.0	1.2877281038	-1.6981598514	-1.3735284790
H	1.0	2.0425242598	-2.9210620469	-0.5294262438

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.000000	5.3817344	5.1764259	4.0155961
2 C	5.3817344	0.000000	1.4010881 *	2.4409788 *

3 C	5.1764259	1.4010881 *	0.0000000	1.4321196 *
4 C	4.0155961	2.4409788 *	1.4321196 *	0.0000000
5 C	2.8188941 *	2.8385045 *	2.4731603 *	1.4078967 *
6 C	3.1392453	2.5314906 *	2.9233052 *	2.5081333 *
7 C	4.5509328	1.4437654 *	2.4789239 *	2.8439980 *
8 C	5.4467372	2.4830637 *	3.7772095	4.2870595
9 C	5.3041477	3.7761979	4.9536835	5.1783551
10 C	4.1646740	4.2905421	5.1839866	5.0068466
11 C	2.8977070 *	3.8348821	4.3844289	3.8941483
12 N	1.9400050 *	5.0522494	5.3257680	4.4950445
13 C	2.8629757 *	6.2322237	6.5893944	5.7684744
14 C	3.2670710	7.5558005	7.7801790	6.8126929
15 C	3.0145256	8.0429887	8.0637681	6.9559881
16 C	4.2852950	9.4366942	9.4140634	8.2616821
17 C	5.4461761	10.3421828	10.4373685	9.3375034
18 C	5.6149168	10.0107380	10.2614486	9.2694812
19 C	4.7014897	8.6961397	9.0232220	8.1113578
20 O	1.9536923 *	7.2732420	7.1219561	5.9523421
21 N	1.9800098 *	4.3424731	3.8158378	2.4753997 *
22 H	6.4430813	1.1053145 *	2.1795875 *	3.4509990
23 H	6.1245582	2.1860503 *	1.1042252 *	2.2020561 *
24 H	4.3432497	3.4377720	2.1932339 *	1.1077832 *
25 H	6.4950557	2.6775913 *	4.0766831	4.8876670
26 H	6.2743242	4.6654636	5.9273546	6.2515093
27 H	4.5207630	5.3899137	6.2668374	6.0084609
28 H	3.8794383	6.3972109	6.9363572	6.2776832
29 H	4.6182764	9.9369745	9.7928342	8.5832815
30 H	6.4262606	11.4213451	11.4823730	10.3521516
31 H	6.6806933	10.8819884	11.1963807	10.2430541
32 H	5.2846137	8.6460625	9.1095773	8.3196813
33 H	2.6580388 *	7.9575285	7.7093364	6.5089448
34 H	2.5027745 *	4.7738953	4.3252565	3.0595556
35 H	2.6241265 *	4.7363805	3.9164851	2.4849379 *

C C C C

1 CO	2.8188941 *	3.1392453	4.5509328	5.4467372
2 C	2.8385045 *	2.5314906 *	1.4437654 *	2.4830637 *
3 C	2.4731603 *	2.9233052 *	2.4789239 *	3.7772095
4 C	1.4078967 *	2.5081333 *	2.8439980 *	4.2870595
5 C	0.0000000	1.4580557 *	2.4745618 *	3.8146154
6 C	1.4580557 *	0.0000000	1.4666890 *	2.5271095 *
7 C	2.4745618 *	1.4666890 *	0.0000000	1.4438105 *
8 C	3.8146154	2.5271095 *	1.4438105 *	0.0000000
9 C	4.3652061	2.9130682 *	2.4774790 *	1.4012327 *
10 C	3.8874506	2.5043360 *	2.8482476 *	2.4435504 *

11 C	2.6262988 *	1.4665176 *	2.4960019 *	2.8582995 *
12 N	3.0960074	2.5304505 *	3.8346917	4.3054369
13 C	4.3614966	3.7348644	4.9310840	5.1497258
14 C	5.4214922	5.0296807	6.3071556	6.5820039
15 C	5.6504376	5.5585641	6.9275955	7.3993432
16 C	6.9926058	6.9613153	8.3321490	8.7824710
17 C	8.0090019	7.8209020	9.1414938	9.4316556
18 C	7.8852828	7.4920522	8.7217555	8.8460011
19 C	6.7092553	6.1986809	7.3804924	7.4667620
20 O	4.7676152	4.9346548	6.3280271	7.0163786
21 N	1.5098986 *	2.5937237 *	3.8869290	5.1119170
22 H	3.9435005	3.5196009	2.1964288 *	2.6773260 *
23 H	3.4674512	4.0273460	3.4855404	4.6679019
24 H	2.1836709 *	3.5078724	3.9513729	5.3941912
25 H	4.6705380	3.5163634	2.1963946 *	1.1049125 *
26 H	5.4690964	4.0169208	3.4830166	2.1839558 *
27 H	4.8040354	3.5055751	3.9493195	3.4291471
28 H	4.9012306	4.0410675	5.0210091	4.9744593
29 H	7.4062084	7.5369303	8.9272110	9.4815309
30 H	9.0459155	8.9049707	10.2341234	10.5287016
31 H	8.8502855	8.3855072	9.5583487	9.5787705
32 H	6.9196348	6.2355185	7.2805475	7.1953191
33 H	5.4394004	5.7310648	7.0991755	7.8336558
34 H	2.1110040 *	2.9617991 *	4.2445758	5.3770335
35 H	2.0882435 *	3.4243107	4.5619849	5.8885672

C C C N

1 CO	5.3041477	4.1646740	2.8977070 *	1.9400050 *
2 C	3.7761979	4.2905421	3.8348821	5.0522494
3 C	4.9536835	5.1839866	4.3844289	5.3257680
4 C	5.1783551	5.0068466	3.8941483	4.4950445
5 C	4.3652061	3.8874506	2.6262988 *	3.0960074
6 C	2.9130682 *	2.5043360 *	1.4665176 *	2.5304505 *
7 C	2.4774790 *	2.8482476 *	2.4960019 *	3.8346917
8 C	1.4012327 *	2.4435504 *	2.8582995 *	4.3054369
9 C	0.0000000	1.4291935 *	2.4823645 *	3.7930166
10 C	1.4291935 *	0.0000000	1.4146793 *	2.4681277 *
11 C	2.4823645 *	1.4146793 *	0.0000000	1.4535162 *
12 N	3.7930166	2.4681277 *	1.4535162 *	0.0000000
13 C	4.3374219	2.9144915 *	2.4427731 *	1.3320859 *
14 C	5.7463547	4.3182238	3.8319611	2.5075741 *
15 C	6.7170071	5.3058791	4.5877051	3.1499847
16 C	8.0468361	6.6308157	5.9840234	4.5511223
17 C	8.5405749	7.1245459	6.6879074	5.3115405
18 C	7.8380522	6.4574820	6.2285219	4.9858050

19 C	6.4612433	5.0840737	4.8943100	3.7424552
20 O	6.5807190	5.2634295	4.2855328	2.9366677 *
21 N	5.3900471	4.5678522	3.1582260	2.9053526 *
22 H	4.0762690	4.8904745	4.6917844	6.0002474
23 H	5.9287032	6.2572730	5.4882410	6.4075063
24 H	6.2662461	6.0083289	4.8034814	5.1785188
25 H	2.1804536 *	3.4521469	3.9630228	5.4090716
26 H	1.1040577 *	2.1965896 *	3.4737036	4.6627673
27 H	2.1796541 *	1.1041068 *	2.1886426 *	2.6878943 *
28 H	3.9789725	2.6432307 *	2.6539289 *	2.0964110 *
29 H	8.8395121	7.4458825	6.6967543	5.2664965
30 H	9.6262484	8.2149526	7.7874031	6.4039589
31 H	8.4928831	7.1634353	7.0749890	5.9181810
32 H	6.0935105	4.8104321	4.8681780	3.9698966
33 H	7.4438911	6.1597936	5.1825785	3.8863990
34 H	5.5616562	4.6900265	3.3372197	3.0120245
35 H	6.3035139	5.5581832	4.1548138	3.8932458

C C C C

1 CO	2.8629757 *	3.2670710	3.0145256	4.2852950
2 C	6.2322237	7.5558005	8.0429887	9.4366942
3 C	6.5893944	7.7801790	8.0637681	9.4140634
4 C	5.7684744	6.8126929	6.9559881	8.2616821
5 C	4.3614966	5.4214922	5.6504376	6.9926058
6 C	3.7348644	5.0296807	5.5585641	6.9613153
7 C	4.9310840	6.3071556	6.9275955	8.3321490
8 C	5.1497258	6.5820039	7.3993432	8.7824710
9 C	4.3374219	5.7463547	6.7170071	8.0468361
10 C	2.9144915 *	4.3182238	5.3058791	6.6308157
11 C	2.4427731 *	3.8319611	4.5877051	5.9840234
12 N	1.3320859 *	2.5075741 *	3.1499847	4.5511223
13 C	0.0000000	1.4659160 *	2.6041798 *	3.8825868
14 C	1.4659160 *	0.0000000	1.4371357 *	2.5000650 *
15 C	2.6041798 *	1.4371357 *	0.0000000	1.4064860 *
16 C	3.8825868	2.5000650 *	1.4064860 *	0.0000000
17 C	4.3432757	2.8823841 *	2.4418893 *	1.4285552 *
18 C	3.7921565	2.4974454 *	2.8249328 *	2.4724032 *
19 C	2.4689658 *	1.4426865 *	2.4454355 *	2.8451384 *
20 O	3.0454130	2.5024088 *	1.4662437 *	2.4607781 *
21 N	4.0021703	4.7303873	4.7156542	5.9558856
22 H	7.1253231	8.4907160	9.0406488	10.4389843
23 H	7.6783361	8.8427862	9.0665646	10.3942066
24 H	6.4212005	7.3152405	7.2884745	8.5105706
25 H	6.2355374	7.6685562	8.4933725	9.8724188
26 H	4.9952169	6.3388241	7.3959662	8.6635922

27 H	2.6313524 *	3.8772432	4.9947447	6.2128503
28 H	1.1082312 *	2.1748045 *	3.5301581	4.6713748
29 H	4.7924157	3.5012829	2.1927540 *	1.1066138 *
30 H	5.4483738	3.9877668	3.4409699	2.1928920 *
31 H	4.6562035	3.4931374	3.9290860	3.4743572
32 H	2.6399296 *	2.1974226 *	3.4503077	3.9513734
33 H	4.0121021	3.3286465	2.0460036 *	2.5110390 *
34 H	3.8773811	4.5873454	4.7264724	5.9305100
35 H	4.9644992	5.5510560	5.3346668	6.4626987

C C C O

1 CO	5.4461761	5.6149168	4.7014897	1.9536923 *
2 C	10.3421828	10.0107380	8.6961397	7.2732420
3 C	10.4373685	10.2614486	9.0232220	7.1219561
4 C	9.3375034	9.2694812	8.1113578	5.9523421
5 C	8.0090019	7.8852828	6.7092553	4.7676152
6 C	7.8209020	7.4920522	6.1986809	4.9346548
7 C	9.1414938	8.7217555	7.3804924	6.3280271
8 C	9.4316556	8.8460011	7.4667620	7.0163786
9 C	8.5405749	7.8380522	6.4612433	6.5807190
10 C	7.1245459	6.4574820	5.0840737	5.2634295
11 C	6.6879074	6.2285219	4.8943100	4.2855328
12 N	5.3115405	4.9858050	3.7424552	2.9366677 *
13 C	4.3432757	3.7921565	2.4689658 *	3.0454130
14 C	2.8823841 *	2.4974454 *	1.4426865 *	2.5024088 *
15 C	2.4418893 *	2.8249328 *	2.4454355 *	1.4662437 *
16 C	1.4285552 *	2.4724032 *	2.8451384 *	2.4607781 *
17 C	0.0000000	1.4234676 *	2.4561412 *	3.7720732
18 C	1.4234676 *	0.0000000	1.4158964 *	4.2910008
19 C	2.4561412 *	1.4158964 *	0.0000000	3.7950469
20 O	3.7720732	4.2910008	3.7950469	0.0000000
21 N	7.0352416	7.0751207	6.0534970	3.7716753
22 H	11.3068684	10.9163965	9.5752709	8.3072339
23 H	11.4564405	11.3226187	10.1012395	8.0589343
24 H	9.6546143	9.7112410	8.6431717	6.1834972
25 H	10.5104115	9.8982659	8.5155351	8.0907402
26 H	9.0284517	8.2214782	6.8713732	7.3962683
27 H	6.5309608	5.7518270	4.4093272	5.2240058
28 H	4.8513583	3.9947259	2.5797562 *	4.1389291
29 H	2.2016879 *	3.4741707	3.9517420	2.6850312 *
30 H	1.1054200 *	2.2011510 *	3.4614278	4.6518548
31 H	2.1977156 *	1.1041541 *	2.1875196 *	5.3951438
32 H	3.4581318	2.1866771 *	1.1062663 *	4.6918485
33 H	3.9313731	4.7309049	4.4863479	0.9918804 *
34 H	6.8749579	6.8074653	5.7775372	4.0392069

35 H	7.6265509	7.8084967	6.8876926	4.2407349
	N	H	H	H
1 CO	1.9800098 *	6.4430813	6.1245582	4.3432497
2 C	4.3424731	1.1053145 *	2.1860503 *	3.4377720
3 C	3.8158378	2.1795875 *	1.1042252 *	2.1932339 *
4 C	2.4753997 *	3.4509990	2.2020561 *	1.1077832 *
5 C	1.5098986 *	3.9435005	3.4674512	2.1836709 *
6 C	2.5937237 *	3.5196009	4.0273460	3.5078724
7 C	3.8869290	2.1964288 *	3.4855404	3.9513729
8 C	5.1119170	2.6773260 *	4.6679019	5.3941912
9 C	5.3900471	4.0762690	5.9287032	6.2662461
10 C	4.5678522	4.8904745	6.2572730	6.0083289
11 C	3.1582260	4.6917844	5.4882410	4.8034814
12 N	2.9053526 *	6.0002474	6.4075063	5.1785188
13 C	4.0021703	7.1253231	7.6783361	6.4212005
14 C	4.7303873	8.4907160	8.8427862	7.3152405
15 C	4.7156542	9.0406488	9.0665646	7.2884745
16 C	5.9558856	10.4389843	10.3942066	8.5105706
17 C	7.0352416	11.3068684	11.4564405	9.6546143
18 C	7.0751207	10.9163965	11.3226187	9.7112410
19 C	6.0534970	9.5752709	10.1012395	8.6431717
20 O	3.7716753	8.3072339	8.0589343	6.1834972
21 N	0.0000000	5.4466921	4.6764177	2.6543883 *
22 H	5.4466921	0.0000000	2.5296371 *	4.3588637
23 H	4.6764177	2.5296371 *	0.0000000	2.5184584 *
24 H	2.6543883 *	4.3588637	2.5184584 *	0.0000000
25 H	6.0565070	2.3952304 *	4.7757653	5.9720991
26 H	6.4739082	4.7734483	6.8479149	7.3467257
27 H	5.2620771	5.9641751	7.3459724	6.9671658
28 H	4.7548211	7.1874686	8.0356635	7.0258374
29 H	6.2809165	10.9624121	10.7172123	8.7182196
30 H	8.0155886	12.3931298	12.4870051	10.6189575
31 H	8.0784874	11.7521593	12.2678634	10.7113799
32 H	6.4414954	9.4502966	10.2015139	8.9432350
33 H	4.3898570	8.9926264	8.5845083	6.6253490
34 H	1.0443538 *	5.8502449	5.1798348	3.2166627
35 H	1.0397320 *	5.8197039	4.5848354	2.2127133 *

H H H H

1 CO	6.4950557	6.2743242	4.5207630	3.8794383
2 C	2.6775913 *	4.6654636	5.3899137	6.3972109
3 C	4.0766831	5.9273546	6.2668374	6.9363572
4 C	4.8876670	6.2515093	6.0084609	6.2776832

5 C	4.6705380	5.4690964	4.8040354	4.9012306
6 C	3.5163634	4.0169208	3.5055751	4.0410675
7 C	2.1963946 *	3.4830166	3.9493195	5.0210091
8 C	1.1049125 *	2.1839558 *	3.4291471	4.9744593
9 C	2.1804536 *	1.1040577 *	2.1796541 *	3.9789725
10 C	3.4521469	2.1965896 *	1.1041068 *	2.6432307 *
11 C	3.9630228	3.4737036	2.1886426 *	2.6539289 *
12 N	5.4090716	4.6627673	2.6878943 *	2.0964110 *
13 C	6.2355374	4.9952169	2.6313524 *	1.1082312 *
14 C	7.6685562	6.3388241	3.8772432	2.1748045 *
15 C	8.4933725	7.3959662	4.9947447	3.5301581
16 C	9.8724188	8.6635922	6.2128503	4.6713748
17 C	10.5104115	9.0284517	6.5309608	4.8513583
18 C	9.8982659	8.2214782	5.7518270	3.9947259
19 C	8.5155351	6.8713732	4.4093272	2.5797562 *
20 O	8.0907402	7.3962683	5.2240058	4.1389291
21 N	6.0565070	6.4739082	5.2620771	4.7548211
22 H	2.3952304 *	4.7734483	5.9641751	7.1874686
23 H	4.7757653	6.8479149	7.3459724	8.0356635
24 H	5.9720991	7.3467257	6.9671658	7.0258374
25 H	0.0000000	2.5278793 *	4.3461047	6.0043189
26 H	2.5278793 *	0.0000000	2.4978644 *	4.4676383
27 H	4.3461047	2.4978644 *	0.0000000	2.1350588 *
28 H	6.0043189	4.4676383	2.1350588 *	0.0000000
29 H	10.5655578	9.5038638	7.1039232	5.6673653
30 H	11.6051274	10.0891759	7.5939923	5.9312408
31 H	10.6012615	8.7718681	6.3706568	4.6530839
32 H	8.1937482	6.3800617	4.0404539	2.2631817 *
33 H	8.8864284	8.2548946	6.1154806	5.0948350
34 H	6.3349238	6.6139729	5.3220728	4.5149129
35 H	6.7583111	7.3995957	6.2764327	5.7633083

H H H H

1 CO	4.6182764	6.4262606	6.6806933	5.2846137
2 C	9.9369745	11.4213451	10.8819884	8.6460625
3 C	9.7928342	11.4823730	11.1963807	9.1095773
4 C	8.5832815	10.3521516	10.2430541	8.3196813
5 C	7.4062084	9.0459155	8.8502855	6.9196348
6 C	7.5369303	8.9049707	8.3855072	6.2355185
7 C	8.9272110	10.2341234	9.5583487	7.2805475
8 C	9.4815309	10.5287016	9.5787705	7.1953191
9 C	8.8395121	9.6262484	8.4928831	6.0935105
10 C	7.4458825	8.2149526	7.1634353	4.8104321
11 C	6.6967543	7.7874031	7.0749890	4.8681780
12 N	5.2664965	6.4039589	5.9181810	3.9698966

13 C	4.7924157	5.4483738	4.6562035	2.6399296 *
14 C	3.5012829	3.9877668	3.4931374	2.1974226 *
15 C	2.1927540 *	3.4409699	3.9290860	3.4503077
16 C	1.1066138 *	2.1928920 *	3.4743572	3.9513734
17 C	2.2016879 *	1.1054200 *	2.1977156 *	3.4581318
18 C	3.4741707	2.2011510 *	1.1041541 *	2.1866771 *
19 C	3.9517420	3.4614278	2.1875196 *	1.1062663 *
20 O	2.6850312 *	4.6518548	5.3951438	4.6918485
21 N	6.2809165	8.0155886	8.0784874	6.4414954
22 H	10.9624121	12.3931298	11.7521593	9.4502966
23 H	10.7172123	12.4870051	12.2678634	10.2015139
24 H	8.7182196	10.6189575	10.7113799	8.9432350
25 H	10.5655578	11.6051274	10.6012615	8.1937482
26 H	9.5038638	10.0891759	8.7718681	6.3800617
27 H	7.1039232	7.5939923	6.3706568	4.0404539
28 H	5.6673653	5.9312408	4.6530839	2.2631817 *
29 H	0.0000000	2.5234161 *	4.3878975	5.0579758
30 H	2.5234161 *	0.0000000	2.5409468 *	4.3756601
31 H	4.3878975	2.5409468 *	0.0000000	2.5156712 *
32 H	5.0579758	4.3756601	2.5156712 *	0.0000000
33 H	2.3082731 *	4.6339425	5.8167484	5.4648075
34 H	6.3478093	7.8545781	7.7494391	6.0903110
35 H	6.6331023	8.5434866	8.8325351	7.3516187

H H H

1 CO	2.6580388 *	2.5027745 *	2.6241265 *
2 C	7.9575285	4.7738953	4.7363805
3 C	7.7093364	4.3252565	3.9164851
4 C	6.5089448	3.0595556	2.4849379 *
5 C	5.4394004	2.1110040 *	2.0882435 *
6 C	5.7310648	2.9617991 *	3.4243107
7 C	7.0991755	4.2445758	4.5619849
8 C	7.8336558	5.3770335	5.8885672
9 C	7.4438911	5.5616562	6.3035139
10 C	6.1597936	4.6900265	5.5581832
11 C	5.1825785	3.3372197	4.1548138
12 N	3.8863990	3.0120245	3.8932458
13 C	4.0121021	3.8773811	4.9644992
14 C	3.3286465	4.5873454	5.5510560
15 C	2.0460036 *	4.7264724	5.3346668
16 C	2.5110390 *	5.9305100	6.4626987
17 C	3.9313731	6.8749579	7.6265509
18 C	4.7309049	6.8074653	7.8084967
19 C	4.4863479	5.7775372	6.8876926
20 O	0.9918804 *	4.0392069	4.2407349

21 N	4.3898570	1.0443538 *	1.0397320 *
22 H	8.9926264	5.8502449	5.8197039
23 H	8.5845083	5.1798348	4.5848354
24 H	6.6253490	3.2166627	2.2127133 *
25 H	8.8864284	6.3349238	6.7583111
26 H	8.2548946	6.6139729	7.3995957
27 H	6.1154806	5.3220728	6.2764327
28 H	5.0948350	4.5149129	5.7633083
29 H	2.3082731 *	6.3478093	6.6331023
30 H	4.6339425	7.8545781	8.5434866
31 H	5.8167484	7.7494391	8.8325351
32 H	5.4648075	6.0903110	7.3516187
33 H	0.0000000	4.7404655	4.6723644
34 H	4.7404655	0.0000000	1.6666480 *
35 H	4.6723644	1.6666480 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.79 , TOTAL = 7320.1 SECONDS (122.0 MIN)
WALL CLOCK TIME: STEP = 0.78 , TOTAL = 6766.3 SECONDS (112.8 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.11 , TOTAL = 7321.2 SECONDS (122.0 MIN)
WALL CLOCK TIME: STEP = 1.11 , TOTAL = 6767.4 SECONDS (112.8 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636861541	-284.636861541	0.010000912	0.000329135	198023352
11337522						
2	1	-284.636877508	-0.000015967	0.002400644	0.000049790	151942862
15214311						
3	2	-284.636877120	0.000000387	0.001143578	0.000089307	137603087
16325789						

4 3	-284.636877902	-0.000000782	0.000469281	0.000044103	132220232
16753059					
5 4	-284.636877816	0.000000086	0.000285330	0.000091431	124495657
17375006					
6 5	-284.636877937	-0.000000121	0.000123784	0.000008759	119419850
17766357					
7 6	-284.636877934	0.000000003	0.000079870	0.000016543	113648782
18140064					
8 7	-284.636877949	-0.000000015	0.000037167	0.000007154	107764981
18553993					
9 8	-284.636877970	-0.000000021	0.000073844	0.000005937	99193237
19214737					
10 9	-284.636877974	-0.000000004	0.000188860	0.000005951	129118227
17167984					
11 10	-284.636877978	-0.000000005	0.000100517	0.000005518	156744514
15002516					
12 11	-284.636877980	-0.000000002	0.000037890	0.000005274	154872861
15073898					
13 12	-284.636877981	-0.000000001	0.000050230	0.000003996	148853543
15569551					

-----DISABLING FDIFF OPTION-----

14 13	-284.636877921	0.000000060	0.000061364	0.000002565	198025251
11337250					
15 14	-284.636877922	-0.000000001	0.000042386	0.000001625	198025287
11337248					
16 15	-284.636877922	0.000000000	0.000013583	0.000001852	198025283
11337249					
17 16	-284.636877922	0.000000000	0.000021303	0.000001621	198025282
11337248					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 56.1 SECONDS (3.3 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 18.5 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.2
 TIME TO SOLVE SCF EQUATIONS= 1.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6368779220 AFTER 17 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6018649046
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998597400

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 59.26 , TOTAL = 7380.4 SECONDS (123.0 MIN)
WALL CLOCK TIME: STEP = 54.74 , TOTAL = 6822.2 SECONDS (113.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.80 , TOTAL = 7384.2 SECONDS (123.1 MIN)
WALL CLOCK TIME: STEP = 3.77 , TOTAL = 6825.9 SECONDS (113.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.88 , TOTAL = 7387.1 SECONDS (123.1 MIN)
WALL CLOCK TIME: STEP = 2.71 , TOTAL = 6828.7 SECONDS (113.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 77 ENERGY= -284.6368779

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000025	0.0000065	0.0001302
2 C	6.0	-0.0003857	-0.0000366	-0.0000969
3 C	6.0	-0.0000062	0.0001152	0.0000885
4 C	6.0	0.0001632	-0.0000649	0.0000888
5 C	6.0	-0.0000805	-0.0001319	0.0000196
6 C	6.0	0.0006186	0.0004447	-0.0000572
7 C	6.0	-0.0001979	-0.0003458	-0.0002156
8 C	6.0	-0.0002601	-0.0000695	0.0000656

9 C	6.0	-0.0000264	-0.0003837	-0.0001600
10 C	6.0	-0.0001805	0.0000467	-0.0003194
11 C	6.0	-0.0004053	0.0001394	-0.0002613
12 N	7.0	0.0001171	0.0000500	0.0000785
13 C	6.0	0.0001047	-0.0000506	-0.0000166
14 C	6.0	0.0000525	0.0000390	0.0000049
15 C	6.0	0.0000497	0.0000849	-0.0001811
16 C	6.0	-0.0001917	0.0002326	-0.0000048
17 C	6.0	-0.0002371	-0.0001396	0.0000074
18 C	6.0	0.0000857	0.0001592	0.0000722
19 C	6.0	-0.0000301	-0.0001301	0.0001508
20 O	8.0	-0.0001327	-0.0000802	-0.0000352
21 N	7.0	0.0002578	-0.0001329	0.0001293
22 H	1.0	0.0001411	0.0001635	-0.0001481
23 H	1.0	0.0001038	0.0000715	0.0001960
24 H	1.0	0.0001782	0.0000735	0.0000108
25 H	1.0	-0.0000277	-0.0001251	0.0001402
26 H	1.0	-0.0000300	-0.0002359	0.0002419
27 H	1.0	-0.0000550	-0.0000215	0.0000376
28 H	1.0	-0.0000861	0.0000979	0.0001082
29 H	1.0	0.0002424	0.0001551	0.0000336
30 H	1.0	-0.0001901	0.0000076	0.0000549
31 H	1.0	0.0000117	-0.0000328	-0.0000154
32 H	1.0	0.0001126	0.0002645	0.0000564
33 H	1.0	0.0000160	0.0000314	0.0001079
34 H	1.0	0.0000109	-0.0000488	-0.0001685
35 H	1.0	0.0002596	-0.0001531	-0.0001433

MAXIMUM GRADIENT = 0.0006186 RMS GRADIENT = 0.0001648
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000105880
 PREDICTED ENERGY CHANGE WAS -0.0000091434 RATIO= 1.158
 GDIIS STEP HAS LENGTH = 0.011848
 RADIUS OF STEP TAKEN= 0.01185 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 7387.1 SECONDS (123.1 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6828.7 SECONDS (113.8
 MIN)
 CPU UTILIZATION: STEP = 85.83% , TOTAL = 100.00%

INSERCH= 78

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM CHARGE X Y Z

CO	27.0	0.1572474782	-1.7364631093	0.8589486165
C	6.0	4.9806560023	0.6318951146	0.5569577971
C	6.0	5.1887161429	-0.7096698750	0.2102906375
C	6.0	4.0555198518	-1.5354079234	-0.0814194053
C	6.0	2.7453914942	-1.0265751410	-0.0020494733
C	6.0	2.4689789266	0.3408412847	0.4211212300
C	6.0	3.6484773241	1.1772677901	0.6709268367
C	6.0	3.4982958145	2.5613767237	1.0522937334
C	6.0	2.2297008466	3.1339041532	1.2155724644
C	6.0	1.0668084637	2.3247292124	1.0283129373
C	6.0	1.1617244126	0.9716033410	0.6260561558
N	7.0	-0.0507509005	0.1712038898	0.5730824975
C	6.0	-1.2468946393	0.6993379115	0.3184743684
C	6.0	-2.5512995229	0.0407049910	0.4369079607
C	6.0	-2.8226926719	-1.2849264616	0.9216771302
C	6.0	-4.1234615029	-1.8041248947	1.0507260392
C	6.0	-5.2339030725	-0.9844666754	0.6816515545
C	6.0	-5.0191127456	0.3332937878	0.1882584557
C	6.0	-3.6998307867	0.8340476613	0.0721958290
O	8.0	-1.6998953945	-2.1460721655	1.3065956135
N	7.0	1.6429998106	-1.9658723224	-0.4282212018
H	1.0	5.8398666634	1.2979394116	0.7554095351
H	1.0	6.2078564241	-1.1279462699	0.1390631042
H	1.0	4.2243480099	-2.5808838066	-0.4065774818
H	1.0	4.4096609222	3.1593867869	1.2318652365
H	1.0	2.1192307139	4.1863909393	1.5305848539
H	1.0	0.0820222048	2.7665166302	1.2606957400
H	1.0	-1.2913998291	1.7530129186	-0.0219070941
H	1.0	-4.2944896682	-2.8291421974	1.4312609030
H	1.0	-6.2592001837	-1.3858201032	0.7811496963
H	1.0	-5.8763340861	0.9661034370	-0.1007011276
H	1.0	-3.5344491660	1.8620780511	-0.3002002442
H	1.0	-2.0161611292	-2.9552488929	1.7847668488
H	1.0	1.2864764523	-1.6972549652	-1.3721199828
H	1.0	2.0418943404	-2.9206542323	-0.5287627642

 INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3819689	5.1759771	4.0151267
2 C	5.3819689	0.0000000	1.4011651 *	2.4414350 *
3 C	5.1759771	1.4011651 *	0.0000000	1.4321564 *
4 C	4.0151267	2.4414350 *	1.4321564 *	0.0000000

5 C	2.8184656 *	2.8389118 *	2.4729239 *	1.4077097 *
6 C	3.1386285	2.5321307 *	2.9231821 *	2.5079813 *
7 C	4.5512488	1.4439946 *	2.4789222 *	2.8443484 *
8 C	5.4471473	2.4830724 *	3.7770671	4.2871259
9 C	5.3049713	3.7764503	4.9537283	5.1786367
10 C	4.1652453	4.2902291	5.1833253	5.0064519
11 C	2.8977296 *	3.8346336	4.3836290	3.8935433
12 N	1.9401485 *	5.0524798	5.3253705	4.4947031
13 C	2.8630149 *	6.2324802	6.5889372	5.7679809
14 C	3.2669055	7.5560752	7.7796054	6.8119643
15 C	3.0146084	8.0435984	8.0634770	6.9554835
16 C	4.2855368	9.4373172	9.4138630	8.2613376
17 C	5.4462315	10.3424074	10.4368906	9.3369798
18 C	5.6150177	10.0110178	10.2609955	9.2689659
19 C	4.7014422	8.6963619	9.0226604	8.1106955
20 O	1.9537520 *	7.2738453	7.1216645	5.9518317
21 N	1.9791146 *	4.3426861	3.8154746	2.4750402 *
22 H	6.4428627	1.1050978 *	2.1798272 *	3.4513814
23 H	6.1235934	2.1857947 *	1.1039363 *	2.2016335 *
24 H	4.3423392	3.4383645	2.1936212 *	1.1078134 *
25 H	6.4954933	2.6776388 *	4.0767807	4.8878656
26 H	6.2754023	4.6658488	5.9275905	6.2519401
27 H	4.5214916	5.3896632	6.2662227	6.0080372
28 H	3.8795526	6.3977085	6.9361823	6.2774838
29 H	4.6194645	9.9383858	9.7935756	8.5839740
30 H	6.4264923	11.4217251	11.4820663	10.3518043
31 H	6.6804865	10.8820239	11.1955468	10.2420532
32 H	5.2841034	8.6461024	9.1086827	8.3185579
33 H	2.6582481 *	7.9580505	7.7092060	6.5087564
34 H	2.5008723 *	4.7742270	4.3251384	3.0593633
35 H	2.6229650 *	4.7366355	3.9162660	2.4846954 *

C C C C

1 CO	2.8184656 *	3.1386285	4.5512488	5.4471473
2 C	2.8389118 *	2.5321307 *	1.4439946 *	2.4830724 *
3 C	2.4729239 *	2.9231821 *	2.4789222 *	3.7770671
4 C	1.4077097 *	2.5079813 *	2.8443484 *	4.2871259
5 C	0.0000000	1.4578426 *	2.4749515 *	3.8146957
6 C	1.4578426 *	0.0000000	1.4673884 *	2.5275778 *
7 C	2.4749515 *	1.4673884 *	0.0000000	1.4435210 *
8 C	3.8146957	2.5275778 *	1.4435210 *	0.0000000
9 C	4.3655616	2.9136930 *	2.4774970 *	1.4013496 *
10 C	3.8872263	2.5041116 *	2.8477020 *	2.4430939 *
11 C	2.6258780 *	1.4658695 *	2.4956465 *	2.8580804 *
12 N	3.0957816	2.5300015 *	3.8348439	4.3056129

13 C	4.3611764	3.7345378	4.9312581	5.1500011
14 C	5.4209507	5.0292670	6.3074379	6.5825595
15 C	5.6500954	5.5583689	6.9282983	7.4004057
16 C	6.9924289	6.9611460	8.3328256	8.7834385
17 C	8.0086430	7.8204033	9.1416570	9.4319499
18 C	7.8849849	7.4917154	8.7219481	8.8463077
19 C	6.7088240	6.1983235	7.3806443	7.4670800
20 O	4.7672215	4.9344013	6.3288035	7.0175449
21 N	1.5096917 *	2.5931741 *	3.8870807	5.1117543
22 H	3.9437151	3.5200383	2.1963347 *	2.6771941 *
23 H	3.4668216	4.0269217	3.4852995	4.6676346
24 H	2.1833073 *	3.5075466	3.9517523	5.3942840
25 H	4.6706119	3.5167814	2.1960984 *	1.1047390 *
26 H	5.4695576	4.0176468	3.4831637	2.1843201 *
27 H	4.8037076	3.5051888	3.9488152	3.4287664
28 H	4.9012435	4.0411572	5.0213432	4.9747908
29 H	7.4069935	7.5374853	8.9286143	9.4830805
30 H	9.0457244	8.9046106	10.2344341	10.5291315
31 H	8.8495566	8.3849568	9.5583488	9.5790386
32 H	6.9187867	6.2350313	7.2805553	7.1956765
33 H	5.4391983	5.7306388	7.0997509	7.8344694
34 H	2.1107671 *	2.9610577 *	4.2445223	5.3764180
35 H	2.0880303 *	3.4237456	4.5621627	5.8884215

C C C N

1 CO	5.3049713	4.1652453	2.8977296 *	1.9401485 *
2 C	3.7764503	4.2902291	3.8346336	5.0524798
3 C	4.9537283	5.1833253	4.3836290	5.3253705
4 C	5.1786367	5.0064519	3.8935433	4.4947031
5 C	4.3655616	3.8872263	2.6258780 *	3.0957816
6 C	2.9136930 *	2.5041116 *	1.4658695 *	2.5300015 *
7 C	2.4774970 *	2.8477020 *	2.4956465 *	3.8348439
8 C	1.4013496 *	2.4430939 *	2.8580804 *	4.3056129
9 C	0.0000000	1.4290378 *	2.4826695 *	3.7935269
10 C	1.4290378 *	0.0000000	1.4148389 *	2.4685714 *
11 C	2.4826695 *	1.4148389 *	0.0000000	1.4538026 *
12 N	3.7935269	2.4685714 *	1.4538026 *	0.0000000
13 C	4.3380426	2.9153027 *	2.4433953 *	1.3321076 *
14 C	5.7473615	4.3194018	3.8326095	2.5076517 *
15 C	6.7185652	5.3074669	4.5885616	3.1504754
16 C	8.0482282	6.6322576	5.9848310	4.5515974
17 C	8.5411611	7.1253012	6.6882996	5.3115373
18 C	7.8386281	6.4583236	6.2291134	4.9858783
19 C	6.4618879	5.0849918	4.8949363	3.7424635
20 O	6.5824131	5.2649935	4.2862457	2.9372585 *

21 N	5.3901759	4.5675759	3.1578300	2.9049088 *
22 H	4.0762500	4.8898730	4.6912943	6.0001793
23 H	5.9285718	6.2563653	5.4871412	6.4067410
24 H	6.2664814	6.0078287	4.8027243	5.1778558
25 H	2.1801699 *	3.4514851	3.9626371	5.4091132
26 H	1.1041580 *	2.1967371 *	3.4741689	4.6634063
27 H	2.1793424 *	1.1040751 *	2.1886612 *	2.6881386 *
28 H	3.9794932	2.6440439 *	2.6548589 *	2.0965071 *
29 H	8.8413520	7.4477027	6.6980813	5.2676243
30 H	9.6269451	8.2158182	7.7879151	6.4040970
31 H	8.4935115	7.1643398	7.0754840	5.9180461
32 H	6.0943034	4.8115034	4.8687722	3.9696136
33 H	7.4450729	6.1607705	5.1828308	3.8866082
34 H	5.5611081	4.6889966	3.3363267	3.0105030
35 H	6.3036223	5.5578165	4.1542719	3.8926615

C C C C

1 CO	2.8630149 *	3.2669055	3.0146084	4.2855368
2 C	6.2324802	7.5560752	8.0435984	9.4373172
3 C	6.5889372	7.7796054	8.0634770	9.4138630
4 C	5.7679809	6.8119643	6.9554835	8.2613376
5 C	4.3611764	5.4209507	5.6500954	6.9924289
6 C	3.7345378	5.0292670	5.5583689	6.9611460
7 C	4.9312581	6.3074379	6.9282983	8.3328256
8 C	5.1500011	6.5825595	7.4004057	8.7834385
9 C	4.3380426	5.7473615	6.7185652	8.0482282
10 C	2.9153027 *	4.3194018	5.3074669	6.6322576
11 C	2.4433953 *	3.8326095	4.5885616	5.9848310
12 N	1.3321076 *	2.5076517 *	3.1504754	4.5515974
13 C	0.0000000	1.4660477 *	2.6046685 *	3.8830601
14 C	1.4660477 *	0.0000000	1.4373427 *	2.5003726 *
15 C	2.6046685 *	1.4373427 *	0.0000000	1.4064922 *
16 C	3.8830601	2.5003726 *	1.4064922 *	0.0000000
17 C	4.3431937	2.8822280 *	2.4416847 *	1.4286833 *
18 C	3.7921727	2.4975061 *	2.8250311 *	2.4727717 *
19 C	2.4689462 *	1.4427514 *	2.4456167 *	2.8455120 *
20 O	3.0459730	2.5026466 *	1.4664269 *	2.4609083 *
21 N	4.0015484	4.7293708	4.7146922	5.9552937
22 H	7.1254068	8.4908039	9.0409499	10.4392492
23 H	7.6775302	8.8417911	9.0657567	10.3934824
24 H	6.4202843	7.3139316	7.2872867	8.5095835
25 H	6.2356030	7.6689702	8.4944144	9.8733701
26 H	4.9959534	6.3400863	7.3978841	8.6653188
27 H	2.6319250 *	3.8785382	4.9966482	6.2145752
28 H	1.1081838 *	2.1748234 *	3.5304794	4.6716533

29 H	4.7933601	3.5019241	2.1932771 *	1.1066697 *
30 H	5.4484089	3.9877316	3.4408591	2.1929501 *
31 H	4.6560264	3.4930274	3.9290099	3.4745520
32 H	2.6396266 *	2.1971144 *	3.4501042	3.9513265
33 H	4.0122050	3.3284886	2.0458236 *	2.5108997 *
34 H	3.8755304	4.5849331	4.7240651	5.9286620
35 H	4.9636969	5.5497386	5.3332530	6.4616589

C C C O

1 CO	5.4462315	5.6150177	4.7014422	1.9537520 *
2 C	10.3424074	10.0110178	8.6963619	7.2738453
3 C	10.4368906	10.2609955	9.0226604	7.1216645
4 C	9.3369798	9.2689659	8.1106955	5.9518317
5 C	8.0086430	7.8849849	6.7088240	4.7672215
6 C	7.8204033	7.4917154	6.1983235	4.9344013
7 C	9.1416570	8.7219481	7.3806443	6.3288035
8 C	9.4319499	8.8463077	7.4670800	7.0175449
9 C	8.5411611	7.8386281	6.4618879	6.5824131
10 C	7.1253012	6.4583236	5.0849918	5.2649935
11 C	6.6882996	6.2291134	4.8949363	4.2862457
12 N	5.3115373	4.9858783	3.7424635	2.9372585 *
13 C	4.3431937	3.7921727	2.4689462 *	3.0459730
14 C	2.8822280 *	2.4975061 *	1.4427514 *	2.5026466 *
15 C	2.4416847 *	2.8250311 *	2.4456167 *	1.4664269 *
16 C	1.4286833 *	2.4727717 *	2.8455120 *	2.4609083 *
17 C	0.0000000	1.4233988 *	2.4559740 *	3.7721470
18 C	1.4233988 *	0.0000000	1.4158848 *	4.2912862
19 C	2.4559740 *	1.4158848 *	0.0000000	3.7953391
20 O	3.7721470	4.2912862	3.7953391	0.0000000
21 N	7.0346832	7.0745993	6.0527521	3.7705450
22 H	11.3067765	10.9164846	9.5753749	8.3074084
23 H	11.4555161	11.3217702	10.1003048	8.0580551
24 H	9.6535643	9.7101919	8.6419668	6.1822879
25 H	10.5105939	9.8983680	8.5156263	8.0919811
26 H	9.0292321	8.2221740	6.8721598	7.3983771
27 H	6.5317861	5.7525884	4.4101452	5.2259799
28 H	4.8509918	3.9944481	2.5795139 *	4.1394024
29 H	2.2016447 *	3.4743539	3.9521686	2.6858975 *
30 H	1.1055400 *	2.2010655 *	3.4613293	4.6520250
31 H	2.1976162 *	1.1039810 *	2.1873497 *	5.3952536
32 H	3.4575994	2.1863209 *	1.1058374 *	4.6917639
33 H	3.9312478	4.7308636	4.4862469	0.9916848 *
34 H	6.8732375	6.8057596	5.7755347	4.0367525
35 H	7.6256903	7.8076961	6.8866788	4.2390457

	N	H	H	H
1 CO	1.9791146 *	6.4428627	6.1235934	4.3423392
2 C	4.3426861	1.1050978 *	2.1857947 *	3.4383645
3 C	3.8154746	2.1798272 *	1.1039363 *	2.1936212 *
4 C	2.4750402 *	3.4513814	2.2016335 *	1.1078134 *
5 C	1.5096917 *	3.9437151	3.4668216	2.1833073 *
6 C	2.5931741 *	3.5200383	4.0269217	3.5075466
7 C	3.8870807	2.1963347 *	3.4852995	3.9517523
8 C	5.1117543	2.6771941 *	4.6676346	5.3942840
9 C	5.3901759	4.0762500	5.9285718	6.2664814
10 C	4.5675759	4.8898730	6.2563653	6.0078287
11 C	3.1578300	4.6912943	5.4871412	4.8027243
12 N	2.9049088 *	6.0001793	6.4067410	5.1778558
13 C	4.0015484	7.1254068	7.6775302	6.4202843
14 C	4.7293708	8.4908039	8.8417911	7.3139316
15 C	4.7146922	9.0409499	9.0657567	7.2872867
16 C	5.9552937	10.4392492	10.3934824	8.5095835
17 C	7.0346832	11.3067765	11.4555161	9.6535643
18 C	7.0745993	10.9164846	11.3217702	9.7101919
19 C	6.0527521	9.5753749	10.1003048	8.6419668
20 O	3.7705450	8.3074084	8.0580551	6.1822879
21 N	0.0000000	5.4467550	4.6756655	2.6536891 *
22 H	5.4467550	0.0000000	2.5298658 *	4.3595165
23 H	4.6756655	2.5298658 *	0.0000000	2.5185426 *
24 H	2.6536891 *	4.3595165	2.5185426 *	0.0000000
25 H	6.0562845	2.3953047 *	4.7758715	5.9723983
26 H	6.4741069	4.7735920	6.8480196	7.3471167
27 H	5.2616154	5.9636236	7.3451171	6.9665884
28 H	4.7545662	7.1879256	8.0352151	7.0252478
29 H	6.2814560	10.9633369	10.7174212	8.7183644
30 H	8.0152232	12.3931693	12.4862434	10.6180816
31 H	8.0773841	11.7521232	12.2666292	10.7097366
32 H	6.4401531	9.4504160	10.2002802	8.9414853
33 H	4.3892643	8.9925725	8.5838127	6.6246580
34 H	1.0441308 *	5.8507208	5.1795528	3.2162341
35 H	1.0396316 *	5.8198131	4.5842157	2.2121205 *

	H	H	H	H
1 CO	6.4954933	6.2754023	4.5214916	3.8795526
2 C	2.6776388 *	4.6658488	5.3896632	6.3977085
3 C	4.0767807	5.9275905	6.2662227	6.9361823
4 C	4.8878656	6.2519401	6.0080372	6.2774838
5 C	4.6706119	5.4695576	4.8037076	4.9012435
6 C	3.5167814	4.0176468	3.5051888	4.0411572

7 C	2.1960984 *	3.4831637	3.9488152	5.0213432
8 C	1.1047390 *	2.1843201 *	3.4287664	4.9747908
9 C	2.1801699 *	1.1041580 *	2.1793424 *	3.9794932
10 C	3.4514851	2.1967371 *	1.1040751 *	2.6440439 *
11 C	3.9626371	3.4741689	2.1886612 *	2.6548589 *
12 N	5.4091132	4.6634063	2.6881386 *	2.0965071 *
13 C	6.2356030	4.9959534	2.6319250 *	1.1081838 *
14 C	7.6689702	6.3400863	3.8785382	2.1748234 *
15 C	8.4944144	7.3978841	4.9966482	3.5304794
16 C	9.8733701	8.6653188	6.2145752	4.6716533
17 C	10.5105939	9.0292321	6.5317861	4.8509918
18 C	9.8983680	8.2221740	5.7525884	3.9944481
19 C	8.5156263	6.8721598	4.4101452	2.5795139 *
20 O	8.0919811	7.3983771	5.2259799	4.1394024
21 N	6.0562845	6.4741069	5.2616154	4.7545662
22 H	2.3953047 *	4.7735920	5.9636236	7.1879256
23 H	4.7758715	6.8480196	7.3451171	8.0352151
24 H	5.9723983	7.3471167	6.9665884	7.0252478
25 H	0.0000000	2.5278531 *	4.3455305	6.0043256
26 H	2.5278531 *	0.0000000	2.4978194 *	4.4681048
27 H	4.3455305	2.4978194 *	0.0000000	2.1350756 *
28 H	6.0043256	4.4681048	2.1350756 *	0.0000000
29 H	10.5671413	9.5059655	7.1059374	5.6680148
30 H	11.6054577	10.0900591	7.5949303	5.9309538
31 H	10.6013168	8.7727078	6.3715696	4.6526398
32 H	8.1938465	6.3810893	4.0414441	2.2628771 *
33 H	8.8873876	8.2564577	6.1168312	5.0948090
34 H	6.3341921	6.6133550	5.3204967	4.5136315
35 H	6.7581823	7.3997963	6.2759201	5.7628914

H H H H

1 CO	4.6194645	6.4264923	6.6804865	5.2841034
2 C	9.9383858	11.4217251	10.8820239	8.6461024
3 C	9.7935756	11.4820663	11.1955468	9.1086827
4 C	8.5839740	10.3518043	10.2420532	8.3185579
5 C	7.4069935	9.0457244	8.8495566	6.9187867
6 C	7.5374853	8.9046106	8.3849568	6.2350313
7 C	8.9286143	10.2344341	9.5583488	7.2805553
8 C	9.4830805	10.5291315	9.5790386	7.1956765
9 C	8.8413520	9.6269451	8.4935115	6.0943034
10 C	7.4477027	8.2158182	7.1643398	4.8115034
11 C	6.6980813	7.7879151	7.0754840	4.8687722
12 N	5.2676243	6.4040970	5.9180461	3.9696136
13 C	4.7933601	5.4484089	4.6560264	2.6396266 *
14 C	3.5019241	3.9877316	3.4930274	2.1971144 *

15 C	2.1932771 *	3.4408591	3.9290099	3.4501042
16 C	1.1066697 *	2.1929501 *	3.4745520	3.9513265
17 C	2.2016447 *	1.1055400 *	2.1976162 *	3.4575994
18 C	3.4743539	2.2010655 *	1.1039810 *	2.1863209 *
19 C	3.9521686	3.4613293	2.1873497 *	1.1058374 *
20 O	2.6858975 *	4.6520250	5.3952536	4.6917639
21 N	6.2814560	8.0152232	8.0773841	6.4401531
22 H	10.9633369	12.3931693	11.7521232	9.4504160
23 H	10.7174212	12.4862434	12.2666292	10.2002802
24 H	8.7183644	10.6180816	10.7097366	8.9414853
25 H	10.5671413	11.6054577	10.6013168	8.1938465
26 H	9.5059655	10.0900591	8.7727078	6.3810893
27 H	7.1059374	7.5949303	6.3715696	4.0414441
28 H	5.6680148	5.9309538	4.6526398	2.2628771 *
29 H	0.0000000	2.5230756 *	4.3878273	5.0579805
30 H	2.5230756 *	0.0000000	2.5408250 *	4.3752061
31 H	4.3878273	2.5408250 *	0.0000000	2.5153519 *
32 H	5.0579805	4.3752061	2.5153519 *	0.0000000
33 H	2.3090367 *	4.6339761	5.8166080	5.4643321
34 H	6.3472274	7.8530757	7.7469890	6.0876257
35 H	6.6332367	8.5428190	8.8311077	7.3499916

H H H

1 CO	2.6582481 *	2.5008723 *	2.6229650 *
2 C	7.9580505	4.7742270	4.7366355
3 C	7.7092060	4.3251384	3.9162660
4 C	6.5087564	3.0593633	2.4846954 *
5 C	5.4391983	2.1107671 *	2.0880303 *
6 C	5.7306388	2.9610577 *	3.4237456
7 C	7.0997509	4.2445223	4.5621627
8 C	7.8344694	5.3764180	5.8884215
9 C	7.4450729	5.5611081	6.3036223
10 C	6.1607705	4.6889966	5.5578165
11 C	5.1828308	3.3363267	4.1542719
12 N	3.8866082	3.0105030	3.8926615
13 C	4.0122050	3.8755304	4.9636969
14 C	3.3284886	4.5849331	5.5497386
15 C	2.0458236 *	4.7240651	5.3332530
16 C	2.5108997 *	5.9286620	6.4616589
17 C	3.9312478	6.8732375	7.6256903
18 C	4.7308636	6.8057596	7.8076961
19 C	4.4862469	5.7755347	6.8866788
20 O	0.9916848 *	4.0367525	4.2390457
21 N	4.3892643	1.0441308 *	1.0396316 *
22 H	8.9925725	5.8507208	5.8198131

23 H	8.5838127	5.1795528	4.5842157
24 H	6.6246580	3.2162341	2.2121205 *
25 H	8.8873876	6.3341921	6.7581823
26 H	8.2564577	6.6133550	7.3997963
27 H	6.1168312	5.3204967	6.2759201
28 H	5.0948090	4.5136315	5.7628914
29 H	2.3090367 *	6.3472274	6.6332367
30 H	4.6339761	7.8530757	8.5428190
31 H	5.8166080	7.7469890	8.8311077
32 H	5.4643321	6.0876257	7.3499916
33 H	0.0000000	4.7387655	4.6713414
34 H	4.7387655	0.0000000	1.6669173 *
35 H	4.6713414	1.6669173 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 7387.9 SECONDS (123.1 MIN)
WALL CLOCK TIME: STEP = 0.78 , TOTAL = 6829.5 SECONDS (113.8 MIN)

CPU UTILIZATION: STEP = 99.90%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.43 , TOTAL = 7389.3 SECONDS (123.2 MIN)
WALL CLOCK TIME: STEP = 1.43 , TOTAL = 6830.9 SECONDS (113.8 MIN)

CPU UTILIZATION: STEP = 99.93%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636877639	-284.636877639	0.009161924	0.000354196	198023956
11337263					
2 1	-284.636883624	-0.000005985	0.001410027	0.000054494	148236041
15475032					
3 2	-284.636883261	0.000000363	0.000801447	0.000115925	135631625
16482320					
4 3	-284.636883876	-0.000000615	0.000362019	0.000024512	131093840
16841307					

5	4	-284.636883862	0.000000014	0.000160949	0.000055832	119839689
17716705						
6	5	-284.636883914	-0.000000052	0.000149885	0.000007489	114936464
18101245						
7	6	-284.636883890	0.000000024	0.000100032	0.000012880	107649648
18590663						
8	7	-284.636883897	-0.000000007	0.000052276	0.000004915	127525418
17148258						
9	8	-284.636883891	0.000000006	0.000029567	0.000004205	123882258
17428016						
10	9	-284.636883893	-0.000000002	0.000095623	0.000003416	142989901
16065180						

-----DISABLING FDIFF OPTION-----

11	10	-284.636883892	0.000000001	0.000045318	0.000002615	198025043
11337180						
12	11	-284.636883893	-0.000000001	0.000019271	0.000002476	198025019
11337181						
13	12	-284.636883893	0.000000000	0.000030074	0.000002148	198024950
11337183						

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 42.4 SECONDS (3.3 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 14.2 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
 TIME TO SOLVE SCF EQUATIONS= 1.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6368838932 AFTER 13 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6021660144
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998603145

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
 PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 45.10 , TOTAL = 7434.4 SECONDS (123.9 MIN)

WALL CLOCK TIME: STEP = 41.39 , TOTAL = 6872.3 SECONDS (114.5 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.78 , TOTAL = 7438.2 SECONDS (124.0 MIN)

WALL CLOCK TIME: STEP = 3.75 , TOTAL = 6876.0 SECONDS (114.6 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.86 , TOTAL = 7441.1 SECONDS (124.0 MIN)

WALL CLOCK TIME: STEP = 2.70 , TOTAL = 6878.7 SECONDS (114.6 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 78 ENERGY= -284.6368839

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0001767	-0.0000236	-0.0000364
2 C	6.0	-0.0000036	0.0001216	-0.0001362
3 C	6.0	0.0000609	0.0000520	0.0000430
4 C	6.0	0.0000773	-0.0001048	0.0000657
5 C	6.0	0.0000032	-0.0001324	0.0000113
6 C	6.0	-0.0000125	0.0001017	-0.0000963
7 C	6.0	-0.0000876	0.0000820	-0.0001099
8 C	6.0	-0.0001645	-0.0002156	0.0000084
9 C	6.0	-0.0001029	-0.0003090	-0.0001175
10 C	6.0	-0.0000169	0.0000991	-0.0003016
11 C	6.0	0.0000296	-0.0000206	-0.0001993
12 N	7.0	0.0000663	0.0000265	0.0000508
13 C	6.0	0.0000747	0.0000519	-0.0000427
14 C	6.0	0.0001163	0.0000688	-0.0000440
15 C	6.0	-0.0000730	0.0000085	-0.0002580
16 C	6.0	-0.0001027	0.0000541	-0.0000554
17 C	6.0	-0.0001225	0.0000179	0.0000279

18 C	6.0	-0.0000610	0.0002816	0.0001901
19 C	6.0	-0.0000559	0.0001853	0.0001339
20 O	8.0	-0.0001208	-0.0002971	0.0000422
21 N	7.0	0.0002317	-0.0000750	0.0000556
22 H	1.0	-0.0000001	0.0000932	-0.0000839
23 H	1.0	-0.0000940	0.0001327	0.0002211
24 H	1.0	0.0001165	0.0000368	0.0000012
25 H	1.0	-0.0001503	-0.0001583	0.0001015
26 H	1.0	-0.0000378	-0.0001588	0.0002605
27 H	1.0	-0.0000203	-0.0000004	0.0000017
28 H	1.0	-0.0000951	0.0000639	0.0001131
29 H	1.0	0.0001743	0.0001377	0.0001014
30 H	1.0	-0.0002600	-0.0000253	0.0000417
31 H	1.0	0.0001163	-0.0001286	-0.0000935
32 H	1.0	0.0000715	-0.0000271	0.0000969
33 H	1.0	0.0000355	0.0001986	0.0000481
34 H	1.0	-0.0000067	-0.0000350	0.0000214
35 H	1.0	0.0002373	-0.0001023	-0.0000628

MAXIMUM GRADIENT = 0.0003090 RMS GRADIENT = 0.0001220
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000059712
 PREDICTED ENERGY CHANGE WAS -0.0000040076 RATIO= 1.490
 GDIIS STEP HAS LENGTH = 0.020933
 RADIUS OF STEP TAKEN= 0.02093 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 7441.1 SECONDS (124.0 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6878.8 SECONDS (114.6
 MIN)
 CPU UTILIZATION: STEP = 84.70%, TOTAL = 100.00%

INSERCH= 79

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1571074014	-1.7367446740	0.8589570892
C	6.0	4.9811252905	0.6315209626	0.5580405914
C	6.0	5.1883157361	-0.7097785728	0.2095337015
C	6.0	4.0548518309	-1.5349152478	-0.0830268652
C	6.0	2.7448572655	-1.0261946468	-0.0025767573
C	6.0	2.4691752641	0.3406347524	0.4224009504
C	6.0	3.6489930741	1.1772337908	0.6721755779
C	6.0	3.4990881842	2.5618066049	1.0528217799

C	6.0	2.2305413724	3.1346960766	1.2164924490
C	6.0	1.0677410856	2.3248679701	1.0299654766
C	6.0	1.1620642849	0.9715440083	0.6280048525
N	7.0	-0.0507040447	0.1711023377	0.5735727775
C	6.0	-1.2469334909	0.6990075610	0.3186327214
C	6.0	-2.5512909797	0.0397947097	0.4365105901
C	6.0	-2.8227454042	-1.2857531906	0.9224361306
C	6.0	-4.1235766943	-1.8046754547	1.0521174252
C	6.0	-5.2336214939	-0.9844039186	0.6824199458
C	6.0	-5.0190207313	0.3324193377	0.1868158121
C	6.0	-3.6996271206	0.8328828592	0.0704670150
O	8.0	-1.6997310860	-2.1467630703	1.3071484246
N	7.0	1.6419092351	-1.9648237973	-0.4287921762
H	1.0	5.8406768741	1.2965837885	0.7581088504
H	1.0	6.2072508441	-1.1285989371	0.1376716648
H	1.0	4.2233972836	-2.5801565944	-0.4087373793
H	1.0	4.4101643836	3.1605895862	1.2313467463
H	1.0	2.1199717639	4.1877112863	1.5299929856
H	1.0	0.0830445649	2.7675562421	1.2602263576
H	1.0	-1.2909256299	1.7525628298	-0.0219083062
H	1.0	-4.2961883635	-2.8289012831	1.4341802942
H	1.0	-6.2587816286	-1.3853435011	0.7822860667
H	1.0	-5.8758759676	0.9651316585	-0.1039894296
H	1.0	-3.5343485398	1.8603116577	-0.3037193757
H	1.0	-2.0158760578	-2.9556137004	1.7858323010
H	1.0	1.2844578574	-1.6948716339	-1.3717188025
H	1.0	2.0405106361	-2.9193147972	-0.5308024852

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3824141	5.1758543	4.0150318
2 C	5.3824141	0.0000000	1.4012385 *	2.4418018 *
3 C	5.1758543	1.4012385 *	0.0000000	1.4321950 *
4 C	4.0150318	2.4418018 *	1.4321950 *	0.0000000
5 C	2.8184342 *	2.8395788 *	2.4729738 *	1.4076060 *
6 C	3.1387489	2.5323716 *	2.9227394 *	2.5074918 *
7 C	4.5518593	1.4440933 *	2.4787835 *	2.8444339 *
8 C	5.4482990	2.4833939 *	3.7772866	4.2874416
9 C	5.3064013	3.7769242	4.9540267	5.1790085
10 C	4.1659567	4.2900715	5.1827911	5.0059474
11 C	2.8979484 *	3.8348061	4.3832254	3.8930867
12 N	1.9402345 *	5.0528737	5.3250168	4.4941304
13 C	2.8628954 *	6.2330239	6.5885517	5.7672064

14 C	3.2664928	7.5566001	7.7791317	6.8110758
15 C	3.0144561	8.0441980	8.0633168	6.9551694
16 C	4.2855784	9.4379427	9.4138243	8.2612358
17 C	5.4458369	10.3425207	10.4362741	9.3362042
18 C	5.6147588	10.0115029	10.2604293	9.2679511
19 C	4.7009684	8.6967659	9.0218996	8.1093756
20 O	1.9536734 *	7.2741918	7.1214375	5.9516527
21 N	1.9786245 *	4.3434098	3.8157041	2.4752105 *
22 H	6.4431525	1.1050633 *	2.1799082 *	3.4516760
23 H	6.1232614	2.1858902 *	1.1039943 *	2.2015046 *
24 H	4.3420164	3.4385584	2.1935452 *	1.1077113 *
25 H	6.4970032	2.6787172 *	4.0779126	4.8889253
26 H	6.2771255	4.6666241	5.9282168	6.2525234
27 H	4.5227457	5.3895182	6.2657487	6.0075655
28 H	3.8791739	6.3977886	6.9352188	6.2760325
29 H	4.6212045	9.9403567	9.7952161	8.5858133
30 H	6.4259624	11.4216258	11.4813097	10.3509504
31 H	6.6801415	10.8822818	11.1946397	10.2406068
32 H	5.2836993	8.6467249	9.1078902	8.3169846
33 H	2.6583071 *	7.9582055	7.7090124	6.5088214
34 H	2.4997175 *	4.7750837	4.3256068	3.0596398
35 H	2.6224247 *	4.7372174	3.9164812	2.4848814 *

C C C C

1 CO	2.8184342 *	3.1387489	4.5518593	5.4482990
2 C	2.8395788 *	2.5323716 *	1.4440933 *	2.4833939 *
3 C	2.4729738 *	2.9227394 *	2.4787835 *	3.7772866
4 C	1.4076060 *	2.5074918 *	2.8444339 *	4.2874416
5 C	0.0000000	1.4576794 *	2.4754493 *	3.8152960
6 C	1.4576794 *	0.0000000	1.4677382 *	2.5281921 *
7 C	2.4754493 *	1.4677382 *	0.0000000	1.4437468 *
8 C	3.8152960	2.5281921 *	1.4437468 *	0.0000000
9 C	4.3661954	2.9144993 *	2.4778912 *	1.4014997 *
10 C	3.8869632	2.5040635 *	2.8474444 *	2.4429718 *
11 C	2.6256097 *	1.4658986 *	2.4958113 *	2.8585110 *
12 N	3.0952595	2.5300960 *	3.8353333	4.3065266
13 C	4.3604921	3.7347909	4.9319154	5.1510946
14 C	5.4201769	5.0294915	6.3081557	6.5838797
15 C	5.6498866	5.5587406	6.9290933	7.4017766
16 C	6.9924100	6.9615571	8.3336054	8.7847132
17 C	8.0079392	7.8202567	9.1418611	9.4325513
18 C	7.8841298	7.4919054	8.7225999	8.8475032
19 C	6.7076735	6.1984102	7.3812499	7.4683131
20 O	4.7671185	4.9345421	6.3293756	7.0187629
21 N	1.5096949 *	2.5930750 *	3.8875495	5.1122086

22 H	3.9443683	3.5204490	2.1966126 *	2.6778129 *
23 H	3.4667457	4.0265280	3.4852893	4.6680550
24 H	2.1830815 *	3.5070084	3.9517459	5.3944939
25 H	4.6717210	3.5176665	2.1967600 *	1.1047498 *
26 H	5.4702895	4.0185446	3.4837812	2.1847701 *
27 H	4.8033805	3.5050705	3.9485337	3.4285133
28 H	4.8999398	4.0409541	5.0215090	4.9753545
29 H	7.4088019	7.5392175	8.9306034	9.4853309
30 H	9.0449163	8.9042546	10.2343992	10.5294448
31 H	8.8483166	8.3849248	9.5587944	9.5800593
32 H	6.9174440	6.2353000	7.2814396	7.1973281
33 H	5.4392689	5.7306094	7.1000987	7.8354363
34 H	2.1105557 *	2.9606937 *	4.2447050	5.3760854
35 H	2.0878291 *	3.4233932	4.5624645	5.8888035

C C C N

1 CO	5.3064013	4.1659567	2.8979484 *	1.9402345 *
2 C	3.7769242	4.2900715	3.8348061	5.0528737
3 C	4.9540267	5.1827911	4.3832254	5.3250168
4 C	5.1790085	5.0059474	3.8930867	4.4941304
5 C	4.3661954	3.8869632	2.6256097 *	3.0952595
6 C	2.9144993 *	2.5040635 *	1.4658986 *	2.5300960 *
7 C	2.4778912 *	2.8474444 *	2.4958113 *	3.8353333
8 C	1.4014997 *	2.4429718 *	2.8585110 *	4.3065266
9 C	0.0000000	1.4292370 *	2.4833823 *	3.7947746
10 C	1.4292370 *	0.0000000	1.4149046 *	2.4693967 *
11 C	2.4833823 *	1.4149046 *	0.0000000	1.4541240 *
12 N	3.7947746	2.4693967 *	1.4541240 *	0.0000000
13 C	4.3395348	2.9166993 *	2.4440249 *	1.3321574 *
14 C	5.7491484	4.3210116	3.8332537	2.5077804 *
15 C	6.7203086	5.3088636	4.5892035	3.1509280
16 C	8.0497967	6.6335059	5.9854212	4.5520319
17 C	8.5420106	7.1259553	6.6883099	5.3112782
18 C	7.8402257	6.4598314	6.2296822	4.9859578
19 C	6.4636380	5.0866941	4.8955203	3.7424201
20 O	6.5840011	5.2660437	4.2866010	2.9376731 *
21 N	5.3905985	4.5671762	3.1574241	2.9037658 *
22 H	4.0769904	4.8900092	4.6916941	6.0007609
23 H	5.9290604	6.2559717	5.4867964	6.4063432
24 H	6.2667685	6.0072704	4.8022048	5.1770939
25 H	2.1798274 *	3.4511996	3.9630918	5.4100876
26 H	1.1042415 *	2.1971350 *	3.4748959	4.6647316
27 H	2.1790931 *	1.1039113 *	2.1885263 *	2.6890435 *
28 H	3.9805350	2.6452373 *	2.6550964 *	2.0961309 *
29 H	8.8436464	7.4495950	6.6996884	5.2692318

30 H	9.6274554	8.2161396	7.7876617	6.4036171
31 H	8.4949799	7.1657906	7.0759070	5.9179558
32 H	6.0966430	4.8139128	4.8697342	3.9697416
33 H	7.4463469	6.1614541	5.1828985	3.8868789
34 H	5.5604528	4.6875751	3.3352132	3.0081016
35 H	6.3039828	5.5573132	4.1537073	3.8914652

C C C C

1 CO	2.8628954 *	3.2664928	3.0144561	4.2855784
2 C	6.2330239	7.5566001	8.0441980	9.4379427
3 C	6.5885517	7.7791317	8.0633168	9.4138243
4 C	5.7672064	6.8110758	6.9551694	8.2612358
5 C	4.3604921	5.4201769	5.6498866	6.9924100
6 C	3.7347909	5.0294915	5.5587406	6.9615571
7 C	4.9319154	6.3081557	6.9290933	8.3336054
8 C	5.1510946	6.5838797	7.4017766	8.7847132
9 C	4.3395348	5.7491484	6.7203086	8.0497967
10 C	2.9166993 *	4.3210116	5.3088636	6.6335059
11 C	2.4440249 *	3.8332537	4.5892035	5.9854212
12 N	1.3321574 *	2.5077804 *	3.1509280	4.5520319
13 C	0.0000000	1.4662214 *	2.6051942 *	3.8834913
14 C	1.4662214 *	0.0000000	1.4376677 *	2.5006248 *
15 C	2.6051942 *	1.4376677 *	0.0000000	1.4065062 *
16 C	3.8834913	2.5006248 *	1.4065062 *	0.0000000
17 C	4.3427982	2.8817271 *	2.4414632 *	1.4288881 *
18 C	3.7921504	2.4975321 *	2.8254637 *	2.4734068 *
19 C	2.4688489 *	1.4427933 *	2.4460972 *	2.8460648 *
20 O	3.0464076	2.5028383 *	1.4664592 *	2.4611161 *
21 N	4.0000067	4.7275969	4.7138197	5.9547938
22 H	7.1263214	8.4916470	9.0415902	10.4398563
23 H	7.6770930	8.8411822	9.0653949	10.3932328
24 H	6.4192292	7.3126596	7.2866748	8.5092563
25 H	6.2366008	7.6702664	8.4959034	9.8747515
26 H	4.9974492	6.3420510	7.3998913	8.6671195
27 H	2.6333123 *	3.8805817	4.9987033	6.2164519
28 H	1.1080985 *	2.1753720 *	3.5312353	4.6724070
29 H	4.7946368	3.5027744	2.1941336 *	1.1067093 *
30 H	5.4477624	3.9869871	3.4403350	2.1926578 *
31 H	4.6558071	3.4930294	3.9295850	3.4754809
32 H	2.6397380 *	2.1974131 *	3.4507333	3.9519127
33 H	4.0125059	3.3286348	2.0457090 *	2.5110552 *
34 H	3.8724525	4.5816733	4.7222498	5.9273836
35 H	4.9619639	5.5476721	5.3321370	6.4609619

C C C O

1 CO	5.4458369	5.6147588	4.7009684	1.9536734 *
2 C	10.3425207	10.0115029	8.6967659	7.2741918
3 C	10.4362741	10.2604293	9.0218996	7.1214375
4 C	9.3362042	9.2679511	8.1093756	5.9516527
5 C	8.0079392	7.8841298	6.7076735	4.7671185
6 C	7.8202567	7.4919054	6.1984102	4.9345421
7 C	9.1418611	8.7225999	7.3812499	6.3293756
8 C	9.4325513	8.8475032	7.4683131	7.0187629
9 C	8.5420106	7.8402257	6.4636380	6.5840011
10 C	7.1259553	6.4598314	5.0866941	5.2660437
11 C	6.6883099	6.2296822	4.8955203	4.2866010
12 N	5.3112782	4.9859578	3.7424201	2.9376731 *
13 C	4.3427982	3.7921504	2.4688489 *	3.0464076
14 C	2.8817271 *	2.4975321 *	1.4427933 *	2.5028383 *
15 C	2.4414632 *	2.8254637 *	2.4460972 *	1.4664592 *
16 C	1.4288881 *	2.4734068 *	2.8460648 *	2.4611161 *
17 C	0.0000000	1.4232710 *	2.4556377 *	3.7722335
18 C	1.4232710 *	0.0000000	1.4159097 *	4.2917566
19 C	2.4556377 *	1.4159097 *	0.0000000	3.7956890
20 O	3.7722335	4.2917566	3.7956890	0.0000000
21 N	7.0334158	7.0727850	6.0504903	3.7700334
22 H	11.3070207	10.9173724	9.5762869	8.3075769
23 H	11.4547415	11.3210496	10.0994138	8.0575863
24 H	9.6525776	9.7087627	8.6401847	6.1818722
25 H	10.5111797	9.8994507	8.5167235	8.0934888
26 H	9.0301988	8.2239051	6.8740687	7.4003618
27 H	6.5328404	5.7544046	4.4121529	5.2279083
28 H	4.8509706	3.9948800	2.5799588 *	4.1398377
29 H	2.2013848 *	3.4745292	3.9527538	2.6875714 *
30 H	1.1052959 *	2.2005229 *	3.4607060	4.6519009
31 H	2.1980945 *	1.1041257 *	2.1872320 *	5.3958674
32 H	3.4572252	2.1861682 *	1.1058673 *	4.6922664
33 H	3.9315484	4.7314789	4.4866694	0.9916276 *
34 H	6.8709249	6.8024100	5.7715289	4.0355816
35 H	7.6242237	7.8054938	6.8840173	4.2384322

N H H H

1 CO	1.9786245 *	6.4431525	6.1232614	4.3420164
2 C	4.3434098	1.1050633 *	2.1858902 *	3.4385584
3 C	3.8157041	2.1799082 *	1.1039943 *	2.1935452 *
4 C	2.4752105 *	3.4516760	2.2015046 *	1.1077113 *
5 C	1.5096949 *	3.9443683	3.4667457	2.1830815 *
6 C	2.5930750 *	3.5204490	4.0265280	3.5070084
7 C	3.8875495	2.1966126 *	3.4852893	3.9517459

8 C	5.1122086	2.6778129 *	4.6680550	5.3944939
9 C	5.3905985	4.0769904	5.9290604	6.2667685
10 C	4.5671762	4.8900092	6.2559717	6.0072704
11 C	3.1574241	4.6916941	5.4867964	4.8022048
12 N	2.9037658 *	6.0007609	6.4063432	5.1770939
13 C	4.0000067	7.1263214	7.6770930	6.4192292
14 C	4.7275969	8.4916470	8.8411822	7.3126596
15 C	4.7138197	9.0415902	9.0653949	7.2866748
16 C	5.9547938	10.4398563	10.3932328	8.5092563
17 C	7.0334158	11.3070207	11.4547415	9.6525776
18 C	7.0727850	10.9173724	11.3210496	9.7087627
19 C	6.0504903	9.5762869	10.0994138	8.6401847
20 O	3.7700334	8.3075769	8.0575863	6.1818722
21 N	0.0000000	5.4474915	4.6757349	2.6538872 *
22 H	5.4474915	0.0000000	2.5299862 *	4.3596146
23 H	4.6757349	2.5299862 *	0.0000000	2.5181853 *
24 H	2.6538872 *	4.3596146	2.5181853 *	0.0000000
25 H	6.0571578	2.3968391 *	4.7773197	5.9733512
26 H	6.4744939	4.7747324	6.8489096	7.3475921
27 H	5.2610135	5.9637414	7.3447979	6.9660601
28 H	4.7524771	7.1886089	8.0342523	7.0235213
29 H	6.2831759	10.9650689	10.7188711	8.7201811
30 H	8.0139518	12.3931519	12.4853278	10.6170707
31 H	8.0750994	11.7529011	12.2655640	10.7078130
32 H	6.4374645	9.4517919	10.1993711	8.9393181
33 H	4.3892618	8.9923758	8.5833695	6.6246235
34 H	1.0439139 *	5.8518461	5.1800401	3.2168972
35 H	1.0393951 *	5.8203399	4.5842388	2.2124471 *

H H H H

1 CO	6.4970032	6.2771255	4.5227457	3.8791739
2 C	2.6787172 *	4.6666241	5.3895182	6.3977886
3 C	4.0779126	5.9282168	6.2657487	6.9352188
4 C	4.8889253	6.2525234	6.0075655	6.2760325
5 C	4.6717210	5.4702895	4.8033805	4.8999398
6 C	3.5176665	4.0185446	3.5050705	4.0409541
7 C	2.1967600 *	3.4837812	3.9485337	5.0215090
8 C	1.1047498 *	2.1847701 *	3.4285133	4.9753545
9 C	2.1798274 *	1.1042415 *	2.1790931 *	3.9805350
10 C	3.4511996	2.1971350 *	1.1039113 *	2.6452373 *
11 C	3.9630918	3.4748959	2.1885263 *	2.6550964 *
12 N	5.4100876	4.6647316	2.6890435 *	2.0961309 *
13 C	6.2366008	4.9974492	2.6333123 *	1.1080985 *
14 C	7.6702664	6.3420510	3.8805817	2.1753720 *
15 C	8.4959034	7.3998913	4.9987033	3.5312353

16 C	9.8747515	8.6671195	6.2164519	4.6724070
17 C	10.5111797	9.0301988	6.5328404	4.8509706
18 C	9.8994507	8.2239051	5.7544046	3.9948800
19 C	8.5167235	6.8740687	4.4121529	2.5799588 *
20 O	8.0934888	7.4003618	5.2279083	4.1398377
21 N	6.0571578	6.4744939	5.2610135	4.7524771
22 H	2.3968391 *	4.7747324	5.9637414	7.1886089
23 H	4.7773197	6.8489096	7.3447979	8.0342523
24 H	5.9733512	7.3475921	6.9660601	7.0235213
25 H	0.0000000	2.5276770 *	4.3450288	6.0046328
26 H	2.5276770 *	0.0000000	2.4977363 *	4.4690678
27 H	4.3450288	2.4977363 *	0.0000000	2.1358546 *
28 H	6.0046328	4.4690678	2.1358546 *	0.0000000
29 H	10.5695658	9.5083722	7.1083245	5.6693572
30 H	11.6057560	10.0906647	7.5956410	5.9306642
31 H	10.6021594	8.7743090	6.3732686	4.6528007
32 H	8.1952691	6.3836219	4.0440761	2.2636196 *
33 H	8.8887228	8.2581949	6.1185295	5.0951355
34 H	6.3341531	6.6123216	5.3182508	4.5099216
35 H	6.7591173	7.4002035	6.2753454	5.7605452

H H H H

1 CO	4.6212045	6.4259624	6.6801415	5.2836993
2 C	9.9403567	11.4216258	10.8822818	8.6467249
3 C	9.7952161	11.4813097	11.1946397	9.1078902
4 C	8.5858133	10.3509504	10.2406068	8.3169846
5 C	7.4088019	9.0449163	8.8483166	6.9174440
6 C	7.5392175	8.9042546	8.3849248	6.2353000
7 C	8.9306034	10.2343992	9.5587944	7.2814396
8 C	9.4853309	10.5294448	9.5800593	7.1973281
9 C	8.8436464	9.6274554	8.4949799	6.0966430
10 C	7.4495950	8.2161396	7.1657906	4.8139128
11 C	6.6996884	7.7876617	7.0759070	4.8697342
12 N	5.2692318	6.4036171	5.9179558	3.9697416
13 C	4.7946368	5.4477624	4.6558071	2.6397380 *
14 C	3.5027744	3.9869871	3.4930294	2.1974131 *
15 C	2.1941336 *	3.4403350	3.9295850	3.4507333
16 C	1.1067093 *	2.1926578 *	3.4754809	3.9519127
17 C	2.2013848 *	1.1052959 *	2.1980945 *	3.4572252
18 C	3.4745292	2.2005229 *	1.1041257 *	2.1861682 *
19 C	3.9527538	3.4607060	2.1872320 *	1.1058673 *
20 O	2.6875714 *	4.6519009	5.3958674	4.6922664
21 N	6.2831759	8.0139518	8.0750994	6.4374645
22 H	10.9650689	12.3931519	11.7529011	9.4517919
23 H	10.7188711	12.4853278	12.2655640	10.1993711

24 H	8.7201811	10.6170707	10.7078130	8.9393181
25 H	10.5695658	11.6057560	10.6021594	8.1952691
26 H	9.5083722	10.0906647	8.7743090	6.3836219
27 H	7.1083245	7.5956410	6.3732686	4.0440761
28 H	5.6693572	5.9306642	4.6528007	2.2636196 *
29 H	0.0000000	2.5220225 *	4.3881733	5.0585979
30 H	2.5220225 *	0.0000000	2.5410302 *	4.3744966
31 H	4.3881733	2.5410302 *	0.0000000	2.5147545 *
32 H	5.0585979	4.3744966	2.5147545 *	0.0000000
33 H	2.3107443 *	4.6341236	5.8174969	5.4648991
34 H	6.3484412	7.8508602	7.7429410	6.0828321
35 H	6.6349895	8.5414004	8.8283787	7.3467987

H H H

1 CO	2.6583071 *	2.4997175 *	2.6224247 *
2 C	7.9582055	4.7750837	4.7372174
3 C	7.7090124	4.3256068	3.9164812
4 C	6.5088214	3.0596398	2.4848814 *
5 C	5.4392689	2.1105557 *	2.0878291 *
6 C	5.7306094	2.9606937 *	3.4233932
7 C	7.1000987	4.2447050	4.5624645
8 C	7.8354363	5.3760854	5.8888035
9 C	7.4463469	5.5604528	6.3039828
10 C	6.1614541	4.6875751	5.5573132
11 C	5.1828985	3.3352132	4.1537073
12 N	3.8868789	3.0081016	3.8914652
13 C	4.0125059	3.8724525	4.9619639
14 C	3.3286348	4.5816733	5.5476721
15 C	2.0457090 *	4.7222498	5.3321370
16 C	2.5110552 *	5.9273836	6.4609619
17 C	3.9315484	6.8709249	7.6242237
18 C	4.7314789	6.8024100	7.8054938
19 C	4.4866694	5.7715289	6.8840173
20 O	0.9916276 *	4.0355816	4.2384322
21 N	4.3892618	1.0439139 *	1.0393951 *
22 H	8.9923758	5.8518461	5.8203399
23 H	8.5833695	5.1800401	4.5842388
24 H	6.6246235	3.2168972	2.2124471 *
25 H	8.8887228	6.3341531	6.7591173
26 H	8.2581949	6.6123216	7.4002035
27 H	6.1185295	5.3182508	6.2753454
28 H	5.0951355	4.5099216	5.7605452
29 H	2.3107443 *	6.3484412	6.6349895
30 H	4.6341236	7.8508602	8.5414004
31 H	5.8174969	7.7429410	8.8283787

32 H	5.4648991	6.0828321	7.3467987
33 H	0.0000000	4.7383334	4.6714438
34 H	4.7383334	0.0000000	1.6667385 *
35 H	4.6714438	1.6667385 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80 , TOTAL = 7441.9 SECONDS (124.0 MIN)
WALL CLOCK TIME: STEP = 0.81 , TOTAL = 6879.6 SECONDS (114.7 MIN)
CPU UTILIZATION: STEP = 99.21% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.02 , TOTAL = 7442.9 SECONDS (124.0 MIN)
WALL CLOCK TIME: STEP = 1.01 , TOTAL = 6880.6 SECONDS (114.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
INTEGRALS	SKIPPED				

-----START SECOND ORDER SCF-----

1	0	-284.636879514	-284.636879514	0.004949174	0.000338515	198014452
11337988						
2	1	-284.636891622	-0.000012108	0.001625218	0.000040843	150563763
15304827						
3	2	-284.636891317	0.000000305	0.001030694	0.000084647	135686402
16495175						
4	3	-284.636891878	-0.000000560	0.000140119	0.000015536	130385462
16915037						
5	4	-284.636891877	0.000000001	0.000113424	0.000039819	119251666
17749543						
6	5	-284.636891922	-0.000000045	0.000087408	0.000008179	113206949
18233297						
7	6	-284.636891935	-0.000000013	0.000046756	0.000010732	107149213
18600440						
8	7	-284.636891949	-0.000000014	0.000029352	0.000003078	101624732
18984108						
9	8	-284.636891946	0.000000003	0.000030883	0.000002689	95606090
19459230						

10 9 -284.636891943 0.000000004 0.000095591 0.000001893 122810205
17508006
11 10 -284.636891943 -0.000000001 0.000031077 0.000001757 152520531
15253448
12 11 -284.636891943 0.000000000 0.000039948 0.000002483 145697912
15752846

-----DISABLING FDIFF OPTION-----

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 37.6 SECONDS (3.1 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 13.1 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.6 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6368919433 AFTER 12 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6016430361
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998592413

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 40.60 , TOTAL = 7483.5 SECONDS (124.7 MIN)
WALL CLOCK TIME: STEP = 37.33 , TOTAL = 6917.9 SECONDS (115.3
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.69 , TOTAL = 7487.2 SECONDS (124.8 MIN)
WALL CLOCK TIME: STEP = 3.68 , TOTAL = 6921.6 SECONDS (115.4
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.91 , TOTAL = 7490.1 SECONDS (124.8 MIN)

WALL CLOCK TIME: STEP = 2.75 , TOTAL = 6924.3 SECONDS (115.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 79 ENERGY= -284.6368919

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0002328	-0.0000617	-0.0001210
2 C	6.0	0.0001547	0.0002149	-0.0001211
3 C	6.0	0.0000072	0.0000786	0.0000278
4 C	6.0	0.0000112	-0.0000969	0.0000139
5 C	6.0	-0.0000179	-0.0001600	-0.0000776
6 C	6.0	-0.0000420	-0.0001821	-0.0001014
7 C	6.0	-0.0000440	0.0000736	-0.0001023
8 C	6.0	-0.0000410	-0.0002043	-0.0000813
9 C	6.0	-0.0000940	-0.0000161	0.0000050
10 C	6.0	0.0000052	0.0000298	-0.0001724
11 C	6.0	0.0000443	-0.0000454	-0.0000733
12 N	7.0	-0.0000162	-0.0000615	-0.0000963
13 C	6.0	-0.0000352	0.0001848	-0.0000318
14 C	6.0	0.0001061	0.0000661	-0.0000680
15 C	6.0	-0.0001251	-0.0001270	-0.0001790
16 C	6.0	0.0000217	-0.0002014	-0.0000581
17 C	6.0	-0.0001623	0.0001463	0.0000841
18 C	6.0	-0.0001461	0.0001836	0.0002292
19 C	6.0	-0.0000705	0.0002302	0.0001465
20 O	8.0	-0.0000806	-0.0003605	0.0000319
21 N	7.0	0.0001319	-0.0001808	-0.0000434
22 H	1.0	-0.0000067	0.0000541	-0.0000287
23 H	1.0	-0.0000669	0.0001100	0.0002058
24 H	1.0	0.0000888	0.0000880	0.0000602
25 H	1.0	-0.0002114	-0.0000682	0.0001073
26 H	1.0	-0.0000449	-0.0000821	0.0002465
27 H	1.0	0.0001074	0.0000061	-0.0001119
28 H	1.0	-0.0000014	0.0000003	0.0001071
29 H	1.0	0.0000596	0.0001261	0.0001388
30 H	1.0	-0.0000950	0.0000404	0.0000052

31 H	1.0	0.0000841	-0.0000251	-0.0001724
32 H	1.0	0.0000267	-0.0000135	0.0000539
33 H	1.0	0.0000321	0.0002500	0.0000244
34 H	1.0	0.0000205	-0.0000568	0.0001814
35 H	1.0	0.0001667	0.0000604	-0.0000290

MAXIMUM GRADIENT = 0.0003605 RMS GRADIENT = 0.0001175
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000080501
 PREDICTED ENERGY CHANGE WAS -0.0000058308 RATIO= 1.381
 GDIIS STEP HAS LENGTH = 0.029098
 RADIUS OF STEP TAKEN= 0.02910 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 7490.1 SECONDS (124.8 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6924.4 SECONDS (115.4
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 80

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z

CO	27.0	0.1565896645	-1.7367297726	0.8594108672
C	6.0	4.9815216983	0.6304675029	0.5599220851
C	6.0	5.1878050003	-0.7102923862	0.2082998881
C	6.0	4.0537676050	-1.5341185975	-0.0854487626
C	6.0	2.7440019016	-1.0251959452	-0.0033984841
C	6.0	2.4692808294	0.3409172267	0.4241204075
C	6.0	3.6497522133	1.1771457908	0.6743434429
C	6.0	3.5003047535	2.5626099058	1.0542291642
C	6.0	2.2316874422	3.1355994179	1.2177998008
C	6.0	1.0688376045	2.3253719280	1.0323235581
C	6.0	1.1624024840	0.9718336185	0.6304213781
N	7.0	-0.0505061538	0.1711653433	0.5743301827
C	6.0	-1.2468952482	0.6984763030	0.3188140801
C	6.0	-2.5512654855	0.0385852503	0.4360726134
C	6.0	-2.8224953236	-1.2862518100	0.9239665325
C	6.0	-4.1234346807	-1.8048403811	1.0540490346
C	6.0	-5.2330452156	-0.9846495879	0.6830132785
C	6.0	-5.0188012101	0.3307685624	0.1841289534
C	6.0	-3.6994296654	0.8307446449	0.0675244825
O	8.0	-1.6994175874	-2.1470820099	1.3086137032
N	7.0	1.6402029681	-1.9632090446	-0.4296155758

H	1.0	5.8418425373	1.2942269782	0.7617935450
H	1.0	6.2063529148	-1.1298893830	0.1350686356
H	1.0	4.2219073383	-2.5792386846	-0.4117441476
H	1.0	4.4111856106	3.1621403151	1.2310642992
H	1.0	2.1211868838	4.1894617058	1.5286682319
H	1.0	0.0839979519	2.7695067195	1.2595471621
H	1.0	-1.2902563424	1.7521165658	-0.0219585212
H	1.0	-4.2980956403	-2.8282067844	1.4372626238
H	1.0	-6.2581519226	-1.3851438804	0.7839816409
H	1.0	-5.8754998817	0.9633812353	-0.1074908209
H	1.0	-3.5345718122	1.8576610666	-0.3084685229
H	1.0	-2.0150539665	-2.9562220724	1.7872522074
H	1.0	1.2817728430	-1.6923671886	-1.3717696072
H	1.0	2.0385168916	-2.9176375525	-0.5332403564

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3826839	5.1759682	4.0151970
2 C	5.3826839	0.0000000	1.4013665 *	2.4418567 *
3 C	5.1759682	1.4013665 *	0.0000000	1.4321378 *
4 C	4.0151970	2.4418567 *	1.4321378 *	0.0000000
5 C	2.8187626 *	2.8399025 *	2.4730859 *	1.4075584 *
6 C	3.1392093	2.5325157 *	2.9226690 *	2.5071933 *
7 C	4.5527031	1.4441466 *	2.4789566 *	2.8445504 *
8 C	5.4500189	2.4842539 *	3.7782460	4.2881664
9 C	5.3079248	3.7775756	4.9546549	5.1792566
10 C	4.1668652	4.2901003	5.1826794	5.0054859
11 C	2.8983463 *	3.8349932	4.3831039	3.8925902
12 N	1.9401607 *	5.0529665	5.3245516	4.4931464
13 C	2.8622095 *	6.2334530	6.5880354	5.7658421
14 C	3.2654920	7.5570197	7.7785545	6.8096875
15 C	3.0136432	8.0441919	8.0628047	6.9543763
16 C	4.2849891	9.4379615	9.4134219	8.2606527
17 C	5.4447135	10.3422015	10.4352644	9.3347385
18 C	5.6138423	10.0118679	10.2595908	9.2661740
19 C	4.6997760	8.6972112	9.0209508	8.1072836
20 O	1.9531859 *	7.2739446	7.1210175	5.9513254
21 N	1.9783808 *	4.3440481	3.8160472	2.4754522 *
22 H	6.4434718	1.1052062 *	2.1799583 *	3.4517489
23 H	6.1231170	2.1862224 *	1.1040219 *	2.2012843 *
24 H	4.3419424	3.4385117	2.1932563 *	1.1077074 *
25 H	6.4991262	2.6805004 *	4.0798186	4.8903785
26 H	6.2791156	4.6675930	5.9291744	6.2529684

27 H	4.5245493	5.3898704	6.2660170	6.0074351
28 H	3.8784306	6.3978029	6.9341009	6.2739114
29 H	4.6227109	9.9420044	9.7968475	8.5876035
30 H	6.4248122	11.4211714	11.4802772	10.3495791
31 H	6.6791918	10.8826095	11.1936420	10.2385714
32 H	5.2828270	8.6477717	9.1072110	8.3148543
33 H	2.6578350 *	7.9575594	7.7083376	6.5084547
34 H	2.4992342 *	4.7765192	4.3264509	3.0600031
35 H	2.6221500 *	4.7376504	3.9166657	2.4851313 *

C C C C

1 CO	2.8187626 *	3.1392093	4.5527031	5.4500189
2 C	2.8399025 *	2.5325157 *	1.4441466 *	2.4842539 *
3 C	2.4730859 *	2.9226690 *	2.4789566 *	3.7782460
4 C	1.4075584 *	2.5071933 *	2.8445504 *	4.2881664
5 C	0.0000000	1.4575696 *	2.4758891 *	3.8161396
6 C	1.4575696 *	0.0000000	1.4681289 *	2.5290247 *
7 C	2.4758891 *	1.4681289 *	0.0000000	1.4443540 *
8 C	3.8161396	2.5290247 *	1.4443540 *	0.0000000
9 C	4.3664642	2.9148973 *	2.4782641 *	1.4015927 *
10 C	3.8865410	2.5038396 *	2.8474011 *	2.4431116 *
11 C	2.6251307 *	1.4657921 *	2.4961953 *	2.8593652 *
12 N	3.0942408	2.5299615 *	3.8358716	4.3078496
13 C	4.3591429	3.7348230	4.9328168	5.1528378
14 C	5.4189134	5.0296553	6.3091769	6.5859183
15 C	5.6492519	5.5588146	6.9296917	7.4032767
16 C	6.9919758	6.9616797	8.3341978	8.7861268
17 C	8.0066276	7.8198452	9.1420744	9.4335705
18 C	7.8825705	7.4919338	8.7235591	8.8494834
19 C	6.7057703	6.1983934	7.3823233	7.4705501
20 O	4.7669677	4.9346241	6.3298031	7.0201867
21 N	1.5099343 *	2.5933054 *	3.8882955	5.1131997
22 H	3.9448521	3.5209367	2.1969560 *	2.6790134 *
23 H	3.4666999	4.0264787	3.4856041	4.6692723
24 H	2.1831169 *	3.5068048	3.9518821	5.3952196
25 H	4.6730274	3.5187288	2.1977084 *	1.1047223 *
26 H	5.4706290	4.0190160	3.4843120	2.1848811 *
27 H	4.8031678	3.5050762	3.9487568	3.4287190
28 H	4.8978617	4.0403700	5.0218634	4.9763998
29 H	7.4106336	7.5410336	8.9327029	9.4880276
30 H	9.0436886	8.9037559	10.2344474	10.5302075
31 H	8.8465296	8.3848338	9.5596751	9.5819016
32 H	6.9155202	6.2356591	7.2830991	7.2002351
33 H	5.4391088	5.7304899	7.1002341	7.8367092
34 H	2.1108460 *	2.9613581 *	4.2459404	5.3770051

35 H 2.0880078 * 3.4234889 4.5630679 5.8898213

C C C N

1 CO	5.3079248	4.1668652	2.8983463 *	1.9401607 *
2 C	3.7775756	4.2901003	3.8349932	5.0529665
3 C	4.9546549	5.1826794	4.3831039	5.3245516
4 C	5.1792566	5.0054859	3.8925902	4.4931464
5 C	4.3664642	3.8865410	2.6251307 *	3.0942408
6 C	2.9148973 *	2.5038396 *	1.4657921 *	2.5299615 *
7 C	2.4782641 *	2.8474011 *	2.4961953 *	3.8358716
8 C	1.4015927 *	2.4431116 *	2.8593652 *	4.3078496
9 C	0.0000000	1.4293669 *	2.4840020 *	3.7960941
10 C	1.4293669 *	0.0000000	1.4150427 *	2.4704846 *
11 C	2.4840020 *	1.4150427 *	0.0000000	1.4544288 *
12 N	3.7960941	2.4704846 *	1.4544288 *	0.0000000
13 C	4.3414608	2.9186476 *	2.4446961 *	1.3321757 *
14 C	5.7514548	4.3231996	3.8340649	2.5080849 *
15 C	6.7218948	5.3101826	4.5896110	3.1512274
16 C	8.0512320	6.6346678	5.9857709	4.5523044
17 C	8.5431073	7.1268497	6.6882243	5.3109727
18 C	7.8425211	6.4619829	6.2303628	4.9861494
19 C	6.4663466	5.0893144	4.8963426	3.7425312
20 O	6.5854808	5.2671071	4.2869096	2.9380865 *
21 N	5.3908885	4.5667988	3.1569680	2.9020611 *
22 H	4.0782121	4.8906055	4.6923720	6.0013484
23 H	5.9299804	6.2560339	5.4867158	6.4057770
24 H	6.2670378	6.0068615	4.8017490	5.1759619
25 H	2.1797001 *	3.4512272	3.9639383	5.4114623
26 H	1.1042985 *	2.1974139 *	3.4755209	4.6662316
27 H	2.1790679 *	1.1039907 *	2.1886946 *	2.6905374 *
28 H	3.9818480	2.6467823 *	2.6551792 *	2.0956974 *
29 H	8.8460848	7.4516657	6.7013685	5.2709489
30 H	9.6282236	8.2167133	7.7873970	6.4031959
31 H	8.4971415	7.1678462	7.0764861	5.9180265
32 H	6.1001940	4.8174532	4.8711161	3.9701782
33 H	7.4477767	6.1624297	5.1830598	3.8873101
34 H	5.5603479	4.6869215	3.3348139	3.0058319
35 H	6.3043742	5.5570151	4.1532723	3.8899143

C C C C

1 CO	2.8622095 *	3.2654920	3.0136432	4.2849891
2 C	6.2334530	7.5570197	8.0441919	9.4379615
3 C	6.5880354	7.7785545	8.0628047	9.4134219
4 C	5.7658421	6.8096875	6.9543763	8.2606527

5 C	4.3591429	5.4189134	5.6492519	6.9919758
6 C	3.7348230	5.0296553	5.5588146	6.9616797
7 C	4.9328168	6.3091769	6.9296917	8.3341978
8 C	5.1528378	6.5859183	7.4032767	8.7861268
9 C	4.3414608	5.7514548	6.7218948	8.0512320
10 C	2.9186476 *	4.3231996	5.3101826	6.6346678
11 C	2.4446961 *	3.8340649	4.5896110	5.9857709
12 N	1.3321757 *	2.5080849 *	3.1512274	4.5523044
13 C	0.0000000	1.4664881 *	2.6053543 *	3.8835092
14 C	1.4664881 *	0.0000000	1.4376367 *	2.5003658 *
15 C	2.6053543 *	1.4376367 *	0.0000000	1.4065201 *
16 C	3.8835092	2.5003658 *	1.4065201 *	0.0000000
17 C	4.3422282	2.8809602 *	2.4412647 *	1.4288513 *
18 C	3.7921793	2.4975146 *	2.8259289 *	2.4737154 *
19 C	2.4689201 *	1.4427838 *	2.4462585 *	2.8459303 *
20 O	3.0465853	2.5028212 *	1.4663852 *	2.4612581 *
21 N	3.9975057	4.7249343	4.7123382	5.9536426
22 H	7.1275068	8.4927612	9.0418981	10.4401332
23 H	7.6764309	8.8403516	9.0645965	10.3925259
24 H	6.4175488	7.3107910	7.2855711	8.5084062
25 H	6.2382465	7.6723095	8.4975668	9.8763341
26 H	4.9994703	6.3447105	7.4019657	8.6690380
27 H	2.6354169 *	3.8833820	5.0009494	6.2184701
28 H	1.1082256 *	2.1762643 *	3.5318852	4.6729685
29 H	4.7956485	3.5031834	2.1951069 *	1.1066336 *
30 H	5.4470678	3.9861074	3.4399290	2.1922817 *
31 H	4.6557375	3.4930278	3.9300878	3.4759111
32 H	2.6402002 *	2.1977874 *	3.4511067	3.9518515
33 H	4.0128791	3.3289758	2.0459776 *	2.5116799 *
34 H	3.8688975	4.5778459	4.7202067	5.9256658
35 H	4.9594565	5.5448105	5.3305076	6.4596790

C C C O

1 CO	5.4447135	5.6138423	4.6997760	1.9531859 *
2 C	10.3422015	10.0118679	8.6972112	7.2739446
3 C	10.4352644	10.2595908	9.0209508	7.1210175
4 C	9.3347385	9.2661740	8.1072836	5.9513254
5 C	8.0066276	7.8825705	6.7057703	4.7669677
6 C	7.8198452	7.4919338	6.1983934	4.9346241
7 C	9.1420744	8.7235591	7.3823233	6.3298031
8 C	9.4335705	8.8494834	7.4705501	7.0201867
9 C	8.5431073	7.8425211	6.4663466	6.5854808
10 C	7.1268497	6.4619829	5.0893144	5.2671071
11 C	6.6882243	6.2303628	4.8963426	4.2869096
12 N	5.3109727	4.9861494	3.7425312	2.9380865 *

13 C	4.3422282	3.7921793	2.4689201 *	3.0465853
14 C	2.8809602 *	2.4975146 *	1.4427838 *	2.5028212 *
15 C	2.4412647 *	2.8259289 *	2.4462585 *	1.4663852 *
16 C	1.4288513 *	2.4737154 *	2.8459303 *	2.4612581 *
17 C	0.0000000	1.4230639 *	2.4548848 *	3.7721545
18 C	1.4230639 *	0.0000000	1.4157380 *	4.2921460
19 C	2.4548848 *	1.4157380 *	0.0000000	3.7957611
20 O	3.7721545	4.2921460	3.7957611	0.0000000
21 N	7.0311494	7.0697491	6.0469002	3.7693920
22 H	11.3071934	10.9185865	9.5777190	8.3073596
23 H	11.4534347	11.3198946	10.0981769	8.0568664
24 H	9.6507687	9.7063846	8.6374339	6.1813008
25 H	10.5122507	9.9013833	8.5188797	8.0952657
26 H	9.0316826	8.2265867	6.8771723	7.4025150
27 H	6.5342964	5.7569547	4.4152057	5.2302795
28 H	4.8510265	3.9955912	2.5809009 *	4.1402397
29 H	2.2003922 *	3.4740302	3.9525320	2.6895370 *
30 H	1.1051851 *	2.2000384 *	3.4598457	4.6516499
31 H	2.1982877 *	1.1041619 *	2.1871224 *	5.3962947
32 H	3.4563822	2.1856326 *	1.1059413 *	4.6926233
33 H	3.9321634	4.7325267	4.4872822	0.9916798 *
34 H	6.8677399	6.7978770	5.7662847	4.0346892
35 H	7.6217669	7.8020830	6.8800667	4.2377277

N H H H

1 CO	1.9783808 *	6.4434718	6.1231170	4.3419424
2 C	4.3440481	1.1052062 *	2.1862224 *	3.4385117
3 C	3.8160472	2.1799583 *	1.1040219 *	2.1932563 *
4 C	2.4754522 *	3.4517489	2.2012843 *	1.1077074 *
5 C	1.5099343 *	3.9448521	3.4666999	2.1831169 *
6 C	2.5933054 *	3.5209367	4.0264787	3.5068048
7 C	3.8882955	2.1969560 *	3.4856041	3.9518821
8 C	5.1131997	2.6790134 *	4.6692723	5.3952196
9 C	5.3908885	4.0782121	5.9299804	6.2670378
10 C	4.5667988	4.8906055	6.2560339	6.0068615
11 C	3.1569680	4.6923720	5.4867158	4.8017490
12 N	2.9020611 *	6.0013484	6.4057770	5.1759619
13 C	3.9975057	7.1275068	7.6764309	6.4175488
14 C	4.7249343	8.4927612	8.8403516	7.3107910
15 C	4.7123382	9.0418981	9.0645965	7.2855711
16 C	5.9536426	10.4401332	10.3925259	8.5084062
17 C	7.0311494	11.3071934	11.4534347	9.6507687
18 C	7.0697491	10.9185865	11.3198946	9.7063846
19 C	6.0469002	9.5777190	10.0981769	8.6374339
20 O	3.7693920	8.3073596	8.0568664	6.1813008

21 N	0.0000000	5.4483135	4.6757903	2.6542437 *
22 H	5.4483135	0.0000000	2.5302158 *	4.3594859
23 H	4.6757903	2.5302158 *	0.0000000	2.5174674 *
24 H	2.6542437 *	4.3594859	2.5174674 *	0.0000000
25 H	6.0584989	2.3991862 *	4.7796811	5.9747869
26 H	6.4746875	4.7763751	6.8502699	7.3480291
27 H	5.2605744	5.9646444	7.3452687	6.9659591
28 H	4.7494653	7.1896290	8.0330421	7.0211480
29 H	6.2846516	10.9667253	10.7202346	8.7218841
30 H	8.0119278	12.3931185	12.4839947	10.6154258
31 H	8.0718328	11.7542004	12.2642482	10.7051557
32 H	6.4336630	9.4541031	10.1984213	8.9364262
33 H	4.3887904	8.9915908	8.5823501	6.6240009
34 H	1.0437824 *	5.8537229	5.1805822	3.2175427
35 H	1.0393872 *	5.8208420	4.5840525	2.2127966 *

H H H H

1 CO	6.4991262	6.2791156	4.5245493	3.8784306
2 C	2.6805004 *	4.6675930	5.3898704	6.3978029
3 C	4.0798186	5.9291744	6.2660170	6.9341009
4 C	4.8903785	6.2529684	6.0074351	6.2739114
5 C	4.6730274	5.4706290	4.8031678	4.8978617
6 C	3.5187288	4.0190160	3.5050762	4.0403700
7 C	2.1977084 *	3.4843120	3.9487568	5.0218634
8 C	1.1047223 *	2.1848811 *	3.4287190	4.9763998
9 C	2.1797001 *	1.1042985 *	2.1790679 *	3.9818480
10 C	3.4512272	2.1974139 *	1.1039907 *	2.6467823 *
11 C	3.9639383	3.4755209	2.1886946 *	2.6551792 *
12 N	5.4114623	4.6662316	2.6905374 *	2.0956974 *
13 C	6.2382465	4.9994703	2.6354169 *	1.1082256 *
14 C	7.6723095	6.3447105	3.8833820	2.1762643 *
15 C	8.4975668	7.4019657	5.0009494	3.5318852
16 C	9.8763341	8.6690380	6.2184701	4.6729685
17 C	10.5122507	9.0316826	6.5342964	4.8510265
18 C	9.9013833	8.2265867	5.7569547	3.9955912
19 C	8.5188797	6.8771723	4.4152057	2.5809009 *
20 O	8.0952657	7.4025150	5.2302795	4.1402397
21 N	6.0584989	6.4746875	5.2605744	4.7494653
22 H	2.3991862 *	4.7763751	5.9646444	7.1896290
23 H	4.7796811	6.8502699	7.3452687	8.0330421
24 H	5.9747869	7.3480291	6.9659591	7.0211480
25 H	0.0000000	2.5274595 *	4.3450576	6.0053870
26 H	2.5274595 *	0.0000000	2.4977664 *	4.4702393
27 H	4.3450576	2.4977664 *	0.0000000	2.1368000 *
28 H	6.0053870	4.4702393	2.1368000 *	0.0000000

29 H	10.5725284	9.5112152	7.1111689	5.6706072
30 H	11.6065688	10.0917840	7.5967196	5.9305926
31 H	10.6038752	8.7767654	6.3754605	4.6533727
32 H	8.1979808	6.3874856	4.0477380	2.2649900 *
33 H	8.8904588	8.2605176	6.1211487	5.0957853
34 H	6.3351568	6.6115858	5.3166542	4.5057510
35 H	6.7606232	7.4006190	6.2751766	5.7574946

H H H H

1 CO	4.6227109	6.4248122	6.6791918	5.2828270
2 C	9.9420044	11.4211714	10.8826095	8.6477717
3 C	9.7968475	11.4802772	11.1936420	9.1072110
4 C	8.5876035	10.3495791	10.2385714	8.3148543
5 C	7.4106336	9.0436886	8.8465296	6.9155202
6 C	7.5410336	8.9037559	8.3848338	6.2356591
7 C	8.9327029	10.2344474	9.5596751	7.2830991
8 C	9.4880276	10.5302075	9.5819016	7.2002351
9 C	8.8460848	9.6282236	8.4971415	6.1001940
10 C	7.4516657	8.2167133	7.1678462	4.8174532
11 C	6.7013685	7.7873970	7.0764861	4.8711161
12 N	5.2709489	6.4031959	5.9180265	3.9701782
13 C	4.7956485	5.4470678	4.6557375	2.6402002 *
14 C	3.5031834	3.9861074	3.4930278	2.1977874 *
15 C	2.1951069 *	3.4399290	3.9300878	3.4511067
16 C	1.1066336 *	2.1922817 *	3.4759111	3.9518515
17 C	2.2003922 *	1.1051851 *	2.1982877 *	3.4563822
18 C	3.4740302	2.2000384 *	1.1041619 *	2.1856326 *
19 C	3.9525320	3.4598457	2.1871224 *	1.1059413 *
20 O	2.6895370 *	4.6516499	5.3962947	4.6926233
21 N	6.2846516	8.0119278	8.0718328	6.4336630
22 H	10.9667253	12.3931185	11.7542004	9.4541031
23 H	10.7202346	12.4839947	12.2642482	10.1984213
24 H	8.7218841	10.6154258	10.7051557	8.9364262
25 H	10.5725284	11.6065688	10.6038752	8.1979808
26 H	9.5112152	10.0917840	8.7767654	6.3874856
27 H	7.1111689	7.5967196	6.3754605	4.0477380
28 H	5.6706072	5.9305926	4.6533727	2.2649900 *
29 H	0.0000000	2.5201244 *	4.3875514	5.0584487
30 H	2.5201244 *	0.0000000	2.5410069 *	4.3734563
31 H	4.3875514	2.5410069 *	0.0000000	2.5139755 *
32 H	5.0584487	4.3734563	2.5139755 *	0.0000000
33 H	2.3132574 *	4.6345139	5.8186239	5.4657525
34 H	6.3494666	7.8480644	7.7380846	6.0770458
35 H	6.6365306	8.5392227	8.8246944	7.3425688

	H	H	H
1 CO	2.6578350 *	2.4992342 *	2.6221500 *
2 C	7.9575594	4.7765192	4.7376504
3 C	7.7083376	4.3264509	3.9166657
4 C	6.5084547	3.0600031	2.4851313 *
5 C	5.4391088	2.1108460 *	2.0880078 *
6 C	5.7304899	2.9613581 *	3.4234889
7 C	7.1002341	4.2459404	4.5630679
8 C	7.8367092	5.3770051	5.8898213
9 C	7.4477767	5.5603479	6.3043742
10 C	6.1624297	4.6869215	5.5570151
11 C	5.1830598	3.3348139	4.1532723
12 N	3.8873101	3.0058319	3.8899143
13 C	4.0128791	3.8688975	4.9594565
14 C	3.3289758	4.5778459	5.5448105
15 C	2.0459776 *	4.7202067	5.3305076
16 C	2.5116799 *	5.9256658	6.4596790
17 C	3.9321634	6.8677399	7.6217669
18 C	4.7325267	6.7978770	7.8020830
19 C	4.4872822	5.7662847	6.8800667
20 O	0.9916798 *	4.0346892	4.2377277
21 N	4.3887904	1.0437824 *	1.0393872 *
22 H	8.9915908	5.8537229	5.8208420
23 H	8.5823501	5.1805822	4.5840525
24 H	6.6240009	3.2175427	2.2127966 *
25 H	8.8904588	6.3351568	6.7606232
26 H	8.2605176	6.6115858	7.4006190
27 H	6.1211487	5.3166542	6.2751766
28 H	5.0957853	4.5057510	5.7574946
29 H	2.3132574 *	6.3494666	6.6365306
30 H	4.6345139	7.8480644	8.5392227
31 H	5.8186239	7.7380846	8.8246944
32 H	5.4657525	6.0770458	7.3425688
33 H	0.0000000	4.7377014	4.6709326
34 H	4.7377014	0.0000000	1.6664574 *
35 H	4.6709326	1.6664574 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.66 , TOTAL = 7490.8 SECONDS (124.8 MIN)
WALL CLOCK TIME: STEP = 0.66 , TOTAL = 6925.0 SECONDS (115.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.91 , TOTAL = 7491.7 SECONDS (124.9 MIN)
WALL CLOCK TIME: STEP = 0.91 , TOTAL = 6925.9 SECONDS (115.4 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

		NONZERO BLOCKS				
ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD	
-----START SECOND ORDER SCF-----						
1	0	-284.636875251	-284.636875251	0.007528211	0.000509631	198004772
11338901						
2	1	-284.636899823	-0.000024572	0.001409374	0.000042821	152530898
15154525						
3	2	-284.636899579	0.000000244	0.001126334	0.000101975	136610143
16416192						
4	3	-284.636900183	-0.000000604	0.000268541	0.000031713	131100996
16870955						
5	4	-284.636900154	0.000000029	0.000234476	0.000064699	123687053
17443103						
6	5	-284.636900245	-0.000000091	0.000107723	0.000010101	118359654
17852324						
7	6	-284.636900233	0.000000012	0.000063343	0.000010060	111315719
18281507						
8	7	-284.636900244	-0.000000010	0.000034772	0.000006038	130320477
16877006						
9	8	-284.636900244	-0.000000001	0.000081701	0.000005958	124000081
17431839						
10	9	-284.636900248	-0.000000004	0.000193722	0.000005528	152104033
15352763						
-----DISABLING FDIFF OPTION-----						
11	10	-284.636900216	0.000000032	0.000111656	0.000007350	198000593
11339150						
12	11	-284.636900218	-0.000000002	0.000036174	0.000007185	198000583
11339152						
13	12	-284.636900219	-0.000000001	0.000024768	0.000005053	198000600
11339150						
14	13	-284.636900220	-0.000000001	0.000029650	0.000002780	198000597
11339151						
15	14	-284.636900220	0.000000000	0.000038896	0.000001677	198000623
11339151						

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 49.1 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 16.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.9 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6369002201 AFTER 15 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6010462293
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998572748

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 52.76 , TOTAL = 7544.5 SECONDS (125.7 MIN)
WALL CLOCK TIME: STEP = 48.43 , TOTAL = 6974.3 SECONDS (116.2
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.78 , TOTAL = 7548.3 SECONDS (125.8 MIN)
WALL CLOCK TIME: STEP = 3.75 , TOTAL = 6978.1 SECONDS (116.3
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.90 , TOTAL = 7551.2 SECONDS (125.9 MIN)
WALL CLOCK TIME: STEP = 2.74 , TOTAL = 6980.8 SECONDS (116.3
MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 80 ENERGY= -284.6369002

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0001256	-0.0000773	-0.0001374
2 C	6.0	0.0001014	0.0001649	-0.0000637
3 C	6.0	0.0000585	0.0000032	-0.0000268
4 C	6.0	-0.0000303	0.0000370	-0.0000490
5 C	6.0	0.0000073	-0.0000864	-0.0001440
6 C	6.0	-0.0001914	-0.0003296	-0.0000833
7 C	6.0	0.0000697	-0.0001292	-0.0001403
8 C	6.0	0.0000775	0.0002014	-0.0000353
9 C	6.0	-0.0001415	0.0001236	0.0001049
10 C	6.0	0.0002137	-0.0000025	0.0000521
11 C	6.0	0.0000894	-0.0001609	0.0000024
12 N	7.0	-0.0000571	-0.0001651	-0.0002802
13 C	6.0	-0.0001063	0.0000850	0.0000227
14 C	6.0	-0.0000857	-0.0000995	-0.0000050
15 C	6.0	-0.0000317	-0.0000093	-0.0001073
16 C	6.0	0.0001146	-0.0003141	-0.0000398
17 C	6.0	-0.0000025	0.0002624	0.0001224
18 C	6.0	-0.0001602	0.0001175	0.0001159
19 C	6.0	-0.0001414	0.0000249	0.0001516
20 O	8.0	-0.0000317	-0.0003159	-0.0000362
21 N	7.0	-0.0000354	-0.0001549	-0.0001107
22 H	1.0	0.0000867	0.0000706	0.0000260
23 H	1.0	-0.0000600	0.0000736	0.0001672
24 H	1.0	0.0001102	0.0000760	0.0001382
25 H	1.0	-0.0002738	0.0000024	0.0000766
26 H	1.0	-0.0000267	-0.0000177	0.0001885
27 H	1.0	0.0000834	0.0000838	-0.0002343
28 H	1.0	0.0001222	0.0000657	0.0000793
29 H	1.0	-0.0001060	0.0001809	0.0000936
30 H	1.0	-0.0000207	0.0000843	0.0000015
31 H	1.0	0.0000740	0.0000387	-0.0001389
32 H	1.0	-0.0000578	0.0000403	0.0000293
33 H	1.0	0.0000562	0.0001875	0.0000370
34 H	1.0	0.0000357	-0.0001256	0.0002668
35 H	1.0	0.0001342	0.0000643	-0.0000437

MAXIMUM GRADIENT = 0.0003296 RMS GRADIENT = 0.0001244

HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000082768
 PREDICTED ENERGY CHANGE WAS -0.0000068146 RATIO= 1.215
 GDIIS STEP HAS LENGTH = 0.028489
 RADIUS OF STEP TAKEN= 0.02849 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 7551.2 SECONDS (125.9 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 6980.9 SECONDS (116.3 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

INSERCH= 81

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1562253294	-1.7364154970	0.8596226130
C	6.0	4.9815368049	0.6292241863	0.5617682087
C	6.0	5.1871632238	-0.7108113845	0.2071984895
C	6.0	4.0526574891	-1.5336769421	-0.0876720480
C	6.0	2.7431890473	-1.0241576325	-0.0041789090
C	6.0	2.4694775455	0.3416489114	0.4253475453
C	6.0	3.6501787115	1.1771352124	0.6765772036
C	6.0	3.5012530843	2.5626844071	1.0561991906
C	6.0	2.2325380483	3.1360179263	1.2190325580
C	6.0	1.0692050356	2.3259903258	1.0337744610
C	6.0	1.1625294854	0.9725220989	0.6319478928
N	7.0	-0.0502738534	0.1715487014	0.5751457378
C	6.0	-1.2466775478	0.6982386515	0.3186246081
C	6.0	-2.5508575866	0.0379098836	0.4356371876
C	6.0	-2.8220770399	-1.2862242560	0.9259299678
C	6.0	-4.1231063777	-1.8044987925	1.0564710507
C	6.0	-5.2323802434	-0.9852054980	0.6834847218
C	6.0	-5.0183330920	0.3289137379	0.1814328172
C	6.0	-3.6990181878	0.8289315576	0.0642872602
O	8.0	-1.6988094620	-2.1464986864	1.3105729296
N	7.0	1.6388081096	-1.9615708675	-0.4309238512
H	1.0	5.8422203805	1.2919448081	0.7651940043
H	1.0	6.2054822460	-1.1311909417	0.1323661055
H	1.0	4.2200176419	-2.5785990127	-0.4149976424
H	1.0	4.4123585056	3.1625929980	1.2323474570
H	1.0	2.1220544704	4.1905921210	1.5279047514
H	1.0	0.0843500437	2.7708355103	1.2590156689
H	1.0	-1.2900275456	1.7516014074	-0.0224600267

H	1.0	-4.2987180683	-2.8275142853	1.4407535852
H	1.0	-6.2572743457	-1.3853915120	0.7855725236
H	1.0	-5.8752954135	0.9613434720	-0.1108436313
H	1.0	-3.5346116749	1.8551255305	-0.3135116659
H	1.0	-2.0140188810	-2.9557796285	1.7895899928
H	1.0	1.2796137393	-1.6899920835	-1.3727031610
H	1.0	2.0366173775	-2.9161694273	-0.5356205963

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3822485	5.1756987	4.0150534
2 C	5.3822485	0.0000000	1.4013198 *	2.4418703 *
3 C	5.1756987	1.4013198 *	0.0000000	1.4321870 *
4 C	4.0150534	2.4418703 *	1.4321870 *	0.0000000
5 C	2.8188376 *	2.8397479 *	2.4730297 *	1.4075825 *
6 C	3.1397583	2.5321437 *	2.9225121 *	2.5072884 *
7 C	4.5530203	1.4442652 *	2.4793104 *	2.8450955 *
8 C	5.4506984	2.4847475 *	3.7787392	4.2886670
9 C	5.3085645	3.7779631	4.9549686	5.1794171
10 C	4.1673735	4.2904714	5.1829501	5.0055631
11 C	2.8987630 *	3.8350483	4.3831154	3.8925219
12 N	1.9400764 *	5.0525998	5.3239733	4.4923454
13 C	2.8615304 *	6.2333407	6.5872714	5.7645014
14 C	3.2643977	7.5566214	7.7775146	6.8080944
15 C	3.0128647	8.0435033	8.0619851	6.9534593
16 C	4.2843978	9.4372806	9.4126795	8.2598743
17 C	5.4435660	10.3414361	10.4340321	9.3331361
18 C	5.6126269	10.0116052	10.2583550	9.2641530
19 C	4.6985600	8.6970918	9.0197257	8.1051518
20 O	1.9526081 *	7.2727142	7.1200599	5.9506312
21 N	1.9784481 *	4.3441330	3.8160743	2.4753957 *
22 H	6.4428583	1.1051502 *	2.1797916 *	3.4516741
23 H	6.1228023	2.1866618 *	1.1042158 *	2.2011511 *
24 H	4.3414672	3.4386207	2.1934286 *	1.1077065 *
25 H	6.5002983	2.6817155 *	4.0809943	4.8915016
26 H	6.2801676	4.6683402	5.9298325	6.2533649
27 H	4.5254826	5.3902775	6.2663296	6.0074836
28 H	3.8776254	6.3979350	6.9332691	6.2722874
29 H	4.6232814	9.9420715	9.7971441	8.5881065
30 H	6.4235255	11.4201419	11.4788817	10.3479099
31 H	6.6782446	10.8827164	11.1926424	10.2366944
32 H	5.2818263	8.6483371	9.1062906	8.3127396
33 H	2.6573762 *	7.9559788	7.7071959	6.5077685

34 H	2.4994870 *	4.7775703	4.3271038	3.0603122
35 H	2.6219072 *	4.7377873	3.9168002	2.4852286 *

	C	C	C	C
--	---	---	---	---

1 CO	2.8188376 *	3.1397583	4.5530203	5.4506984
2 C	2.8397479 *	2.5321437 *	1.4442652 *	2.4847475 *
3 C	2.4730297 *	2.9225121 *	2.4793104 *	3.7787392
4 C	1.4075825 *	2.5072884 *	2.8450955 *	4.2886670
5 C	0.0000000	1.4576826 *	2.4762369 *	3.8163462
6 C	1.4576826 *	0.0000000	1.4680630 *	2.5289392 *
7 C	2.4762369 *	1.4680630 *	0.0000000	1.4443124 *
8 C	3.8163462	2.5289392 *	1.4443124 *	0.0000000
9 C	4.3662423	2.9145453 *	2.4781413 *	1.4017360 *
10 C	3.8862657	2.5037087 *	2.8476101 *	2.4436417 *
11 C	2.6248566 *	1.4658779 *	2.4964489 *	2.8597611 *
12 N	3.0933422	2.5299250 *	3.8359929	4.3083971
13 C	4.3577387	3.7347496	4.9332214	5.1539324
14 C	5.4174122	5.0295256	6.3094166	6.5869285
15 C	5.6485368	5.5588761	6.9296761	7.4037539
16 C	6.9914178	6.9617835	8.3341719	8.7865321
17 C	8.0052548	7.8195774	9.1419702	9.4341290
18 C	7.8807664	7.4917932	8.7239753	8.8508924
19 C	6.7037796	6.1982375	7.3828748	7.4721948
20 O	4.7665053	4.9344827	6.3293102	7.0200970
21 N	1.5101364 *	2.5938454 *	3.8889132	5.1136212
22 H	3.9446496	3.5205045	2.1968343 *	2.6794759 *
23 H	3.4666374	4.0265154	3.4862747	4.6702289
24 H	2.1831360 *	3.5069101	3.9524412	5.3957240
25 H	4.6737571	3.5190568	2.1981450 *	1.1050030 *
26 H	5.4705305	4.0187932	3.4843715	2.1851267 *
27 H	4.8028178	3.5049655	3.9489555	3.4292401
28 H	4.8961218	4.0400961	5.0223801	4.9777235
29 H	7.4113684	7.5420897	8.9334284	9.4890291
30 H	9.0422640	8.9032932	10.2340632	10.5304036
31 H	8.8448780	8.3849125	9.5604004	9.5836289
32 H	6.9135187	6.2358329	7.2843091	7.2027870
33 H	5.4387313	5.7302646	7.0995012	7.8364234
34 H	2.1114561 *	2.9624867 *	4.2472988	5.3777788
35 H	2.0883923 *	3.4240631	4.5637864	5.8904064

	C	C	C	N
--	---	---	---	---

1 CO	5.3085645	4.1673735	2.8987630 *	1.9400764 *
2 C	3.7779631	4.2904714	3.8350483	5.0525998
3 C	4.9549686	5.1829501	4.3831154	5.3239733

4 C	5.1794171	5.0055631	3.8925219	4.4923454
5 C	4.3662423	3.8862657	2.6248566 *	3.0933422
6 C	2.9145453 *	2.5037087 *	1.4658779 *	2.5299250 *
7 C	2.4781413 *	2.8476101 *	2.4964489 *	3.8359929
8 C	1.4017360 *	2.4436417 *	2.8597611 *	4.3083971
9 C	0.0000000	1.4296185 *	2.4840090 *	3.7965640
10 C	1.4296185 *	0.0000000	1.4149383 *	2.4708687 *
11 C	2.4840090 *	1.4149383 *	0.0000000	1.4545366 *
12 N	3.7965640	2.4708687 *	1.4545366 *	0.0000000
13 C	4.3426309	2.9196450 *	2.4449297 *	1.3321363 *
14 C	5.7526390	4.3241107	3.8342250	2.5080353 *
15 C	6.7224451	5.3105368	4.5897113	3.1513560
16 C	8.0516674	6.6348740	5.9858175	4.5524062
17 C	8.5437872	7.1271802	6.6880658	5.3107480
18 C	7.8442067	6.4631975	6.2305905	4.9861194
19 C	6.4683416	5.0908784	4.8966828	3.7425211
20 O	6.5855034	5.2670371	4.2867334	2.9380038 *
21 N	5.3907590	4.5665052	3.1568084	2.9009262 *
22 H	4.0787721	4.8911206	4.6924719	6.0010744
23 H	5.9307842	6.2566751	5.4869448	6.4052844
24 H	6.2671346	6.0067926	4.8015404	5.1748513
25 H	2.1800231 *	3.4519575	3.9646285	5.4123329
26 H	1.1044163 *	2.1975888 *	3.4755433	4.6668480
27 H	2.1793734 *	1.1038841 *	2.1885191 *	2.6911138 *
28 H	3.9832626	2.6479298 *	2.6552307 *	2.0953970 *
29 H	8.8470437	7.4524385	6.7022137	5.2719004
30 H	9.6284965	8.2166453	7.7869664	6.4027492
31 H	8.4991025	7.1692746	7.0769233	5.9182120
32 H	6.1032281	4.8199608	4.8719624	3.9704852
33 H	7.4477365	6.1623551	5.1828708	3.8873322
34 H	5.5601737	4.6865255	3.3348638	3.0046714
35 H	6.3044559	5.5568990	4.1532117	3.8888199

C C C C

1 CO	2.8615304 *	3.2643977	3.0128647	4.2843978
2 C	6.2333407	7.5566214	8.0435033	9.4372806
3 C	6.5872714	7.7775146	8.0619851	9.4126795
4 C	5.7645014	6.8080944	6.9534593	8.2598743
5 C	4.3577387	5.4174122	5.6485368	6.9914178
6 C	3.7347496	5.0295256	5.5588761	6.9617835
7 C	4.9332214	6.3094166	6.9296761	8.3341719
8 C	5.1539324	6.5869285	7.4037539	8.7865321
9 C	4.3426309	5.7526390	6.7224451	8.0516674
10 C	2.9196450 *	4.3241107	5.3105368	6.6348740
11 C	2.4449297 *	3.8342250	4.5897113	5.9858175

12 N	1.3321363 *	2.5080353 *	3.1513560	4.5524062
13 C	0.0000000	1.4664964 *	2.6055319 *	3.8835493
14 C	1.4664964 *	0.0000000	1.4378033 *	2.5003741 *
15 C	2.6055319 *	1.4378033 *	0.0000000	1.4065301 *
16 C	3.8835493	2.5003741 *	1.4065301 *	0.0000000
17 C	4.3419964	2.8807564 *	2.4410968 *	1.4285828 *
18 C	3.7921772	2.4975465 *	2.8260374 *	2.4735747 *
19 C	2.4689558 *	1.4428752 *	2.4464951 *	2.8459155 *
20 O	3.0464595	2.5026265 *	1.4662034 *	2.4614523 *
21 N	3.9953019	4.7225152	4.7113312	5.9528711
22 H	7.1277195	8.4926421	9.0411748	10.4393746
23 H	7.6756883	8.8392453	9.0636971	10.3916821
24 H	6.4156545	7.3085190	7.2841895	8.5071834
25 H	6.2396010	7.6736413	8.4984072	9.8770995
26 H	5.0007246	6.3461741	7.4028594	8.6697981
27 H	2.6365939 *	3.8847334	5.0017995	6.2191155
28 H	1.1080573 *	2.1763006 *	3.5319972	4.6729302
29 H	4.7963589	3.5037025	2.1956974 *	1.1068303 *
30 H	5.4466169	3.9856953	3.4394934	2.1917367 *
31 H	4.6559393	3.4933162	3.9304710	3.4760140
32 H	2.6405731 *	2.1980147 *	3.4513765	3.9517121
33 H	4.0130290	3.3291982	2.0460405 *	2.5122024 *
34 H	3.8660553	4.5747405	4.7191747	5.9248109
35 H	4.9571873	5.5420982	5.3291428	6.4585420

C C C O

1 CO	5.4435660	5.6126269	4.6985600	1.9526081 *
2 C	10.3414361	10.0116052	8.6970918	7.2727142
3 C	10.4340321	10.2583550	9.0197257	7.1200599
4 C	9.3331361	9.2641530	8.1051518	5.9506312
5 C	8.0052548	7.8807664	6.7037796	4.7665053
6 C	7.8195774	7.4917932	6.1982375	4.9344827
7 C	9.1419702	8.7239753	7.3828748	6.3293102
8 C	9.4341290	8.8508924	7.4721948	7.0200970
9 C	8.5437872	7.8442067	6.4683416	6.5855034
10 C	7.1271802	6.4631975	5.0908784	5.2670371
11 C	6.6880658	6.2305905	4.8966828	4.2867334
12 N	5.3107480	4.9861194	3.7425211	2.9380038 *
13 C	4.3419964	3.7921772	2.4689558 *	3.0464595
14 C	2.8807564 *	2.4975465 *	1.4428752 *	2.5026265 *
15 C	2.4410968 *	2.8260374 *	2.4464951 *	1.4662034 *
16 C	1.4285828 *	2.4735747 *	2.8459155 *	2.4614523 *
17 C	0.0000000	1.4229482 *	2.4547297 *	3.7719973
18 C	1.4229482 *	0.0000000	1.4157446 *	4.2920696
19 C	2.4547297 *	1.4157446 *	0.0000000	3.7956881

20	O	3.7719973	4.2920696	3.7956881	0.0000000
21	N	7.0291127	7.0667411	6.0435525	3.7691777
22	H	11.3065852	10.9187833	9.5781462	8.3058692
23	H	11.4520628	11.3184957	10.0968235	8.0558580
24	H	9.6484917	9.7034264	8.6343562	6.1803575
25	H	10.5131569	9.9031361	8.5208434	8.0956129
26	H	9.0326982	8.2286500	6.8795221	7.4030368
27	H	6.5350364	5.7586059	4.4172664	5.2309169
28	H	4.8508365	3.9957321	2.5811007 *	4.1399594
29	H	2.1998370 *	3.4737260	3.9527074	2.6907720 *
30	H	1.1049790 *	2.1997279 *	3.4595019	4.6512914
31	H	2.1984882 *	1.1044353 *	2.1873240 *	5.3964936
32	H	3.4559948	2.1853425 *	1.1058190 *	4.6926343
33	H	3.9324904	4.7329995	4.4877534	0.9918417 *
34	H	6.8651801	6.7937805	5.7616572	4.0347706
35	H	7.6192628	7.7985291	6.8762771	4.2372441

N H H H

1	CO	1.9784481 *	6.4428583	6.1228023	4.3414672
2	C	4.3441330	1.1051502 *	2.1866618 *	3.4386207
3	C	3.8160743	2.1797916 *	1.1042158 *	2.1934286 *
4	C	2.4753957 *	3.4516741	2.2011511 *	1.1077065 *
5	C	1.5101364 *	3.9446496	3.4666374	2.1831360 *
6	C	2.5938454 *	3.5205045	4.0265154	3.5069101
7	C	3.8889132	2.1968343 *	3.4862747	3.9524412
8	C	5.1136212	2.6794759 *	4.6702289	5.3957240
9	C	5.3907590	4.0787721	5.9307842	6.2671346
10	C	4.5665052	4.8911206	6.2566751	6.0067926
11	C	3.1568084	4.6924719	5.4869448	4.8015404
12	N	2.9009262 *	6.0010744	6.4052844	5.1748513
13	C	3.9953019	7.1277195	7.6756883	6.4156545
14	C	4.7225152	8.4926421	8.8392453	7.3085190
15	C	4.7113312	9.0411748	9.0636971	7.2841895
16	C	5.9528711	10.4393746	10.3916821	8.5071834
17	C	7.0291127	11.3065852	11.4520628	9.6484917
18	C	7.0667411	10.9187833	11.3184957	9.7034264
19	C	6.0435525	9.5781462	10.0968235	8.6343562
20	O	3.7691777	8.3058692	8.0558580	6.1803575
21	N	0.0000000	5.4483701	4.6756111	2.6539819 *
22	H	5.4483701	0.0000000	2.5306160 *	4.3595302
23	H	4.6756111	2.5306160 *	0.0000000	2.5172737 *
24	H	2.6539819 *	4.3595302	2.5172737 *	0.0000000
25	H	6.0593819	2.4004295 *	4.7814048	5.9759540
26	H	6.4745383	4.7773966	6.8515170	7.3483514
27	H	5.2600290	5.9652367	7.3459791	6.9658106

28 H	4.7468484	7.1903160	8.0322556	7.0189258
29 H	6.2854794	10.9665380	10.7204298	8.7220771
30 H	8.0099915	12.3921878	12.4824516	10.6131409
31 H	8.0689300	11.7548677	12.2630763	10.7022917
32 H	6.4300256	9.4554618	10.1973684	8.9332239
33 H	4.3888812	8.9896076	8.5811254	6.6231173
34 H	1.0438984 *	5.8549066	5.1808950	3.2175763
35 H	1.0394576 *	5.8209070	4.5838618	2.2126320 *

H H H H

1 CO	6.5002983	6.2801676	4.5254826	3.8776254
2 C	2.6817155 *	4.6683402	5.3902775	6.3979350
3 C	4.0809943	5.9298325	6.2663296	6.9332691
4 C	4.8915016	6.2533649	6.0074836	6.2722874
5 C	4.6737571	5.4705305	4.8028178	4.8961218
6 C	3.5190568	4.0187932	3.5049655	4.0400961
7 C	2.1981450 *	3.4843715	3.9489555	5.0223801
8 C	1.1050030 *	2.1851267 *	3.4292401	4.9777235
9 C	2.1800231 *	1.1044163 *	2.1793734 *	3.9832626
10 C	3.4519575	2.1975888 *	1.1038841 *	2.6479298 *
11 C	3.9646285	3.4755433	2.1885191 *	2.6552307 *
12 N	5.4123329	4.6668480	2.6911138 *	2.0953970 *
13 C	6.2396010	5.0007246	2.6365939 *	1.1080573 *
14 C	7.6736413	6.3461741	3.8847334	2.1763006 *
15 C	8.4984072	7.4028594	5.0017995	3.5319972
16 C	9.8770995	8.6697981	6.2191155	4.6729302
17 C	10.5131569	9.0326982	6.5350364	4.8508365
18 C	9.9031361	8.2286500	5.7586059	3.9957321
19 C	8.5208434	6.8795221	4.4172664	2.5811007 *
20 O	8.0956129	7.4030368	5.2309169	4.1399594
21 N	6.0593819	6.4745383	5.2600290	4.7468484
22 H	2.4004295 *	4.7773966	5.9652367	7.1903160
23 H	4.7814048	6.8515170	7.3459791	8.0322556
24 H	5.9759540	7.3483514	6.9658106	7.0189258
25 H	0.0000000	2.5277715 *	4.3457844	6.0068832
26 H	2.5277715 *	0.0000000	2.4980491 *	4.4715333
27 H	4.3457844	2.4980491 *	0.0000000	2.1377399 *
28 H	6.0068832	4.4715333	2.1377399 *	0.0000000
29 H	10.5739148	9.5125040	7.1123720	5.6711122
30 H	11.6071028	10.0923635	7.5970107	5.9301924
31 H	10.6059174	8.7790175	6.3771585	4.6537083
32 H	8.2008223	6.3908599	4.0507099	2.2657419 *
33 H	8.8906315	8.2611265	6.1219917	5.0957948
34 H	6.3362418	6.6109382	5.3154099	4.5023081
35 H	6.7617460	7.4007767	6.2748779	5.7548227

	H	H	H	H
1 CO	4.6232814	6.4235255	6.6782446	5.2818263
2 C	9.9420715	11.4201419	10.8827164	8.6483371
3 C	9.7971441	11.4788817	11.1926424	9.1062906
4 C	8.5881065	10.3479099	10.2366944	8.3127396
5 C	7.4113684	9.0422640	8.8448780	6.9135187
6 C	7.5420897	8.9032932	8.3849125	6.2358329
7 C	8.9334284	10.2340632	9.5604004	7.2843091
8 C	9.4890291	10.5304036	9.5836289	7.2027870
9 C	8.8470437	9.6284965	8.4991025	6.1032281
10 C	7.4524385	8.2166453	7.1692746	4.8199608
11 C	6.7022137	7.7869664	7.0769233	4.8719624
12 N	5.2719004	6.4027492	5.9182120	3.9704852
13 C	4.7963589	5.4466169	4.6559393	2.6405731 *
14 C	3.5037025	3.9856953	3.4933162	2.1980147 *
15 C	2.1956974 *	3.4394934	3.9304710	3.4513765
16 C	1.1068303 *	2.1917367 *	3.4760140	3.9517121
17 C	2.1998370 *	1.1049790 *	2.1984882 *	3.4559948
18 C	3.4737260	2.1997279 *	1.1044353 *	2.1853425 *
19 C	3.9527074	3.4595019	2.1873240 *	1.1058190 *
20 O	2.6907720 *	4.6512914	5.3964936	4.6926343
21 N	6.2854794	8.0099915	8.0689300	6.4300256
22 H	10.9665380	12.3921878	11.7548677	9.4554618
23 H	10.7204298	12.4824516	12.2630763	10.1973684
24 H	8.7220771	10.6131409	10.7022917	8.9332239
25 H	10.5739148	11.6071028	10.6059174	8.2008223
26 H	9.5125040	10.0923635	8.7790175	6.3908599
27 H	7.1123720	7.5970107	6.3771585	4.0507099
28 H	5.6711122	5.9301924	4.6537083	2.2657419 *
29 H	0.0000000	2.5189131 *	4.3873105	5.0584999
30 H	2.5189131 *	0.0000000	2.5409909 *	4.3728513
31 H	4.3873105	2.5409909 *	0.0000000	2.5137066 *
32 H	5.0584999	4.3728513	2.5137066 *	0.0000000
33 H	2.3147331 *	4.6345859	5.8193606	5.4662645
34 H	6.3503765	7.8457388	7.7339896	6.0717800
35 H	6.6370468	8.5368303	8.8212191	7.3384727

	H	H	H
1 CO	2.6573762 *	2.4994870 *	2.6219072 *
2 C	7.9559788	4.7775703	4.7377873
3 C	7.7071959	4.3271038	3.9168002
4 C	6.5077685	3.0603122	2.4852286 *
5 C	5.4387313	2.1114561 *	2.0883923 *

6 C	5.7302646	2.9624867 *	3.4240631
7 C	7.0995012	4.2472988	4.5637864
8 C	7.8364234	5.3777788	5.8904064
9 C	7.4477365	5.5601737	6.3044559
10 C	6.1623551	4.6865255	5.5568990
11 C	5.1828708	3.3348638	4.1532117
12 N	3.8873322	3.0046714	3.8888199
13 C	4.0130290	3.8660553	4.9571873
14 C	3.3291982	4.5747405	5.5420982
15 C	2.0460405 *	4.7191747	5.3291428
16 C	2.5122024 *	5.9248109	6.4585420
17 C	3.9324904	6.8651801	7.6192628
18 C	4.7329995	6.7937805	7.7985291
19 C	4.4877534	5.7616572	6.8762771
20 O	0.9918417 *	4.0347706	4.2372441
21 N	4.3888812	1.0438984 *	1.0394576 *
22 H	8.9896076	5.8549066	5.8209070
23 H	8.5811254	5.1808950	4.5838618
24 H	6.6231173	3.2175763	2.2126320 *
25 H	8.8906315	6.3362418	6.7617460
26 H	8.2611265	6.6109382	7.4007767
27 H	6.1219917	5.3154099	6.2748779
28 H	5.0957948	4.5023081	5.7548227
29 H	2.3147331 *	6.3503765	6.6370468
30 H	4.6345859	7.8457388	8.5368303
31 H	5.8193606	7.7339896	8.8212191
32 H	5.4662645	6.0717800	7.3384727
33 H	0.0000000	4.7381781	4.6707416
34 H	4.7381781	0.0000000	1.6665151 *
35 H	4.6707416	1.6665151 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.79 , TOTAL = 7552.0 SECONDS (125.9 MIN)

WALL CLOCK TIME: STEP = 0.79 , TOTAL = 6981.7 SECONDS (116.4 MIN)

CPU UTILIZATION: STEP = 99.58% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.07 , TOTAL = 7553.0 SECONDS (125.9 MIN)

WALL CLOCK TIME: STEP = 1.08 , TOTAL = 6982.7 SECONDS (116.4 MIN)

CPU UTILIZATION: STEP = 99.38%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636884233	-284.636884233	0.003380373	0.000595926	198009345
11338532						
2	1	-284.636905492	-0.000021259	0.001592963	0.000053254	149495498
15427997						
3	2	-284.636905227	0.000000265	0.000876038	0.000137023	135427663
16543630						
4	3	-284.636905800	-0.000000573	0.000292693	0.000020454	130458976
16939816						
5	4	-284.636905767	0.000000033	0.000143314	0.000038363	123401298
17429545						
6	5	-284.636905830	-0.000000063	0.000084276	0.000012448	116745870
17908093						
7	6	-284.636905848	-0.000000018	0.000067002	0.000023331	112246889
18262827						
8	7	-284.636905863	-0.000000015	0.000056026	0.000008257	105452851
18747074						
9	8	-284.636905877	-0.000000014	0.000133541	0.000008227	103205949
18962830						
10	9	-284.636905881	-0.000000004	0.000257350	0.000008035	130923448
17008157						
11	10	-284.636905891	-0.000000010	0.000136914	0.000007422	156947848
15005368						
12	11	-284.636905893	-0.000000002	0.000038328	0.000006698	155803602
15013024						
13	12	-284.636905895	-0.000000002	0.000044109	0.000004858	148851778
15538715						

-----DISABLING FDIFF OPTION-----

14	13	-284.636905867	0.000000028	0.000053142	0.000002842	198008201
11338704						
15	14	-284.636905868	-0.000000001	0.000017559	0.000001248	198008203
11338704						
16	15	-284.636905868	0.000000000	0.000008307	0.000000715	198008228
11338697						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 52.9 SECONDS (3.3 SEC/ITER)

OF THE ABOVE TIME, DFT PART= 17.5 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 1.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369058678 AFTER 16 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6006656957
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998546383

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 55.78 , TOTAL = 7608.8 SECONDS (126.8 MIN)
WALL CLOCK TIME: STEP = 51.31 , TOTAL = 7034.0 SECONDS (117.2
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.85 , TOTAL = 7612.7 SECONDS (126.9 MIN)
WALL CLOCK TIME: STEP = 3.83 , TOTAL = 7037.9 SECONDS (117.3
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.87 , TOTAL = 7615.5 SECONDS (126.9 MIN)
WALL CLOCK TIME: STEP = 2.67 , TOTAL = 7040.5 SECONDS (117.3
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 81 ENERGY= -284.6369059

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000379	-0.0001010	-0.0001048
2 C	6.0	0.0000953	0.0000062	-0.0000394
3 C	6.0	0.0000135	0.0001711	-0.0000143
4 C	6.0	-0.0000002	-0.0000100	-0.0001209
5 C	6.0	-0.0000166	-0.0000218	-0.0001391
6 C	6.0	0.0000033	-0.0002160	-0.0000600
7 C	6.0	-0.0000059	0.0000678	-0.0000509
8 C	6.0	0.0000945	0.0000467	-0.0000924
9 C	6.0	-0.0000836	0.0001285	0.0001590
10 C	6.0	0.0000543	-0.0000908	0.0001634
11 C	6.0	0.0000167	-0.0000624	0.0000605
12 N	7.0	-0.0001045	-0.0002237	-0.0003200
13 C	6.0	-0.0001346	0.0001268	-0.0000301
14 C	6.0	0.0000147	-0.0000654	0.0000267
15 C	6.0	-0.0000113	-0.0001482	0.0000688
16 C	6.0	0.0000112	-0.0000438	-0.0000790
17 C	6.0	0.0000864	0.0001606	0.0001442
18 C	6.0	-0.0000563	-0.0001054	0.0000845
19 C	6.0	-0.0001324	0.0001076	0.0000194
20 O	8.0	0.0000913	-0.0001127	-0.0001887
21 N	7.0	-0.0000137	-0.0001500	-0.0000963
22 H	1.0	0.0000428	0.0000396	0.0000447
23 H	1.0	0.0000381	-0.0000285	0.0001071
24 H	1.0	0.0000933	0.0000554	0.0001806
25 H	1.0	-0.0001270	0.0001340	0.0000733
26 H	1.0	-0.0000469	0.0000728	0.0001456
27 H	1.0	0.0001367	0.0000542	-0.0003271
28 H	1.0	0.0001575	-0.0000457	0.0001322
29 H	1.0	-0.0002149	0.0000565	0.0000895
30 H	1.0	0.0001142	0.0001350	0.0000117
31 H	1.0	-0.0000724	0.0001784	-0.0001207
32 H	1.0	-0.0001186	-0.0000288	0.0000582
33 H	1.0	0.0000242	0.0000645	0.0000872
34 H	1.0	-0.0000181	-0.0001427	0.0001737
35 H	1.0	0.0001073	-0.0000088	-0.0000467

MAXIMUM GRADIENT = 0.0003271 RMS GRADIENT = 0.0001088

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0000056477

PREDICTED ENERGY CHANGE WAS -0.0000042090 RATIO= 1.342

GDIIS STEP HAS LENGTH = 0.026867

RADIUS OF STEP TAKEN= 0.02687 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 7615.6 SECONDS (126.9 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7040.6 SECONDS (117.3 MIN)
 CPU UTILIZATION: STEP = 83.65% , TOTAL = 100.00%

INSERCH= 82

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1560321138	-1.7357863384	0.8602439626
C	6.0	4.9813858767	0.6278336706	0.5634740673
C	6.0	5.1864251483	-0.7117268461	0.2061255918
C	6.0	4.0513608276	-1.5332480418	-0.0894868523
C	6.0	2.7424111634	-1.0227404913	-0.0045693387
C	6.0	2.4695591815	0.3428373041	0.4263388387
C	6.0	3.6506266032	1.1770937836	0.6785450106
C	6.0	3.5022619630	2.5628361928	1.0580842091
C	6.0	2.2335726648	3.1365085634	1.2196831762
C	6.0	1.0694210677	2.3270148291	1.0346906004
C	6.0	1.1626600464	0.9735852937	0.6331744402
N	7.0	-0.0497161638	0.1724530575	0.5769808473
C	6.0	-1.2461900830	0.6979576159	0.3186892203
C	6.0	-2.5503733103	0.0375146751	0.4352731068
C	6.0	-2.8216970840	-1.2857925278	0.9275791584
C	6.0	-4.1225837378	-1.8042575251	1.0583798158
C	6.0	-5.2318993998	-0.9860749785	0.6835342819
C	6.0	-5.0177472906	0.3271764144	0.1792527653
C	6.0	-3.6984288445	0.8271574724	0.0612302223
O	8.0	-1.6984471462	-2.1455706921	1.3128955047
N	7.0	1.6374986025	-1.9597159093	-0.4318551912
H	1.0	5.8422285378	1.2895806303	0.7684335985
H	1.0	6.2044295656	-1.1326731911	0.1296295935
H	1.0	4.2173509956	-2.5782515095	-0.4183226512
H	1.0	4.4139875874	3.1624993781	1.2332648590
H	1.0	2.1231678305	4.1914760451	1.5265783330
H	1.0	0.0843771478	2.7719626487	1.2595627666
H	1.0	-1.2902639404	1.7511583030	-0.0230872023
H	1.0	-4.2984459744	-2.8272419471	1.4422407684
H	1.0	-6.2566643247	-1.3861900829	0.7868647340
H	1.0	-5.8752541630	0.9589403832	-0.1124589309
H	1.0	-3.5345500363	1.8526977014	-0.3188975750
H	1.0	-2.0132640909	-2.9553646473	1.7913345414

H 1.0 1.2777886141 -1.6879784482 -1.3736554082
H 1.0 2.0349770517 -2.9145657863 -0.5368638639

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3813391	5.1750771	4.0145481
2 C	5.3813391	0.0000000	1.4014854 *	2.4416344 *
3 C	5.1750771	1.4014854 *	0.0000000	1.4320108 *
4 C	4.0145481	2.4416344 *	1.4320108 *	0.0000000
5 C	2.8188106 *	2.8390273 *	2.4727164 *	1.4075433 *
6 C	3.1402798	2.5316600 *	2.9226632 *	2.5075623 *
7 C	4.5530293	1.4442466 *	2.4798187 *	2.8454198 *
8 C	5.4511055	2.4852930 *	3.7795505	4.2890949
9 C	5.3089197	3.7781659	4.9553559	5.1792767
10 C	4.1678609	4.2910057	5.1836467	5.0057336
11 C	2.8992335 *	3.8349797	4.3833016	3.8924343
12 N	1.9400897 *	5.0516870	5.3232024	4.4913726
13 C	2.8605276 *	6.2327794	6.5862295	5.7627192
14 C	3.2634073	7.5559452	7.7763695	6.8062884
15 C	3.0122914	8.0425519	8.0610215	6.9523077
16 C	4.2837483	9.4362207	9.4115677	8.2585964
17 C	5.4427107	10.3407114	10.4328650	9.3314458
18 C	5.6113775	10.0110282	10.2569575	9.2618639
19 C	4.6972304	8.6966179	9.0183031	8.1026829
20 O	1.9524113 *	7.2714217	7.1191512	5.9499502
21 N	1.9784862 *	4.3436937	3.8156750	2.4750397 *
22 H	6.4415917	1.1049740 *	2.1797936 *	3.4513181
23 H	6.1221446	2.1871080 *	1.1042556 *	2.2009492 *
24 H	4.3403676	3.4389906	2.1938447 *	1.1080244 *
25 H	6.5009640	2.6823666 *	4.0818260	4.8919540
26 H	6.2806101	4.6686751	5.9303069	6.2531641
27 H	4.5259685	5.3909668	6.2671139	6.0076396
28 H	3.8769613	6.3983985	6.9329534	6.2709401
29 H	4.6230261	9.9410793	9.7962322	8.5871930
30 H	6.4226379	11.4192805	11.4776503	10.3462554
31 H	6.6771339	10.8826996	11.1916654	10.2347064
32 H	5.2809080	8.6487014	9.1053463	8.3104333
33 H	2.6570937 *	7.9543749	7.7059927	6.5068871
34 H	2.5001859 *	4.7782935	4.3273797	3.0603485
35 H	2.6214243 *	4.7371576	3.9161407	2.4847512 *

C C C C

1 CO	2.8188106 *	3.1402798	4.5530293	5.4511055
2 C	2.8390273 *	2.5316600 *	1.4442466 *	2.4852930 *
3 C	2.4727164 *	2.9226632 *	2.4798187 *	3.7795505
4 C	1.4075433 *	2.5075623 *	2.8454198 *	4.2890949
5 C	0.0000000	1.4577149 *	2.4760394 *	3.8161454
6 C	1.4577149 *	0.0000000	1.4678256 *	2.5286305 *
7 C	2.4760394 *	1.4678256 *	0.0000000	1.4444183 *
8 C	3.8161454	2.5286305 *	1.4444183 *	0.0000000
9 C	4.3654397	2.9137062 *	2.4779384 *	1.4017085 *
10 C	3.8858484	2.5034854 *	2.8481187 *	2.4443555 *
11 C	2.6244328 *	1.4658135 *	2.4966882 *	2.8600706 *
12 N	3.0923556	2.5295201 *	3.8356427	4.3083571
13 C	4.3559428	3.7342324	4.9333438	5.1548302
14 C	5.4158259	5.0292170	6.3095342	6.5878324
15 C	5.6477781	5.5588731	6.9295599	7.4041497
16 C	6.9906212	6.9617412	8.3339984	8.7869096
17 C	8.0040277	7.8195026	9.1421328	9.4350746
18 C	7.8788404	7.4913987	8.7242397	8.8521792
19 C	6.7015574	6.1977372	7.3832343	7.4737037
20 O	4.7663071	4.9346159	6.3289090	7.0200712
21 N	1.5104065 *	2.5943348 *	3.8891192	5.1137794
22 H	3.9437584	3.5196946	2.1963270 *	2.6796494 *
23 H	3.4663621	4.0267138	3.4868670	4.6712447
24 H	2.1831752 *	3.5072766	3.9530891	5.3964722
25 H	4.6736104	3.5188671	2.1982424 *	1.1052275 *
26 H	5.4695456	4.0177773	3.4840768	2.1849154 *
27 H	4.8023897	3.5048545	3.9495979	3.4301988
28 H	4.8946221	4.0400027	5.0233691	4.9795640
29 H	7.4110157	7.5423705	8.9334031	9.4895502
30 H	9.0411185	8.9031731	10.2340887	10.5311448
31 H	8.8432378	8.3848551	9.5611549	9.5854297
32 H	6.9113811	6.2357344	7.2854716	7.2053521
33 H	5.4384514	5.7303625	7.0989556	7.8364038
34 H	2.1123583 *	2.9638672 *	4.2485910	5.3787605
35 H	2.0887325 *	3.4245140	4.5639041	5.8905617

C C C N

1 CO	5.3089197	4.1678609	2.8992335 *	1.9400897 *
2 C	3.7781659	4.2910057	3.8349797	5.0516870
3 C	4.9553559	5.1836467	4.3833016	5.3232024
4 C	5.1792767	5.0057336	3.8924343	4.4913726
5 C	4.3654397	3.8858484	2.6244328 *	3.0923556
6 C	2.9137062 *	2.5034854 *	1.4658135 *	2.5295201 *
7 C	2.4779384 *	2.8481187 *	2.4966882 *	3.8356427
8 C	1.4017085 *	2.4443555 *	2.8600706 *	4.3083571

9 C	0.0000000	1.4299480 *	2.4837640 *	3.7963271
10 C	1.4299480 *	0.0000000	1.4148075 *	2.4706483 *
11 C	2.4837640 *	1.4148075 *	0.0000000	1.4542444 *
12 N	3.7963271	2.4706483 *	1.4542444 *	0.0000000
13 C	4.3436240	2.9203665 *	2.4448784 *	1.3320734 *
14 C	5.7537120	4.3248149	3.8343200	2.5083013 *
15 C	6.7229327	5.3108051	4.5898327	3.1517103
16 C	8.0521992	6.6351252	5.9859011	4.5527332
17 C	8.5449648	7.1278689	6.6882879	5.3111735
18 C	7.8457940	6.4641122	6.2306761	4.9863273
19 C	6.4702208	5.0921106	4.8968098	3.7426917
20 O	6.5855774	5.2671163	4.2868507	2.9382169 *
21 N	5.3902122	4.5661285	3.1565829	2.9001014 *
22 H	4.0788682	4.8915083	4.6921753	5.9999700
23 H	5.9314277	6.2575466	5.4871962	6.4045153
24 H	6.2671303	6.0068584	4.8012840	5.1734772
25 H	2.1806121 *	3.4530554	3.9651714	5.4125536
26 H	1.1042329 *	2.1973965 *	3.4749916	4.6664447
27 H	2.1802581 *	1.1040188 *	2.1884281 *	2.6909755 *
28 H	3.9851095	2.6492674 *	2.6555857 *	2.0955550 *
29 H	8.8477748	7.4529495	6.7025782	5.2724330
30 H	9.6294475	8.2171063	7.7870748	6.4030950
31 H	8.5011457	7.1705016	7.0773173	5.9186808
32 H	6.1062788	4.8222119	4.8726853	3.9711317
33 H	7.4480418	6.1627097	5.1830953	3.8875981
34 H	5.5600902	4.6865465	3.3353474	3.0047389
35 H	6.3039986	5.5566401	4.1530285	3.8879662

C C C C

1 CO	2.8605276 *	3.2634073	3.0122914	4.2837483
2 C	6.2327794	7.5559452	8.0425519	9.4362207
3 C	6.5862295	7.7763695	8.0610215	9.4115677
4 C	5.7627192	6.8062884	6.9523077	8.2585964
5 C	4.3559428	5.4158259	5.6477781	6.9906212
6 C	3.7342324	5.0292170	5.5588731	6.9617412
7 C	4.9333438	6.3095342	6.9295599	8.3339984
8 C	5.1548302	6.5878324	7.4041497	8.7869096
9 C	4.3436240	5.7537120	6.7229327	8.0521992
10 C	2.9203665 *	4.3248149	5.3108051	6.6351252
11 C	2.4448784 *	3.8343200	4.5898327	5.9859011
12 N	1.3320734 *	2.5083013 *	3.1517103	4.5527332
13 C	0.0000000	1.4665165 *	2.6054239 *	3.8835375
14 C	1.4665165 *	0.0000000	1.4377496 *	2.5004464 *
15 C	2.6054239 *	1.4377496 *	0.0000000	1.4064924 *
16 C	3.8835375	2.5004464 *	1.4064924 *	0.0000000

17 C	4.3422294	2.8809637 *	2.4409965 *	1.4284653 *
18 C	3.7923034	2.4974757 *	2.8256500 *	2.4732959 *
19 C	2.4690996 *	1.4427319 *	2.4461759 *	2.8457968 *
20 O	3.0460853	2.5023711 *	1.4660756 *	2.4612418 *
21 N	3.9927692	4.7200755	4.7102718	5.9517658
22 H	7.1272692	8.4920216	9.0399934	10.4380739
23 H	7.6745479	8.8379483	9.0626228	10.3904190
24 H	6.4130347	7.3056793	7.2821769	8.5049532
25 H	6.2408354	7.6749360	8.4991692	9.8778697
26 H	5.0016237	6.3473088	7.4034424	8.6704927
27 H	2.6376408 *	3.8856877	5.0020853	6.2193879
28 H	1.1081450 *	2.1759008 *	3.5315895	4.6725355
29 H	4.7964222	3.5037940	2.1958438 *	1.1066950 *
30 H	5.4468075	3.9858682	3.4393139	2.1915293 *
31 H	4.6564187	3.4934036	3.9299766	3.4753388
32 H	2.6413127 *	2.1982417 *	3.4513743	3.9517083
33 H	4.0129603	3.3293716	2.0462425 *	2.5122698 *
34 H	3.8635721	4.5721300	4.7183914	5.9238786
35 H	4.9546296	5.5394284	5.3277368	6.4570227

C C C O

1 CO	5.4427107	5.6113775	4.6972304	1.9524113 *
2 C	10.3407114	10.0110282	8.6966179	7.2714217
3 C	10.4328650	10.2569575	9.0183031	7.1191512
4 C	9.3314458	9.2618639	8.1026829	5.9499502
5 C	8.0040277	7.8788404	6.7015574	4.7663071
6 C	7.8195026	7.4913987	6.1977372	4.9346159
7 C	9.1421328	8.7242397	7.3832343	6.3289090
8 C	9.4350746	8.8521792	7.4737037	7.0200712
9 C	8.5449648	7.8457940	6.4702208	6.5855774
10 C	7.1278689	6.4641122	5.0921106	5.2671163
11 C	6.6882879	6.2306761	4.8968098	4.2868507
12 N	5.3111735	4.9863273	3.7426917	2.9382169 *
13 C	4.3422294	3.7923034	2.4690996 *	3.0460853
14 C	2.8809637 *	2.4974757 *	1.4427319 *	2.5023711 *
15 C	2.4409965 *	2.8256500 *	2.4461759 *	1.4660756 *
16 C	1.4284653 *	2.4732959 *	2.8457968 *	2.4612418 *
17 C	0.0000000	1.4229512 *	2.4549147 *	3.7717119
18 C	1.4229512 *	0.0000000	1.4158077 *	4.2915472
19 C	2.4549147 *	1.4158077 *	0.0000000	3.7952214
20 O	3.7717119	4.2915472	3.7952214	0.0000000
21 N	7.0271402	7.0636837	6.0400263	3.7692481
22 H	11.3058448	10.9184445	9.5780016	8.3041251
23 H	11.4506734	11.3168404	10.0951582	8.0549078
24 H	9.6455921	9.6997757	8.6305476	6.1790773

25 H	10.5145617	9.9049291	8.5228392	8.0959130
26 H	9.0340894	8.2304779	6.8816330	7.4032805
27 H	6.5358589	5.7598371	4.4190371	5.2310076
28 H	4.8505928	3.9953470	2.5807257 *	4.1395604
29 H	2.1992878 *	3.4731669	3.9524481	2.6909849 *
30 H	1.1049491 *	2.1999392 *	3.4597719	4.6508828
31 H	2.1978615 *	1.1043276 *	2.1877164 *	5.3958633
32 H	3.4560808	2.1852330 *	1.1059323 *	4.6925657
33 H	3.9325483	4.7329486	4.4878185	0.9918568 *
34 H	6.8629976	6.7901506	5.7573905	4.0354586
35 H	7.6168197	7.7950392	6.8724197	4.2369115

N H H H

1 CO	1.9784862 *	6.4415917	6.1221446	4.3403676
2 C	4.3436937	1.1049740 *	2.1871080 *	3.4389906
3 C	3.8156750	2.1797936 *	1.1042556 *	2.1938447 *
4 C	2.4750397 *	3.4513181	2.2009492 *	1.1080244 *
5 C	1.5104065 *	3.9437584	3.4663621	2.1831752 *
6 C	2.5943348 *	3.5196946	4.0267138	3.5072766
7 C	3.8891192	2.1963270 *	3.4868670	3.9530891
8 C	5.1137794	2.6796494 *	4.6712447	5.3964722
9 C	5.3902122	4.0788682	5.9314277	6.2671303
10 C	4.5661285	4.8915083	6.2575466	6.0068584
11 C	3.1565829	4.6921753	5.4871962	4.8012840
12 N	2.9001014 *	5.9999700	6.4045153	5.1734772
13 C	3.9927692	7.1272692	7.6745479	6.4130347
14 C	4.7200755	8.4920216	8.8379483	7.3056793
15 C	4.7102718	9.0399934	9.0626228	7.2821769
16 C	5.9517658	10.4380739	10.3904190	8.5049532
17 C	7.0271402	11.3058448	11.4506734	9.6455921
18 C	7.0636837	10.9184445	11.3168404	9.6997757
19 C	6.0400263	9.5780016	10.0951582	8.6305476
20 O	3.7692481	8.3041251	8.0549078	6.1790773
21 N	0.0000000	5.4477862	4.6750533	2.6529998 *
22 H	5.4477862	0.0000000	2.5311210 *	4.3599017
23 H	4.6750533	2.5311210 *	0.0000000	2.5176238 *
24 H	2.6529998 *	4.3599017	2.5176238 *	0.0000000
25 H	6.0595879	2.4007842 *	4.7824890	5.9768410
26 H	6.4736774	4.7777812	6.8523520	7.3482960
27 H	5.2594546	5.9658626	7.3469702	6.9657422
28 H	4.7444148	7.1911062	8.0318265	7.0166817
29 H	6.2849244	10.9651960	10.7193706	8.7202345
30 H	8.0082469	12.3912589	12.4809891	10.6103008
31 H	8.0661033	11.7551987	12.2618193	10.6988765
32 H	6.4263010	9.4563929	10.1961434	8.9294550

33 H	4.3888446	8.9874719	8.5798576	6.6215832
34 H	1.0441361 *	5.8556396	5.1807355	3.2165624
35 H	1.0395933 *	5.8201213	4.5829782	2.2113153 *

H H H H

1 CO	6.5009640	6.2806101	4.5259685	3.8769613
2 C	2.6823666 *	4.6686751	5.3909668	6.3983985
3 C	4.0818260	5.9303069	6.2671139	6.9329534
4 C	4.8919540	6.2531641	6.0076396	6.2709401
5 C	4.6736104	5.4695456	4.8023897	4.8946221
6 C	3.5188671	4.0177773	3.5048545	4.0400027
7 C	2.1982424 *	3.4840768	3.9495979	5.0233691
8 C	1.1052275 *	2.1849154 *	3.4301988	4.9795640
9 C	2.1806121 *	1.1042329 *	2.1802581 *	3.9851095
10 C	3.4530554	2.1973965 *	1.1040188 *	2.6492674 *
11 C	3.9651714	3.4749916	2.1884281 *	2.6555857 *
12 N	5.4125536	4.6664447	2.6909755 *	2.0955550 *
13 C	6.2408354	5.0016237	2.6376408 *	1.1081450 *
14 C	7.6749360	6.3473088	3.8856877	2.1759008 *
15 C	8.4991692	7.4034424	5.0020853	3.5315895
16 C	9.8778697	8.6704927	6.2193879	4.6725355
17 C	10.5145617	9.0340894	6.5358589	4.8505928
18 C	9.9049291	8.2304779	5.7598371	3.9953470
19 C	8.5228392	6.8816330	4.4190371	2.5807257 *
20 O	8.0959130	7.4032805	5.2310076	4.1395604
21 N	6.0595879	6.4736774	5.2594546	4.7444148
22 H	2.4007842 *	4.7777812	5.9658626	7.1911062
23 H	4.7824890	6.8523520	7.3469702	8.0318265
24 H	5.9768410	7.3482960	6.9657422	7.0166817
25 H	0.0000000	2.5283752 *	4.3472678	6.0090590
26 H	2.5283752 *	0.0000000	2.4985962 *	4.4730449
27 H	4.3472678	2.4985962 *	0.0000000	2.1393622 *
28 H	6.0090590	4.4730449	2.1393622 *	0.0000000
29 H	10.5748367	9.5134977	7.1129180	5.6708107
30 H	11.6083014	10.0935188	7.5975315	5.9299334
31 H	10.6082581	8.7812576	6.3786126	4.6537868
32 H	8.2039039	6.3941721	4.0537907	2.2659731 *
33 H	8.8909654	8.2618095	6.1225124	5.0957054
34 H	6.3371060	6.6101442	5.3149923	4.4996211
35 H	6.7619352	7.4000947	6.2744398	5.7524061

H H H H

1 CO	4.6230261	6.4226379	6.6771339	5.2809080
2 C	9.9410793	11.4192805	10.8826996	8.6487014

3 C	9.7962322	11.4776503	11.1916654	9.1053463
4 C	8.5871930	10.3462554	10.2347064	8.3104333
5 C	7.4110157	9.0411185	8.8432378	6.9113811
6 C	7.5423705	8.9031731	8.3848551	6.2357344
7 C	8.9334031	10.2340887	9.5611549	7.2854716
8 C	9.4895502	10.5311448	9.5854297	7.2053521
9 C	8.8477748	9.6294475	8.5011457	6.1062788
10 C	7.4529495	8.2171063	7.1705016	4.8222119
11 C	6.7025782	7.7870748	7.0773173	4.8726853
12 N	5.2724330	6.4030950	5.9186808	3.9711317
13 C	4.7964222	5.4468075	4.6564187	2.6413127 *
14 C	3.5037940	3.9858682	3.4934036	2.1982417 *
15 C	2.1958438 *	3.4393139	3.9299766	3.4513743
16 C	1.1066950 *	2.1915293 *	3.4753388	3.9517083
17 C	2.1992878 *	1.1049491 *	2.1978615 *	3.4560808
18 C	3.4731669	2.1999392 *	1.1043276 *	2.1852330 *
19 C	3.9524481	3.4597719	2.1877164 *	1.1059323 *
20 O	2.6909849 *	4.6508828	5.3958633	4.6925657
21 N	6.2849244	8.0082469	8.0661033	6.4263010
22 H	10.9651960	12.3912589	11.7551987	9.4563929
23 H	10.7193706	12.4809891	12.2618193	10.1961434
24 H	8.7202345	10.6103008	10.6988765	8.9294550
25 H	10.5748367	11.6083014	10.6082581	8.2039039
26 H	9.5134977	10.0935188	8.7812576	6.3941721
27 H	7.1129180	7.5975315	6.3786126	4.0537907
28 H	5.6708107	5.9299334	4.6537868	2.2659731 *
29 H	0.0000000	2.5180880 *	4.3861819	5.0583575
30 H	2.5180880 *	0.0000000	2.5404515 *	4.3729865
31 H	4.3861819	2.5404515 *	0.0000000	2.5140236 *
32 H	5.0583575	4.3729865	2.5140236 *	0.0000000
33 H	2.3152404 *	4.6344055	5.8190361	5.4667041
34 H	6.3499279	7.8439088	7.7306414	6.0669189
35 H	6.6360175	8.5346064	8.8179322	7.3344354

H H H

1 CO	2.6570937 *	2.5001859 *	2.6214243 *
2 C	7.9543749	4.7782935	4.7371576
3 C	7.7059927	4.3273797	3.9161407
4 C	6.5068871	3.0603485	2.4847512 *
5 C	5.4384514	2.1123583 *	2.0887325 *
6 C	5.7303625	2.9638672 *	3.4245140
7 C	7.0989556	4.2485910	4.5639041
8 C	7.8364038	5.3787605	5.8905617
9 C	7.4480418	5.5600902	6.3039986
10 C	6.1627097	4.6865465	5.5566401

11	C	5.1830953	3.3353474	4.1530285
12	N	3.8875981	3.0047389	3.8879662
13	C	4.0129603	3.8635721	4.9546296
14	C	3.3293716	4.5721300	5.5394284
15	C	2.0462425 *	4.7183914	5.3277368
16	C	2.5122698 *	5.9238786	6.4570227
17	C	3.9325483	6.8629976	7.6168197
18	C	4.7329486	6.7901506	7.7950392
19	C	4.4878185	5.7573905	6.8724197
20	O	0.9918568 *	4.0354586	4.2369115
21	N	4.3888446	1.0441361 *	1.0395933 *
22	H	8.9874719	5.8556396	5.8201213
23	H	8.5798576	5.1807355	4.5829782
24	H	6.6215832	3.2165624	2.2113153 *
25	H	8.8909654	6.3371060	6.7619352
26	H	8.2618095	6.6101442	7.4000947
27	H	6.1225124	5.3149923	6.2744398
28	H	5.0957054	4.4996211	5.7524061
29	H	2.3152404 *	6.3499279	6.6360175
30	H	4.6344055	7.8439088	8.5346064
31	H	5.8190361	7.7306414	8.8179322
32	H	5.4667041	6.0669189	7.3344354
33	H	0.0000000	4.7386134	4.6701637
34	H	4.7386134	0.0000000	1.6667546 *
35	H	4.6701637	1.6667546 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.73 , TOTAL = 7616.3 SECONDS (126.9 MIN)

WALL CLOCK TIME: STEP = 0.73 , TOTAL = 7041.3 SECONDS (117.4 MIN)

CPU UTILIZATION: STEP = 99.88%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.95 , TOTAL = 7617.3 SECONDS (127.0 MIN)

WALL CLOCK TIME: STEP = 0.94 , TOTAL = 7042.2 SECONDS (117.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636892461	-284.636892461	0.003571244	0.000551661	198021979
11337677						
2	1	-284.636911943	-0.000019481	0.001158545	0.000034363	149912668
15418718						
3	2	-284.636911903	0.000000040	0.000463978	0.000055223	134031015
16623729						
4	3	-284.636912232	-0.000000329	0.000163359	0.000012192	127118912
17113564						
5	4	-284.636912216	0.000000016	0.000127524	0.000027529	119495257
17730407						
6	5	-284.636912251	-0.000000036	0.000103623	0.000011187	110266060
18413308						
7	6	-284.636912290	-0.000000039	0.000054940	0.000015243	113185394
18207392						
8	7	-284.636912286	0.000000004	0.000121605	0.000010799	105189222
18781593						
9	8	-284.636912297	-0.000000011	0.000255941	0.000010606	134733498
16659892						
10	9	-284.636912308	-0.000000011	0.000190070	0.000015416	159002961
14813684						
11	10	-284.636912318	-0.000000009	0.000167895	0.000007909	157527558
14910981						
12	11	-284.636912324	-0.000000006	0.000053927	0.000005705	159477291
14686818						
13	12	-284.636912326	-0.000000003	0.000095962	0.000003594	153371369
15171181						

-----DISABLING FDIFF OPTION-----

14	13	-284.636912311	0.000000015	0.000064211	0.000002120	198021832
11337650						
15	14	-284.636912312	-0.000000001	0.000056139	0.000001220	198021784
11337653						
16	15	-284.636912312	0.000000000	0.000015262	0.000001167	198021781
11337648						
17	16	-284.636912312	0.000000000	0.000017063	0.000001056	198021772
11337649						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 56.0 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 18.5 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369123119 AFTER 17 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6006716612
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998527979

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 58.48 , TOTAL = 7675.7 SECONDS (127.9 MIN)
WALL CLOCK TIME: STEP = 53.73 , TOTAL = 7096.0 SECONDS (118.3
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.77 , TOTAL = 7679.5 SECONDS (128.0 MIN)
WALL CLOCK TIME: STEP = 3.73 , TOTAL = 7099.7 SECONDS (118.3
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.74 , TOTAL = 7682.2 SECONDS (128.0 MIN)
WALL CLOCK TIME: STEP = 2.66 , TOTAL = 7102.3 SECONDS (118.4
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 82 ENERGY= -284.6369123

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
------	------	-------	-------	-------

```

-----
1 CO    27.0 -0.0001259 -0.0001321 -0.0001081
2 C     6.0  0.0000562  0.0000267  0.0000244
3 C     6.0 -0.0000032  0.0000354 -0.0000825
4 C     6.0  0.0000251  0.0002098 -0.0000644
5 C     6.0  0.0001260  0.0001096 -0.0000575
6 C     6.0  0.0000886  0.0000540 -0.0000445
7 C     6.0 -0.0000147  0.0000852 -0.0000254
8 C     6.0 -0.0000021  0.0001002  0.0000114
9 C     6.0  0.0001036  0.0001606  0.0002027
10 C    6.0 -0.0001297 -0.0001780  0.0001466
11 C    6.0 -0.0000470 -0.0001067  0.0000193
12 N    7.0  0.0000454 -0.0000786 -0.0002051
13 C    6.0 -0.0000477 -0.0001165 -0.0000452
14 C    6.0 -0.0000415  0.0000553  0.0000201
15 C    6.0  0.0000044 -0.0000455  0.0001003
16 C    6.0  0.0000165  0.0000053  0.0000935
17 C    6.0  0.0000307  0.0000626  0.0000530
18 C    6.0 -0.0000232 -0.0000583 -0.0000389
19 C    6.0  0.0000320 -0.0000715  0.0000049
20 O    8.0  0.0000264 -0.0000438 -0.0001942
21 N    7.0  0.0000299 -0.0001095 -0.0000256
22 H    1.0 -0.0000838 -0.0000184  0.0000562
23 H    1.0  0.0000485 -0.0000781  0.0000509
24 H    1.0  0.0000812 -0.0001608  0.0001279
25 H    1.0  0.0000417  0.0001833  0.0000220
26 H    1.0 -0.0000572 -0.0000431  0.0000466
27 H    1.0  0.0000219  0.0000345 -0.0003215
28 H    1.0  0.0000917 -0.0000050  0.0001538
29 H    1.0 -0.0002634  0.0001153 -0.0000424
30 H    1.0  0.0001394  0.0001250  0.0000635
31 H    1.0 -0.0000819  0.0001004  0.0000281
32 H    1.0 -0.0001457  0.0000324 -0.0000001
33 H    1.0  0.0000513  0.0000176  0.0000695
34 H    1.0 -0.0001044 -0.0001429 -0.0000082
35 H    1.0  0.0001111 -0.0001244 -0.0000312

```

MAXIMUM GRADIENT = 0.0003215 RMS GRADIENT = 0.0000966
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000064440
 PREDICTED ENERGY CHANGE WAS -0.0000048446 RATIO= 1.330
 GDIIS STEP HAS LENGTH = 0.016768
 RADIUS OF STEP TAKEN= 0.01677 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 0.03 , TOTAL = 7682.3 SECONDS (128.0 MIN)

WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7102.4 SECONDS (118.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

INSERCH= 83

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1558630094	-1.7348956766	0.8612293216
C	6.0	4.9812868124	0.6268486797	0.5643565167
C	6.0	5.1859858977	-0.7124453769	0.2056510226
C	6.0	4.0505144301	-1.5332700239	-0.0900793593
C	6.0	2.7418758601	-1.0220158608	-0.0039560980
C	6.0	2.4696158994	0.3435063962	0.4274427670
C	6.0	3.6509347876	1.1769418400	0.6797144230
C	6.0	3.5030790055	2.5628892456	1.0585493523
C	6.0	2.2344330933	3.1369405697	1.2191946359
C	6.0	1.0698269399	2.3280874414	1.0350378571
C	6.0	1.1629439157	0.9745360212	0.6342897852
N	7.0	-0.0494224785	0.1733760421	0.5791697634
C	6.0	-1.2459127447	0.6979393900	0.3191496574
C	6.0	-2.5500449587	0.0371752915	0.4351032166
C	6.0	-2.8216040163	-1.2856946379	0.9278324840
C	6.0	-4.1224444783	-1.8044791158	1.0586091241
C	6.0	-5.2317787587	-0.9868952609	0.6831406646
C	6.0	-5.0172850221	0.3262474162	0.1784777301
C	6.0	-3.6980524782	0.8262441215	0.0599898894
O	8.0	-1.6985064359	-2.1451881286	1.3136077927
N	7.0	1.6365720395	-1.9582218700	-0.4315487147
H	1.0	5.8422388022	1.2882608707	0.7701236488
H	1.0	6.2038540896	-1.1334266730	0.1276025725
H	1.0	4.2152670728	-2.5778857785	-0.4205980209
H	1.0	4.4153929535	3.1622302785	1.2323771931
H	1.0	2.1242714318	4.1923422073	1.5247777190
H	1.0	0.0845680311	2.7724521252	1.2609334472
H	1.0	-1.2908574052	1.7508341509	-0.0236476753
H	1.0	-4.2978317908	-2.8279894196	1.4420283118
H	1.0	-6.2566119162	-1.3870309350	0.7869045702
H	1.0	-5.8752330361	0.9575159113	-0.1127052865
H	1.0	-3.5342128068	1.8514322944	-0.3210729801
H	1.0	-2.0132364588	-2.9555464256	1.7910896098
H	1.0	1.2770556711	-1.6863722695	-1.3735167265
H	1.0	2.0334520423	-2.9133378411	-0.5363712145

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C	
1	CO	0.0000000	5.3805841	5.1746810	4.0142186
2	C	5.3805841	0.0000000	1.4015277 *	2.4414619 *
3	C	5.1746810	1.4015277 *	0.0000000	1.4319585 *
4	C	4.0142186	2.4414619 *	1.4319585 *	0.0000000
5	C	2.8185468 *	2.8384318 *	2.4725377 *	1.4075983 *
6	C	3.1402832	2.5313078 *	2.9228226 *	2.5078595 *
7	C	4.5527214	1.4442114 *	2.4801012 *	2.8456097 *
8	C	5.4510316	2.4854734 *	3.7798714	4.2892370
9	C	5.3088022	3.7781715	4.9554724	5.1791135
10	C	4.1681376	4.2913020	5.1841573	5.0060432
11	C	2.8994368 *	3.8347777	4.3834352	3.8925397
12	N	1.9398971 *	5.0511279	5.3229406	4.4911043
13	C	2.8596350 *	6.2324309	6.5856957	5.7617623
14	C	3.2624771	7.5554867	7.7756513	6.8051083
15	C	3.0118976	8.0420795	8.0604998	6.9515070
16	C	4.2834234	9.4357598	9.4110016	8.2577416
17	C	5.4422334	10.3404539	10.4323123	9.3304534
18	C	5.6103406	10.0105296	10.2560401	9.2603950
19	C	4.6961778	8.6962679	9.0174786	8.1012417
20	O	1.9523504 *	7.2708461	7.1187467	5.9494556
21	N	1.9782944 *	4.3429867	3.8152747	2.4747330 *
22	H	6.4407022	1.1050088 *	2.1799364 *	3.4512696
23	H	6.1219416	2.1872343 *	1.1042520 *	2.2009388 *
24	H	4.3396400	3.4390761	2.1941629 *	1.1079748 *
25	H	6.5010144	2.6822840 *	4.0818000	4.8918044
26	H	6.2806908	4.6687996	5.9305254	6.2530641
27	H	4.5255973	5.3913531	6.2675829	6.0077625
28	H	3.8763797	6.3991316	6.9332404	6.2705667
29	H	4.6225078	9.9402342	9.7952516	8.5859500
30	H	6.4223336	11.4190896	11.4771933	10.3454019
31	H	6.6762076	10.8826365	11.1910985	10.2335228
32	H	5.2797961	8.6485446	9.1045468	8.3088901
33	H	2.6569947 *	7.9537277	7.7054474	6.5062079
34	H	2.5007034 *	4.7778313	4.3268973	3.0598571
35	H	2.6205636 *	4.7364810	3.9157368	2.4844123 *
	C	C	C	C	
1	CO	2.8185468 *	3.1402832	4.5527214	5.4510316
2	C	2.8384318 *	2.5313078 *	1.4442114 *	2.4854734 *
3	C	2.4725377 *	2.9228226 *	2.4801012 *	3.7798714

4 C	1.4075983 *	2.5078595 *	2.8456097 *	4.2892370
5 C	0.0000000	1.4576973 *	2.4757238 *	3.8157427
6 C	1.4576973 *	0.0000000	1.4675728 *	2.5282408 *
7 C	2.4757238 *	1.4675728 *	0.0000000	1.4443779 *
8 C	3.8157427	2.5282408 *	1.4443779 *	0.0000000
9 C	4.3646895	2.9129807 *	2.4777229 *	1.4017148 *
10 C	3.8856722	2.5034262 *	2.8484221 *	2.4446677 *
11 C	2.6242339 *	1.4657339 *	2.4966237 *	2.8599116 *
12 N	3.0919806	2.5293319 *	3.8353484	4.3081138
13 C	4.3548940	3.7339662	4.9334132	5.1553538
14 C	5.4147101	5.0290051	6.3096000	6.5884919
15 C	5.6471289	5.5589292	6.9296392	7.4047485
16 C	6.9900062	6.9618584	8.3341381	8.7876342
17 C	8.0032808	7.8196438	9.1424725	9.4360819
18 C	7.8775424	7.4910591	8.7242738	8.8528920
19 C	6.7002113	6.1974342	7.3834044	7.4745804
20 O	4.7659716	4.9347880	6.3288932	7.0205084
21 N	1.5103025 *	2.5941822 *	3.8886777	5.1131875
22 H	3.9432003	3.5191727	2.1959916 *	2.6794655 *
23 H	3.4662679	4.0268810	3.4871230	4.6715735
24 H	2.1829346 *	3.5072786	3.9532125	5.3965412
25 H	4.6730178	3.5184048	2.1979997 *	1.1053246 *
26 H	5.4688200	4.0170815	3.4838875	2.1848561 *
27 H	4.8020014	3.5047022	3.9499925	3.4309027
28 H	4.8940804	4.0404472	5.0244782	4.9812057
29 H	7.4101211	7.5422886	8.9332797	9.4901443
30 H	9.0405464	8.9034277	10.2344969	10.5321995
31 H	8.8422247	8.3848239	9.5615872	9.5865425
32 H	6.9098883	6.2353890	7.2857984	7.2064558
33 H	5.4379980	5.7305539	7.0989753	7.8370584
34 H	2.1125255 *	2.9641293 *	4.2484854	5.3783221
35 H	2.0886429 *	3.4243555	4.5634967	5.8900457

C C C N

1 CO	5.3088022	4.1681376	2.8994368 *	1.9398971 *
2 C	3.7781715	4.2913020	3.8347777	5.0511279
3 C	4.9554724	5.1841573	4.3834352	5.3229406
4 C	5.1791135	5.0060432	3.8925397	4.4911043
5 C	4.3646895	3.8856722	2.6242339 *	3.0919806
6 C	2.9129807 *	2.5034262 *	1.4657339 *	2.5293319 *
7 C	2.4777229 *	2.8484221 *	2.4966237 *	3.8353484
8 C	1.4017148 *	2.4446677 *	2.8599116 *	4.3081138
9 C	0.0000000	1.4298478 *	2.4831827 *	3.7958323
10 C	1.4298478 *	0.0000000	1.4146983 *	2.4704891 *
11 C	2.4831827 *	1.4146983 *	0.0000000	1.4542104 *

12 N	3.7958323	2.4704891 *	1.4542104 *	0.0000000
13 C	4.3441472	2.9210493 *	2.4450786 *	1.3320533 *
14 C	5.7545264	4.3256991	3.8346586	2.5084694 *
15 C	6.7236973	5.3116992	4.5903630	3.1520538
16 C	8.0531552	6.6361393	5.9865100	4.5531617
17 C	8.5462094	7.1290375	6.6889519	5.3116717
18 C	7.8466874	6.4648272	6.2308324	4.9863395
19 C	6.4712795	5.0930272	4.8970498	3.7427644
20 O	6.5861833	5.2679659	4.2874293	2.9384719 *
21 N	5.3891624	4.5655803	3.1561692	2.8996274 *
22 H	4.0786693	4.8915574	4.6917667	5.9992586
23 H	5.9316029	6.2580950	5.4873504	6.4043043
24 H	6.2667267	6.0067664	4.8009547	5.1726738
25 H	2.1811463 *	3.4536284	3.9651153	5.4124400
26 H	1.1042596 *	2.1970763 *	3.4743915	4.6659628
27 H	2.1809433 *	1.1041847 *	2.1881680 *	2.6903442 *
28 H	3.9866805	2.6508238 *	2.6564377 *	2.0959303 *
29 H	8.8487586	7.4540278	6.7031122	5.2727319
30 H	9.6307340	8.2182955	7.7878173	6.4036883
31 H	8.5023840	7.1714461	7.0777275	5.9189218
32 H	6.1075553	4.8232166	4.8728787	3.9711552
33 H	7.4490374	6.1639014	5.1838071	3.8878620
34 H	5.5590530	4.6861461	3.3353773	3.0051943
35 H	6.3030369	5.5561172	4.1525648	3.8872356

C C C C

1 CO	2.8596350 *	3.2624771	3.0118976	4.2834234
2 C	6.2324309	7.5554867	8.0420795	9.4357598
3 C	6.5856957	7.7756513	8.0604998	9.4110016
4 C	5.7617623	6.8051083	6.9515070	8.2577416
5 C	4.3548940	5.4147101	5.6471289	6.9900062
6 C	3.7339662	5.0290051	5.5589292	6.9618584
7 C	4.9334132	6.3096000	6.9296392	8.3341381
8 C	5.1553538	6.5884919	7.4047485	8.7876342
9 C	4.3441472	5.7545264	6.7236973	8.0531552
10 C	2.9210493 *	4.3256991	5.3116992	6.6361393
11 C	2.4450786 *	3.8346586	4.5903630	5.9865100
12 N	1.3320533 *	2.5084694 *	3.1520538	4.5531617
13 C	0.0000000	1.4665658 *	2.6053986 *	3.8837268
14 C	1.4665658 *	0.0000000	1.4375365 *	2.5005781 *
15 C	2.6053986 *	1.4375365 *	0.0000000	1.4065652 *
16 C	3.8837268	2.5005781 *	1.4065652 *	0.0000000
17 C	4.3426127	2.8813086 *	2.4409214 *	1.4283006 *
18 C	3.7922543	2.4973372 *	2.8250495 *	2.4729267 *
19 C	2.4691325 *	1.4426576 *	2.4457306 *	2.8457079 *

20 O	3.0458434	2.5019189 *	1.4659126 *	2.4610125 *
21 N	3.9909221	4.7180989	4.7090916	5.9506704
22 H	7.1269734	8.4916359	9.0394851	10.4375848
23 H	7.6739571	8.8371723	9.0621436	10.3898762
24 H	6.4111420	7.3034386	7.2804929	8.5031550
25 H	6.2415620	7.6758674	8.5000535	9.8789203
26 H	5.0022526	6.3483885	7.4045199	8.6718302
27 H	2.6383212 *	3.8865049	5.0025341	6.2199830
28 H	1.1082046 *	2.1754614 *	3.5311481	4.6721962
29 H	4.7965863	3.5039729	2.1959779 *	1.1069527 *
30 H	5.4472931	3.9863224	3.4393908	2.1915193 *
31 H	4.6566603	3.4934219	3.9292954	3.4746024
32 H	2.6413535 *	2.1981622 *	3.4509624	3.9516107
33 H	4.0128981	3.3291509	2.0462346 *	2.5120195 *
34 H	3.8620501	4.5703853	4.7176013	5.9231569
35 H	4.9525218	5.5369428	5.3258506	6.4551214

C C C O

1 CO	5.4422334	5.6103406	4.6961778	1.9523504 *
2 C	10.3404539	10.0105296	8.6962679	7.2708461
3 C	10.4323123	10.2560401	9.0174786	7.1187467
4 C	9.3304534	9.2603950	8.1012417	5.9494556
5 C	8.0032808	7.8775424	6.7002113	4.7659716
6 C	7.8196438	7.4910591	6.1974342	4.9347880
7 C	9.1424725	8.7242738	7.3834044	6.3288932
8 C	9.4360819	8.8528920	7.4745804	7.0205084
9 C	8.5462094	7.8466874	6.4712795	6.5861833
10 C	7.1290375	6.4648272	5.0930272	5.2679659
11 C	6.6889519	6.2308324	4.8970498	4.2874293
12 N	5.3116717	4.9863395	3.7427644	2.9384719 *
13 C	4.3426127	3.7922543	2.4691325 *	3.0458434
14 C	2.8813086 *	2.4973372 *	1.4426576 *	2.5019189 *
15 C	2.4409214 *	2.8250495 *	2.4457306 *	1.4659126 *
16 C	1.4283006 *	2.4729267 *	2.8457079 *	2.4610125 *
17 C	0.0000000	1.4230376 *	2.4552205 *	3.7713584
18 C	1.4230376 *	0.0000000	1.4157721 *	4.2907814
19 C	2.4552205 *	1.4157721 *	0.0000000	3.7946214
20 O	3.7713584	4.2907814	3.7946214	0.0000000
21 N	7.0256851	7.0614974	6.0376386	3.7687234
22 H	11.3056520	10.9180938	9.5778342	8.3034201
23 H	11.4500564	11.3157943	10.0941882	8.0546615
24 H	9.6434519	9.6970562	8.6278440	6.1779782
25 H	10.5159320	9.9060041	8.5240436	8.0966076
26 H	9.0357251	8.2317095	6.8829990	7.4042227
27 H	6.5368250	5.7606017	4.4202046	5.2311867

28 H	4.8503168	3.9945669	2.5800097 *	4.1392535
29 H	2.1994988 *	3.4732381	3.9526179	2.6905765 *
30 H	1.1050604 *	2.2003266 *	3.4602338	4.6506499
31 H	2.1973027 *	1.1042474 *	2.1879605 *	5.3950150
32 H	3.4563389	2.1852329 *	1.1059218 *	4.6920117
33 H	3.9321944	4.7323351	4.4874548	0.9918288 *
34 H	6.8617806	6.7880814	5.7549877	4.0354826
35 H	7.6145892	7.7922278	6.8695170	4.2355626

N H H H

1 CO	1.9782944 *	6.4407022	6.1219416	4.3396400
2 C	4.3429867	1.1050088 *	2.1872343 *	3.4390761
3 C	3.8152747	2.1799364 *	1.1042520 *	2.1941629 *
4 C	2.4747330 *	3.4512696	2.2009388 *	1.1079748 *
5 C	1.5103025 *	3.9432003	3.4662679	2.1829346 *
6 C	2.5941822 *	3.5191727	4.0268810	3.5072786
7 C	3.8886777	2.1959916 *	3.4871230	3.9532125
8 C	5.1131875	2.6794655 *	4.6715735	5.3965412
9 C	5.3891624	4.0786693	5.9316029	6.2667267
10 C	4.5655803	4.8915574	6.2580950	6.0067664
11 C	3.1561692	4.6917667	5.4873504	4.8009547
12 N	2.8996274 *	5.9992586	6.4043043	5.1726738
13 C	3.9909221	7.1269734	7.6739571	6.4111420
14 C	4.7180989	8.4916359	8.8371723	7.3034386
15 C	4.7090916	9.0394851	9.0621436	7.2804929
16 C	5.9506704	10.4375848	10.3898762	8.5031550
17 C	7.0256851	11.3056520	11.4500564	9.6434519
18 C	7.0614974	10.9180938	11.3157943	9.6970562
19 C	6.0376386	9.5778342	10.0941882	8.6278440
20 O	3.7687234	8.3034201	8.0546615	6.1779782
21 N	0.0000000	5.4471368	4.6747195	2.6521258 *
22 H	5.4471368	0.0000000	2.5314363 *	4.3602689
23 H	4.6747195	2.5314363 *	0.0000000	2.5182264 *
24 H	2.6521258 *	4.3602689	2.5182264 *	0.0000000
25 H	6.0588386	2.4002768 *	4.7824459	5.9767307
26 H	6.4725963	4.7777058	6.8526569	7.3479750
27 H	5.2585634	5.9661119	7.3475159	6.9653671
28 H	4.7427126	7.1920170	8.0319697	7.0151830
29 H	6.2836244	10.9643059	10.7184264	8.7180721
30 H	8.0070744	12.3911120	12.4804730	10.6083197
31 H	8.0641431	11.7553360	12.2610821	10.6963571
32 H	6.4236038	9.4565172	10.1951282	8.9265448
33 H	4.3881522	8.9866993	8.5795039	6.6203056
34 H	1.0442500 *	5.8552996	5.1800049	3.2149552
35 H	1.0395903 *	5.8195547	4.5827064	2.2104860 *

	H	H	H	H
1 CO	6.5010144	6.2806908	4.5255973	3.8763797
2 C	2.6822840 *	4.6687996	5.3913531	6.3991316
3 C	4.0818000	5.9305254	6.2675829	6.9332404
4 C	4.8918044	6.2530641	6.0077625	6.2705667
5 C	4.6730178	5.4688200	4.8020014	4.8940804
6 C	3.5184048	4.0170815	3.5047022	4.0404472
7 C	2.1979997 *	3.4838875	3.9499925	5.0244782
8 C	1.1053246 *	2.1848561 *	3.4309027	4.9812057
9 C	2.1811463 *	1.1042596 *	2.1809433 *	3.9866805
10 C	3.4536284	2.1970763 *	1.1041847 *	2.6508238 *
11 C	3.9651153	3.4743915	2.1881680 *	2.6564377 *
12 N	5.4124400	4.6659628	2.6903442 *	2.0959303 *
13 C	6.2415620	5.0022526	2.6383212 *	1.1082046 *
14 C	7.6758674	6.3483885	3.8865049	2.1754614 *
15 C	8.5000535	7.4045199	5.0025341	3.5311481
16 C	9.8789203	8.6718302	6.2199830	4.6721962
17 C	10.5159320	9.0357251	6.5368250	4.8503168
18 C	9.9060041	8.2317095	5.7606017	3.9945669
19 C	8.5240436	6.8829990	4.4202046	2.5800097 *
20 O	8.0966076	7.4042227	5.2311867	4.1392535
21 N	6.0588386	6.4725963	5.2585634	4.7427126
22 H	2.4002768 *	4.7777058	5.9661119	7.1920170
23 H	4.7824459	6.8526569	7.3475159	8.0319697
24 H	5.9767307	7.3479750	6.9653671	7.0151830
25 H	0.0000000	2.5290050 *	4.3484235	6.0109010
26 H	2.5290050 *	0.0000000	2.4992182 *	4.4745601
27 H	4.3484235	2.4992182 *	0.0000000	2.1414124 *
28 H	6.0109010	4.4745601	2.1414124 *	0.0000000
29 H	10.5757728	9.5150046	7.1135904	5.6706019
30 H	11.6097335	10.0952002	7.5984581	5.9297479
31 H	10.6097594	8.7827970	6.3796634	4.6533628
32 H	8.2053416	6.3957383	4.0554404	2.2652208 *
33 H	8.8919417	8.2633048	6.1230562	5.0955982
34 H	6.3363073	6.6088705	5.3144585	4.4978564
35 H	6.7612603	7.3991400	6.2734887	5.7505147

	H	H	H	H
1 CO	4.6225078	6.4223336	6.6762076	5.2797961
2 C	9.9402342	11.4190896	10.8826365	8.6485446
3 C	9.7952516	11.4771933	11.1910985	9.1045468
4 C	8.5859500	10.3454019	10.2335228	8.3088901
5 C	7.4101211	9.0405464	8.8422247	6.9098883

6 C	7.5422886	8.9034277	8.3848239	6.2353890
7 C	8.9332797	10.2344969	9.5615872	7.2857984
8 C	9.4901443	10.5321995	9.5865425	7.2064558
9 C	8.8487586	9.6307340	8.5023840	6.1075553
10 C	7.4540278	8.2182955	7.1714461	4.8232166
11 C	6.7031122	7.7878173	7.0777275	4.8728787
12 N	5.2727319	6.4036883	5.9189218	3.9711552
13 C	4.7965863	5.4472931	4.6566603	2.6413535 *
14 C	3.5039729	3.9863224	3.4934219	2.1981622 *
15 C	2.1959779 *	3.4393908	3.9292954	3.4509624
16 C	1.1069527 *	2.1915193 *	3.4746024	3.9516107
17 C	2.1994988 *	1.1050604 *	2.1973027 *	3.4563389
18 C	3.4732381	2.2003266 *	1.1042474 *	2.1852329 *
19 C	3.9526179	3.4602338	2.1879605 *	1.1059218 *
20 O	2.6905765 *	4.6506499	5.3950150	4.6920117
21 N	6.2836244	8.0070744	8.0641431	6.4236038
22 H	10.9643059	12.3911120	11.7553360	9.4565172
23 H	10.7184264	12.4804730	12.2610821	10.1951282
24 H	8.7180721	10.6083197	10.6963571	8.9265448
25 H	10.5757728	11.6097335	10.6097594	8.2053416
26 H	9.5150046	10.0952002	8.7827970	6.3957383
27 H	7.1135904	7.5984581	6.3796634	4.0554404
28 H	5.6706019	5.9297479	4.6533628	2.2652208 *
29 H	0.0000000	2.5184059 *	4.3858228	5.0585203
30 H	2.5184059 *	0.0000000	2.5400094 *	4.3734100
31 H	4.3858228	2.5400094 *	0.0000000	2.5145336 *
32 H	5.0585203	4.3734100	2.5145336 *	0.0000000
33 H	2.3146253 *	4.6340979	5.8182050	5.4664105
34 H	6.3490120	7.8430334	7.7288436	6.0639924
35 H	6.6337398	8.5326334	8.8153446	7.3313218

H H H

1 CO	2.6569947 *	2.5007034 *	2.6205636 *
2 C	7.9537277	4.7778313	4.7364810
3 C	7.7054474	4.3268973	3.9157368
4 C	6.5062079	3.0598571	2.4844123 *
5 C	5.4379980	2.1125255 *	2.0886429 *
6 C	5.7305539	2.9641293 *	3.4243555
7 C	7.0989753	4.2484854	4.5634967
8 C	7.8370584	5.3783221	5.8900457
9 C	7.4490374	5.5590530	6.3030369
10 C	6.1639014	4.6861461	5.5561172
11 C	5.1838071	3.3353773	4.1525648
12 N	3.8878620	3.0051943	3.8872356
13 C	4.0128981	3.8620501	4.9525218

14 C	3.3291509	4.5703853	5.5369428
15 C	2.0462346 *	4.7176013	5.3258506
16 C	2.5120195 *	5.9231569	6.4551214
17 C	3.9321944	6.8617806	7.6145892
18 C	4.7323351	6.7880814	7.7922278
19 C	4.4874548	5.7549877	6.8695170
20 O	0.9918288 *	4.0354826	4.2355626
21 N	4.3881522	1.0442500 *	1.0395903 *
22 H	8.9866993	5.8552996	5.8195547
23 H	8.5795039	5.1800049	4.5827064
24 H	6.6203056	3.2149552	2.2104860 *
25 H	8.8919417	6.3363073	6.7612603
26 H	8.2633048	6.6088705	7.3991400
27 H	6.1230562	5.3144585	6.2734887
28 H	5.0955982	4.4978564	5.7505147
29 H	2.3146253 *	6.3490120	6.6337398
30 H	4.6340979	7.8430334	8.5326334
31 H	5.8182050	7.7288436	8.8153446
32 H	5.4664105	6.0639924	7.3313218
33 H	0.0000000	4.7383076	4.6684626
34 H	4.7383076	0.0000000	1.6668511 *
35 H	4.6684626	1.6668511 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.60 , TOTAL = 7682.9 SECONDS (128.0 MIN)
WALL CLOCK TIME: STEP = 0.61 , TOTAL = 7103.0 SECONDS (118.4 MIN)
CPU UTILIZATION: STEP = 98.66% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.07 , TOTAL = 7683.9 SECONDS (128.1 MIN)
WALL CLOCK TIME: STEP = 1.07 , TOTAL = 7104.0 SECONDS (118.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636909391	-284.636909391	0.002928577	0.000251948	198033495
11336785						
2	1	-284.636917246	-0.000007855	0.000783226	0.000030047	147966088
15549458						
3	2	-284.636917204	0.000000043	0.000405407	0.000063053	130359563
16894244						
4	3	-284.636917348	-0.000000145	0.000179352	0.000027865	123693127
17409613						
5	4	-284.636917314	0.000000034	0.000146875	0.000044289	118987982
17776414						
6	5	-284.636917364	-0.000000050	0.000065405	0.000006958	113744991
18157533						
7	6	-284.636917388	-0.000000023	0.000059270	0.000006818	108501124
18491497						
8	7	-284.636917384	0.000000004	0.000061154	0.000006627	101084091
19057856						
9	8	-284.636917384	-0.000000001	0.000158879	0.000006151	129508594
17041872						
10	9	-284.636917390	-0.000000005	0.000139609	0.000005612	155425786
15065308						
11	10	-284.636917395	-0.000000005	0.000209750	0.000005489	153603779
15245854						

-----DISABLING FDIFF OPTION-----

12	11	-284.636917378	0.000000017	0.000057294	0.000005863	198034647
11336658						
13	12	-284.636917380	-0.000000002	0.000040608	0.000003404	198034625
11336657						
14	13	-284.636917381	-0.000000001	0.000036146	0.000001782	198034618
11336653						
15	14	-284.636917381	0.000000000	0.000038041	0.000001001	198034668
11336654						

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 48.9 SECONDS (3.3 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 16.3 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
 TIME TO SOLVE SCF EQUATIONS= 2.1 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369173813 AFTER 15 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6009757969
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998520857

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 51.93 , TOTAL = 7735.9 SECONDS (128.9 MIN)
WALL CLOCK TIME: STEP = 47.85 , TOTAL = 7151.9 SECONDS (119.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.90 , TOTAL = 7739.8 SECONDS (129.0 MIN)
WALL CLOCK TIME: STEP = 3.95 , TOTAL = 7155.9 SECONDS (119.3 MIN)
CPU UTILIZATION: STEP = 98.71% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.85 , TOTAL = 7742.6 SECONDS (129.0 MIN)
WALL CLOCK TIME: STEP = 2.68 , TOTAL = 7158.5 SECONDS (119.3 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 83 ENERGY= -284.6369174

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0001306	-0.0001165	-0.0001564
2 C	6.0	-0.0000455	-0.0000480	-0.0000073
3 C	6.0	0.0000033	-0.0000016	-0.0000744
4 C	6.0	0.0001241	0.0001113	-0.0000500
5 C	6.0	0.0001132	0.0001522	-0.0000158
6 C	6.0	0.0001351	0.0002053	-0.0000201

7 C	6.0	-0.0000405	0.0000999	-0.0000017
8 C	6.0	-0.0000476	0.0001017	0.0001158
9 C	6.0	0.0000608	-0.0001046	0.0001199
10 C	6.0	-0.0000417	-0.0000615	0.0000721
11 C	6.0	0.0000377	-0.0000254	-0.0000142
12 N	7.0	0.0000884	-0.0000618	-0.0000642
13 C	6.0	0.0000178	-0.0002240	-0.0000500
14 C	6.0	-0.0000583	0.0000294	0.0000156
15 C	6.0	0.0000532	0.0001059	0.0000412
16 C	6.0	-0.0000673	0.0002449	0.0001080
17 C	6.0	0.0000430	-0.0000154	-0.0000082
18 C	6.0	0.0001065	0.0000198	-0.0000670
19 C	6.0	0.0000939	-0.0001321	-0.0000051
20 O	8.0	-0.0000627	0.0000051	-0.0001884
21 N	7.0	0.0000908	-0.0000343	0.0000576
22 H	1.0	-0.0000990	0.0000151	0.0000994
23 H	1.0	0.0000435	-0.0000797	0.0000024
24 H	1.0	0.0000232	-0.0001324	0.0000988
25 H	1.0	0.0001490	0.0001714	-0.0000422
26 H	1.0	-0.0000829	-0.0000324	0.0000244
27 H	1.0	-0.0001139	-0.0000122	-0.0002494
28 H	1.0	-0.0000023	0.0000118	0.0001448
29 H	1.0	-0.0002770	-0.0000608	-0.0000292
30 H	1.0	0.0000718	0.0000771	0.0001047
31 H	1.0	-0.0000929	0.0000168	0.0001101
32 H	1.0	-0.0001285	0.0000153	-0.0000200
33 H	1.0	0.0000671	0.0000194	0.0000466
34 H	1.0	-0.0001228	-0.0001313	-0.0001015
35 H	1.0	0.0000912	-0.0001286	0.0000038

MAXIMUM GRADIENT = 0.0002770 RMS GRADIENT = 0.0000958
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000050695
 PREDICTED ENERGY CHANGE WAS -0.0000037974 RATIO= 1.335
 GDIIS STEP HAS LENGTH = 0.023012
 RADIUS OF STEP TAKEN= 0.02301 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 7742.6 SECONDS (129.0 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7158.6 SECONDS (119.3
 MIN)
 CPU UTILIZATION: STEP = 84.04% , TOTAL = 100.00%

1NSERCH= 84

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1557237472	-1.7330391717	0.8634677111
C	6.0	4.9815858554	0.6258744984	0.5653366215
C	6.0	5.1856439619	-0.7132609878	0.2053262124
C	6.0	4.0495260326	-1.5333434891	-0.0903527498
C	6.0	2.7411976394	-1.0216857716	-0.0025984737
C	6.0	2.4695579083	0.3436501261	0.4291440081
C	6.0	3.6514716485	1.1763284413	0.6810373055
C	6.0	3.5042250169	2.5626920184	1.0583070537
C	6.0	2.2358159248	3.1378631911	1.2177743651
C	6.0	1.0706064017	2.3294656503	1.0351086922
C	6.0	1.1631906801	0.9755479007	0.6357921198
N	7.0	-0.0494208942	0.1750046889	0.5823075530
C	6.0	-1.2458887368	0.6984292055	0.3202014191
C	6.0	-2.5499285069	0.0367489183	0.4352564561
C	6.0	-2.8219039027	-1.2859759218	0.9279238888
C	6.0	-4.1225449661	-1.8054060036	1.0582188683
C	6.0	-5.2320770449	-0.9882052784	0.6825291556
C	6.0	-5.0172021802	0.3250966604	0.1780584460
C	6.0	-3.6980155946	0.8254410722	0.0592727952
O	8.0	-1.6986109334	-2.1450532898	1.3141835326
N	7.0	1.6350943181	-1.9563109576	-0.4304596581
H	1.0	5.8428738441	1.2868013832	0.7713741845
H	1.0	6.2034958935	-1.1337438625	0.1251193326
H	1.0	4.2133340561	-2.5771514566	-0.4237516513
H	1.0	4.4169619198	3.1615396752	1.2308122533
H	1.0	2.1261480832	4.1936864441	1.5218942252
H	1.0	0.0854793186	2.7730530149	1.2633451086
H	1.0	-1.2918036499	1.7505952213	-0.0247679504
H	1.0	-4.2964804623	-2.8291835713	1.4412206045
H	1.0	-6.2571027649	-1.3883815859	0.7857453160
H	1.0	-5.8751657645	0.9560437354	-0.1131503819
H	1.0	-3.5335481241	1.8502037014	-0.3224988692
H	1.0	-2.0136395556	-2.9564608908	1.7894781400
H	1.0	1.2767123534	-1.6839087381	-1.3726357505
H	1.0	2.0306854775	-2.9118495704	-0.5351328840

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3798049	5.1742821	4.0138944
2 C	5.3798049	0.0000000	1.4016173 *	2.4414927 *

3 C	5.1742821	1.4016173 *	0.0000000	1.4320354 *
4 C	4.0138944	2.4414927 *	1.4320354 *	0.0000000
5 C	2.8179371 *	2.8383700 *	2.4725850 *	1.4075573 *
6 C	3.1392840	2.5314983 *	2.9230599 *	2.5078439 *
7 C	4.5516979	1.4441572 *	2.4800270 *	2.8453140 *
8 C	5.4501128	2.4853324 *	3.7797638	4.2888553
9 C	5.3082960	3.7782290	4.9555720	5.1788911
10 C	4.1677831	4.2916977	5.1846175	5.0061882
11 C	2.8988394 *	3.8350198	4.3837777	3.8926539
12 N	1.9395275 *	5.0511979	5.3232542	4.4913574
13 C	2.8586175 *	6.2327197	6.5856418	5.7611441
14 C	3.2612986	7.5556402	7.7752469	6.8039882
15 C	3.0116916	8.0424557	8.0604573	6.9508724
16 C	4.2833104	9.4360615	9.4107698	8.2568747
17 C	5.4420505	10.3410782	10.4322686	9.3296665
18 C	5.6093557	10.0108049	10.2555838	9.2591255
19 C	4.6950887	8.6966320	9.0171139	8.1000404
20 O	1.9522954 *	7.2707525	7.1184661	5.9487805
21 N	1.9780383 *	4.3426141	3.8152064	2.4746827 *
22 H	6.4398443	1.1050307 *	2.1800484 *	3.4513601
23 H	6.1220798	2.1870327 *	1.1042018 *	2.2012938 *
24 H	4.3397766	3.4391688	2.1943594 *	1.1079364 *
25 H	6.4999996	2.6816517 *	4.0812466	4.8910545
26 H	6.2803005	4.6688124	5.9305986	6.2528070
27 H	4.5243456	5.3916093	6.2678121	6.0075964
28 H	3.8755653	6.4006747	6.9340362	6.2704352
29 H	4.6214125	9.9391707	9.7936330	8.5837488
30 H	6.4225519	11.4198918	11.4773310	10.3448131
31 H	6.6750714	10.8829413	11.1905995	10.2321589
32 H	5.2779611	8.6483953	9.1035301	8.3069427
33 H	2.6571400 *	7.9539190	7.7052687	6.5054596
34 H	2.5018369 *	4.7767063	4.3257216	3.0586623
35 H	2.6193814 *	4.7364900	3.9160994	2.4847184 *

C C C C

1 CO	2.8179371 *	3.1392840	4.5516979	5.4501128
2 C	2.8383700 *	2.5314983 *	1.4441572 *	2.4853324 *
3 C	2.4725850 *	2.9230599 *	2.4800270 *	3.7797638
4 C	1.4075573 *	2.5078439 *	2.8453140 *	4.2888553
5 C	0.0000000	1.4575088 *	2.4753228 *	3.8151665
6 C	1.4575088 *	0.0000000	1.4675570 *	2.5279496 *
7 C	2.4753228 *	1.4675570 *	0.0000000	1.4443054 *
8 C	3.8151665	2.5279496 *	1.4443054 *	0.0000000
9 C	4.3642374	2.9127650 *	2.4778592 *	1.4018250 *
10 C	3.8856051	2.5035419 *	2.8488519 *	2.4448788 *

11 C	2.6242315 *	1.4658082 *	2.4967784 *	2.8597180 *
12 N	3.0922055	2.5292597 *	3.8352317	4.3076706
13 C	4.3542913	3.7339363	4.9338351	5.1559535
14 C	5.4136879	5.0288636	6.3100248	6.5894883
15 C	5.6465759	5.5591394	6.9302588	7.4060213
16 C	6.9893142	6.9620398	8.3347670	8.7890785
17 C	8.0027264	7.8200527	9.1434482	9.4378522
18 C	7.8764984	7.4909922	8.7248776	8.8541737
19 C	6.6991919	6.1974100	7.3840826	7.4758531
20 O	4.7652670	4.9346298	6.3289679	7.0212421
21 N	1.5099848 *	2.5932738 *	3.8877542	5.1118943
22 H	3.9431639	3.5193630	2.1960439 *	2.6794600 *
23 H	3.4664648	4.0270854	3.4868763	4.6712462
24 H	2.1826656 *	3.5070312	3.9528293	5.3960471
25 H	4.6721369	3.5178908	2.1975649 *	1.1051992 *
26 H	5.4683152	4.0168163	3.4839778	2.1849833 *
27 H	4.8016138	3.5045286	3.9503054	3.4313430
28 H	4.8939895	4.0414566	5.0263221	4.9834169
29 H	7.4081425	7.5412498	8.9326339	9.4905190
30 H	9.0402081	8.9040275	10.2356508	10.5341726
31 H	8.8411172	8.3847196	9.5622215	9.5878362
32 H	6.9081488	6.2347376	7.2859935	7.2072544
33 H	5.4372208	5.7306458	7.0994418	7.8385260
34 H	2.1119324 *	2.9631547 *	4.2471180	5.3763290
35 H	2.0883342 *	3.4235533	4.5628080	5.8890555

C C C N

1 CO	5.3082960	4.1677831	2.8988394 *	1.9395275 *
2 C	3.7782290	4.2916977	3.8350198	5.0511979
3 C	4.9555720	5.1846175	4.3837777	5.3232542
4 C	5.1788911	5.0061882	3.8926539	4.4913574
5 C	4.3642374	3.8856051	2.6242315 *	3.0922055
6 C	2.9127650 *	2.5035419 *	1.4658082 *	2.5292597 *
7 C	2.4778592 *	2.8488519 *	2.4967784 *	3.8352317
8 C	1.4018250 *	2.4448788 *	2.8597180 *	4.3076706
9 C	0.0000000	1.4298904 *	2.4829087 *	3.7953466
10 C	1.4298904 *	0.0000000	1.4146091 *	2.4700591 *
11 C	2.4829087 *	1.4146091 *	0.0000000	1.4540141 *
12 N	3.7953466	2.4700591 *	1.4540141 *	0.0000000
13 C	4.3449675	2.9219038 *	2.4454153 *	1.3319940 *
14 C	5.7560919	4.3271984	3.8352069	2.5086405 *
15 C	6.7256892	5.3136186	4.5913843	3.1528681
16 C	8.0554405	6.6382617	5.9875830	4.5539936
17 C	8.5487048	7.1312742	6.6901390	5.3125349
18 C	7.8484990	6.4663315	6.2313612	4.9864613

19	C	6.4730038	5.0945168	4.8975742	3.7428433
20	O	6.5877322	5.2695130	4.2881552	2.9390712 *
21	N	5.3877780	4.5644735	3.1552151	2.8992750 *
22	H	4.0787951	4.8919568	4.6919821	5.9992479
23	H	5.9315265	6.2584707	5.4876748	6.4047492
24	H	6.2663050	6.0066548	4.8008000	5.1727747
25	H	2.1813135 *	3.4538011	3.9647997	5.4118874
26	H	1.1042095 *	2.1969177 *	3.4740293	4.6653753
27	H	2.1815386 *	1.1042359 *	2.1877635 *	2.6892128 *
28	H	3.9890505	2.6531888 *	2.6578253 *	2.0963161 *
29	H	8.8502244	7.4553478	6.7031862	5.2726079
30	H	9.6334422	8.2206990	7.7891850	6.4047543
31	H	8.5041002	7.1727636	7.0781182	5.9188670
32	H	6.1086881	4.8240055	4.8726481	3.9704041
33	H	7.4515437	6.1662522	5.1849720	3.8886363
34	H	5.5569406	4.6847505	3.3345733	3.0059927
35	H	6.3018876	5.5550694	4.1515626	3.8864103

C C C C

1	CO	2.8586175 *	3.2612986	3.0116916	4.2833104
2	C	6.2327197	7.5556402	8.0424557	9.4360615
3	C	6.5856418	7.7752469	8.0604573	9.4107698
4	C	5.7611441	6.8039882	6.9508724	8.2568747
5	C	4.3542913	5.4136879	5.6465759	6.9893142
6	C	3.7339363	5.0288636	5.5591394	6.9620398
7	C	4.9338351	6.3100248	6.9302588	8.3347670
8	C	5.1559535	6.5894883	7.4060213	8.7890785
9	C	4.3449675	5.7560919	6.7256892	8.0554405
10	C	2.9219038 *	4.3271984	5.3136186	6.6382617
11	C	2.4454153 *	3.8352069	4.5913843	5.9875830
12	N	1.3319940 *	2.5086405 *	3.1528681	4.5539936
13	C	0.0000000	1.4668259 *	2.6059574 *	3.8844577
14	C	1.4668259 *	0.0000000	1.4374605 *	2.5009477 *
15	C	2.6059574 *	1.4374605 *	0.0000000	1.4065744 *
16	C	3.8844577	2.5009477 *	1.4065744 *	0.0000000
17	C	4.3434680	2.8819430 *	2.4408647 *	1.4282931 *
18	C	3.7924118	2.4973455 *	2.8243915 *	2.4726778 *
19	C	2.4692391 *	1.4427415 *	2.4454464 *	2.8459576 *
20	O	3.0460385	2.5015026 *	1.4659460 *	2.4609621 *
21	N	3.9888846	4.7155242	4.7073759	5.9488945
22	H	7.1274325	8.4920397	9.0400257	10.4380840
23	H	7.6738678	8.8367798	9.0623127	10.3898472
24	H	6.4098368	7.3015129	7.2793361	8.5016885
25	H	6.2421153	7.6768997	8.5013713	9.8804613
26	H	5.0031511	6.3503231	7.4069372	8.6746913

27 H	2.6393417 *	3.8882471	5.0041084	6.2218833
28 H	1.1082262 *	2.1752631 *	3.5312311	4.6723764
29 H	4.7965452	3.5037090	2.1952994 *	1.1068263 *
30 H	5.4482820	3.9871018	3.4396646	2.1919143 *
31 H	4.6566474	3.4932873	3.9284724	3.4741028
32 H	2.6406502 *	2.1977987 *	3.4504517	3.9518073
33 H	4.0132826	3.3287876	2.0459929 *	2.5114039 *
34 H	3.8606668	4.5686231	4.7169461	5.9224822
35 H	4.9499140	5.5333456	5.3227459	6.4517619

C C C O

1 CO	5.4420505	5.6093557	4.6950887	1.9522954 *
2 C	10.3410782	10.0108049	8.6966320	7.2707525
3 C	10.4322686	10.2555838	9.0171139	7.1184661
4 C	9.3296665	9.2591255	8.1000404	5.9487805
5 C	8.0027264	7.8764984	6.6991919	4.7652670
6 C	7.8200527	7.4909922	6.1974100	4.9346298
7 C	9.1434482	8.7248776	7.3840826	6.3289679
8 C	9.4378522	8.8541737	7.4758531	7.0212421
9 C	8.5487048	7.8484990	6.4730038	6.5877322
10 C	7.1312742	6.4663315	5.0945168	5.2695130
11 C	6.6901390	6.2313612	4.8975742	4.2881552
12 N	5.3125349	4.9864613	3.7428433	2.9390712 *
13 C	4.3434680	3.7924118	2.4692391 *	3.0460385
14 C	2.8819430 *	2.4973455 *	1.4427415 *	2.5015026 *
15 C	2.4408647 *	2.8243915 *	2.4454464 *	1.4659460 *
16 C	1.4282931 *	2.4726778 *	2.8459576 *	2.4609621 *
17 C	0.0000000	1.4231739 *	2.4558310 *	3.7712952
18 C	1.4231739 *	0.0000000	1.4158770 *	4.2901595
19 C	2.4558310 *	1.4158770 *	0.0000000	3.7942399
20 O	3.7712952	4.2901595	3.7942399	0.0000000
21 N	7.0238177	7.0589067	6.0349021	3.7673591
22 H	11.3065506	10.9187065	9.5785444	8.3033885
23 H	11.4500749	11.3152589	10.0936946	8.0548068
24 H	9.6418047	9.6947418	8.6255668	6.1772341
25 H	10.5178396	9.9074291	8.5254162	8.0973521
26 H	9.0388059	8.2340351	6.8851449	7.4061830
27 H	6.5391755	5.7626119	4.4224220	5.2319530
28 H	4.8504692	3.9939678	2.5793078 *	4.1393672
29 H	2.2000352 *	3.4733992	3.9527486	2.6894421 *
30 H	1.1052024 *	2.2006009 *	3.4608814	4.6509834
31 H	2.1969919 *	1.1040826 *	2.1878688 *	5.3942279
32 H	3.4571155	2.1858038 *	1.1058651 *	4.6912474
33 H	3.9316289	4.7314566	4.4870386	0.9917310 *
34 H	6.8609070	6.7863182	5.7528355	4.0353687

35 H	7.6112304	7.7884006	6.8657611	4.2326823
	N	H	H	H
1 CO	1.9780383 *	6.4398443	6.1220798	4.3397766
2 C	4.3426141	1.1050307 *	2.1870327 *	3.4391688
3 C	3.8152064	2.1800484 *	1.1042018 *	2.1943594 *
4 C	2.4746827 *	3.4513601	2.2012938 *	1.1079364 *
5 C	1.5099848 *	3.9431639	3.4664648	2.1826656 *
6 C	2.5932738 *	3.5193630	4.0270854	3.5070312
7 C	3.8877542	2.1960439 *	3.4868763	3.9528293
8 C	5.1118943	2.6794600 *	4.6712462	5.3960471
9 C	5.3877780	4.0787951	5.9315265	6.2663050
10 C	4.5644735	4.8919568	6.2584707	6.0066548
11 C	3.1552151	4.6919821	5.4876748	4.8008000
12 N	2.8992750 *	5.9992479	6.4047492	5.1727747
13 C	3.9888846	7.1274325	7.6738678	6.4098368
14 C	4.7155242	8.4920397	8.8367798	7.3015129
15 C	4.7073759	9.0400257	9.0623127	7.2793361
16 C	5.9488945	10.4380840	10.3898472	8.5016885
17 C	7.0238177	11.3065506	11.4500749	9.6418047
18 C	7.0589067	10.9187065	11.3152589	9.6947418
19 C	6.0349021	9.5785444	10.0936946	8.6255668
20 O	3.7673591	8.3033885	8.0548068	6.1772341
21 N	0.0000000	5.4467964	4.6749949	2.6519442 *
22 H	5.4467964	0.0000000	2.5311525 *	4.3604882
23 H	4.6749949	2.5311525 *	0.0000000	2.5190135 *
24 H	2.6519442 *	4.3604882	2.5190135 *	0.0000000
25 H	6.0573102	2.3997816 *	4.7816024	5.9759202
26 H	6.4711118	4.7777936	6.8525367	7.3475254
27 H	5.2571061	5.9664538	7.3477035	6.9649241
28 H	4.7405138	7.1939259	8.0325210	7.0139233
29 H	6.2808179	10.9634179	10.7170958	8.7154222
30 H	8.0055277	12.3921848	12.4806965	10.6068895
31 H	8.0614206	11.7560298	12.2604263	10.6938192
32 H	6.4199746	9.4568107	10.1938379	8.9233351
33 H	4.3865342	8.9870247	8.5798428	6.6194760
34 H	1.0441917 *	5.8542060	5.1787207	3.2127886
35 H	1.0394724 *	5.8196573	4.5836601	2.2109689 *

H H H H

1 CO	6.4999996	6.2803005	4.5243456	3.8755653
2 C	2.6816517 *	4.6688124	5.3916093	6.4006747
3 C	4.0812466	5.9305986	6.2678121	6.9340362
4 C	4.8910545	6.2528070	6.0075964	6.2704352

5 C	4.6721369	5.4683152	4.8016138	4.8939895
6 C	3.5178908	4.0168163	3.5045286	4.0414566
7 C	2.1975649 *	3.4839778	3.9503054	5.0263221
8 C	1.1051992 *	2.1849833 *	3.4313430	4.9834169
9 C	2.1813135 *	1.1042095 *	2.1815386 *	3.9890505
10 C	3.4538011	2.1969177 *	1.1042359 *	2.6531888 *
11 C	3.9647997	3.4740293	2.1877635 *	2.6578253 *
12 N	5.4118874	4.6653753	2.6892128 *	2.0963161 *
13 C	6.2421153	5.0031511	2.6393417 *	1.1082262 *
14 C	7.6768997	6.3503231	3.8882471	2.1752631 *
15 C	8.5013713	7.4069372	5.0041084	3.5312311
16 C	9.8804613	8.6746913	6.2218833	4.6723764
17 C	10.5178396	9.0388059	6.5391755	4.8504692
18 C	9.9074291	8.2340351	5.7626119	3.9939678
19 C	8.5254162	6.8851449	4.4224220	2.5793078 *
20 O	8.0973521	7.4061830	5.2319530	4.1393672
21 N	6.0573102	6.4711118	5.2571061	4.7405138
22 H	2.3997816 *	4.7777936	5.9664538	7.1939259
23 H	4.7816024	6.8525367	7.3477035	8.0325210
24 H	5.9759202	7.3475254	6.9649241	7.0139233
25 H	0.0000000	2.5294038 *	4.3489909	6.0130899
26 H	2.5294038 *	0.0000000	2.4998752 *	4.4769691
27 H	4.3489909	2.4998752 *	0.0000000	2.1451255 *
28 H	6.0130899	4.4769691	2.1451255 *	0.0000000
29 H	10.5762524	9.5172143	7.1146515	5.6702362
30 H	11.6118700	10.0985293	7.6009201	5.9299496
31 H	10.6112365	8.7850284	6.3816575	4.6525619
32 H	8.2062773	6.3973321	4.0575746	2.2636218 *
33 H	8.8935186	8.2664412	6.1245772	5.0959703
34 H	6.3338361	6.6065097	5.3133736	4.4955355
35 H	6.7600987	7.3979129	6.2718791	5.7478516

H H H H

1 CO	4.6214125	6.4225519	6.6750714	5.2779611
2 C	9.9391707	11.4198918	10.8829413	8.6483953
3 C	9.7936330	11.4773310	11.1905995	9.1035301
4 C	8.5837488	10.3448131	10.2321589	8.3069427
5 C	7.4081425	9.0402081	8.8411172	6.9081488
6 C	7.5412498	8.9040275	8.3847196	6.2347376
7 C	8.9326339	10.2356508	9.5622215	7.2859935
8 C	9.4905190	10.5341726	9.5878362	7.2072544
9 C	8.8502244	9.6334422	8.5041002	6.1086881
10 C	7.4553478	8.2206990	7.1727636	4.8240055
11 C	6.7031862	7.7891850	7.0781182	4.8726481
12 N	5.2726079	6.4047543	5.9188670	3.9704041

13 C	4.7965452	5.4482820	4.6566474	2.6406502 *
14 C	3.5037090	3.9871018	3.4932873	2.1977987 *
15 C	2.1952994 *	3.4396646	3.9284724	3.4504517
16 C	1.1068263 *	2.1919143 *	3.4741028	3.9518073
17 C	2.2000352 *	1.1052024 *	2.1969919 *	3.4571155
18 C	3.4733992	2.2006009 *	1.1040826 *	2.1858038 *
19 C	3.9527486	3.4608814	2.1878688 *	1.1058651 *
20 O	2.6894421 *	4.6509834	5.3942279	4.6912474
21 N	6.2808179	8.0055277	8.0614206	6.4199746
22 H	10.9634179	12.3921848	11.7560298	9.4568107
23 H	10.7170958	12.4806965	12.2604263	10.1938379
24 H	8.7154222	10.6068895	10.6938192	8.9233351
25 H	10.5762524	11.6118700	10.6112365	8.2062773
26 H	9.5172143	10.0985293	8.7850284	6.3973321
27 H	7.1146515	7.6009201	6.3816575	4.0575746
28 H	5.6702362	5.9299496	4.6525619	2.2636218 *
29 H	0.0000000	2.5198409 *	4.3859163	5.0586003
30 H	2.5198409 *	0.0000000	2.5397282 *	4.3742873
31 H	4.3859163	2.5397282 *	0.0000000	2.5152578 *
32 H	5.0586003	4.3742873	2.5152578 *	0.0000000
33 H	2.3127571 *	4.6339327	5.8171361	5.4657656
34 H	6.3474341	7.8424687	7.7269019	6.0606389
35 H	6.6291655	8.5295432	8.8114217	7.3268725

H H H

1 CO	2.6571400 *	2.5018369 *	2.6193814 *
2 C	7.9539190	4.7767063	4.7364900
3 C	7.7052687	4.3257216	3.9160994
4 C	6.5054596	3.0586623	2.4847184 *
5 C	5.4372208	2.1119324 *	2.0883342 *
6 C	5.7306458	2.9631547 *	3.4235533
7 C	7.0994418	4.2471180	4.5628080
8 C	7.8385260	5.3763290	5.8890555
9 C	7.4515437	5.5569406	6.3018876
10 C	6.1662522	4.6847505	5.5550694
11 C	5.1849720	3.3345733	4.1515626
12 N	3.8886363	3.0059927	3.8864103
13 C	4.0132826	3.8606668	4.9499140
14 C	3.3287876	4.5686231	5.5333456
15 C	2.0459929 *	4.7169461	5.3227459
16 C	2.5114039 *	5.9224822	6.4517619
17 C	3.9316289	6.8609070	7.6112304
18 C	4.7314566	6.7863182	7.7884006
19 C	4.4870386	5.7528355	6.8657611
20 O	0.9917310 *	4.0353687	4.2326823

21 N	4.3865342	1.0441917 *	1.0394724 *
22 H	8.9870247	5.8542060	5.8196573
23 H	8.5798428	5.1787207	4.5836601
24 H	6.6194760	3.2127886	2.2109689 *
25 H	8.8935186	6.3338361	6.7600987
26 H	8.2664412	6.6065097	7.3979129
27 H	6.1245772	5.3133736	6.2718791
28 H	5.0959703	4.4955355	5.7478516
29 H	2.3127571 *	6.3474341	6.6291655
30 H	4.6339327	7.8424687	8.5295432
31 H	5.8171361	7.7269019	8.8114217
32 H	5.4657656	6.0606389	7.3268725
33 H	0.0000000	4.7375910	4.6650157
34 H	4.7375910	0.0000000	1.6666509 *
35 H	4.6650157	1.6666509 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 7743.4 SECONDS (129.1 MIN)
WALL CLOCK TIME: STEP = 0.77 , TOTAL = 7159.3 SECONDS (119.3 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.99 , TOTAL = 7744.4 SECONDS (129.1 MIN)
WALL CLOCK TIME: STEP = 0.98 , TOTAL = 7160.3 SECONDS (119.3 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636909751	-284.636909751	0.003386508	0.000350742	198043299
11335935					
2 1	-284.636923788	-0.000014037	0.001722146	0.000053350	150897086
15316287					
3 2	-284.636923231	0.000000557	0.001226923	0.000127454	136541138
16440817					

4 3	-284.636924085	-0.000000854	0.000664187	0.000026627	131775066
16813356					
5 4	-284.636924037	0.000000048	0.000369538	0.000054113	122765342
17510029					
6 5	-284.636924116	-0.000000079	0.000196150	0.000009956	118040877
17867174					
7 6	-284.636924134	-0.000000018	0.000135105	0.000012432	110213867
18434104					
8 7	-284.636924132	0.000000001	0.000059756	0.000008839	104347448
18871051					
9 8	-284.636924133	0.000000000	0.000140813	0.000007921	103320656
18958900					
10 9	-284.636924136	-0.000000003	0.000144548	0.000005747	134473416
16719315					
11 10	-284.636924143	-0.000000007	0.000159023	0.000007248	154212391
15211627					
-----DISABLING FDIFF OPTION-----					
12 11	-284.636924132	0.000000011	0.000076696	0.000007893	198044070
11335948					
13 12	-284.636924134	-0.000000002	0.000073490	0.000006002	198044064
11335950					
14 13	-284.636924135	-0.000000001	0.000053275	0.000002698	198044051
11335945					
15 14	-284.636924136	-0.000000001	0.000061901	0.000002394	198044055
11335946					
16 15	-284.636924136	0.000000000	0.000037562	0.000002418	198044012
11335950					
17 16	-284.636924137	0.000000000	0.000021440	0.000002081	198044052
11335950					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 55.9 SECONDS (3.3 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 18.6 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
 TIME TO SOLVE SCF EQUATIONS= 1.5 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369241365 AFTER 17 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6012985336
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998514633

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 58.55 , TOTAL = 7803.0 SECONDS (130.0 MIN)
WALL CLOCK TIME: STEP = 53.87 , TOTAL = 7214.2 SECONDS (120.2 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.70 , TOTAL = 7806.7 SECONDS (130.1 MIN)
WALL CLOCK TIME: STEP = 3.67 , TOTAL = 7217.9 SECONDS (120.3 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.88 , TOTAL = 7809.5 SECONDS (130.2 MIN)
WALL CLOCK TIME: STEP = 2.71 , TOTAL = 7220.6 SECONDS (120.3 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 84 ENERGY= -284.6369241

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000853	-0.0000510	-0.0002000
2 C	6.0	-0.0000433	0.0000705	-0.0000078
3 C	6.0	0.0000850	-0.0000978	-0.0000441
4 C	6.0	0.0000386	0.0000661	0.0000195
5 C	6.0	0.0001065	0.0000955	-0.0000142
6 C	6.0	0.0000614	0.0001214	-0.0000274
7 C	6.0	0.0000546	0.0000237	0.0000310
8 C	6.0	0.0000880	0.0000369	0.0001687

9 C	6.0	0.0000336	-0.0000859	0.0000683
10 C	6.0	-0.0000941	0.0000043	-0.0000846
11 C	6.0	0.0000254	-0.0000151	-0.0000587
12 N	7.0	0.0001041	0.0000560	0.0000615
13 C	6.0	0.0001973	-0.0001698	0.0000045
14 C	6.0	0.0000022	-0.0000965	-0.0000115
15 C	6.0	-0.0001091	0.0000949	0.0000260
16 C	6.0	-0.0001487	0.0001682	0.0001579
17 C	6.0	-0.0000182	-0.0000804	-0.0000045
18 C	6.0	0.0000636	0.0000619	-0.0000324
19 C	6.0	0.0000674	0.0000348	-0.0000889
20 O	8.0	-0.0000294	-0.0000127	-0.0001418
21 N	7.0	0.0000608	0.0000823	0.0001050
22 H	1.0	-0.0000824	0.0000129	0.0001304
23 H	1.0	0.0000367	-0.0000008	-0.0000415
24 H	1.0	-0.0000063	-0.0000862	0.0000199
25 H	1.0	0.0001100	0.0000884	-0.0001031
26 H	1.0	-0.0001096	-0.0000707	0.0000050
27 H	1.0	-0.0001532	-0.0000995	-0.0001235
28 H	1.0	-0.0000920	-0.0000151	0.0000941
29 H	1.0	-0.0001581	0.0000002	-0.0000639
30 H	1.0	-0.0000284	0.0000431	0.0001037
31 H	1.0	-0.0000137	-0.0000659	0.0001592
32 H	1.0	-0.0000253	-0.0000402	-0.0000305
33 H	1.0	0.0000456	0.0000893	-0.0000195
34 H	1.0	-0.0000191	-0.0001266	-0.0000998
35 H	1.0	0.0000355	-0.0000364	0.0000430

MAXIMUM GRADIENT = 0.0002000 RMS GRADIENT = 0.0000832
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000067552
 PREDICTED ENERGY CHANGE WAS -0.0000047184 RATIO= 1.432
 GDIIS STEP HAS LENGTH = 0.020874
 RADIUS OF STEP TAKEN= 0.02087 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 7809.6 SECONDS (130.2 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7220.6 SECONDS (120.3 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 85

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM CHARGE X Y Z

CO	27.0	0.1558634731	-1.7314094052	0.8651935143
C	6.0	4.9817750277	0.6249348311	0.5666136952
C	6.0	5.1850811456	-0.7138838571	0.2050179516
C	6.0	4.0485882507	-1.5334090534	-0.0911215013
C	6.0	2.7403526706	-1.0216516037	-0.0019982428
C	6.0	2.4693786614	0.3434941273	0.4306112738
C	6.0	3.6517132247	1.1755538029	0.6825710346
C	6.0	3.5047956420	2.5622356845	1.0587211069
C	6.0	2.2367832074	3.1385132337	1.2171723059
C	6.0	1.0712911996	2.3304500998	1.0354455557
C	6.0	1.1632817846	0.9763258347	0.6369592591
N	7.0	-0.0497756599	0.1762282207	0.5840015974
C	6.0	-1.2462223765	0.6990750501	0.3204740426
C	6.0	-2.5498986679	0.0364877627	0.4350079104
C	6.0	-2.8216899946	-1.2861431340	0.9283641358
C	6.0	-4.1221578017	-1.8060925915	1.0586348142
C	6.0	-5.2320508776	-0.9892142621	0.6822994623
C	6.0	-5.0171490513	0.3237980385	0.1767822310
C	6.0	-3.6980319672	0.8244474233	0.0580368518
O	8.0	-1.6983459545	-2.1446568579	1.3160342077
N	7.0	1.6335449054	-1.9548183863	-0.4306228392
H	1.0	5.8437155841	1.2852592260	0.7726309689
H	1.0	6.2029379624	-1.1339757128	0.1229387215
H	1.0	4.2121027782	-2.5762758586	-0.4271135913
H	1.0	4.4177299197	3.1606869496	1.2311701043
H	1.0	2.1277715061	4.1947284119	1.5204233947
H	1.0	0.0864498635	2.7739526015	1.2650018243
H	1.0	-1.2922970989	1.7506149950	-0.0263740429
H	1.0	-4.2950924817	-2.8295945654	1.4431046967
H	1.0	-6.2572106710	-1.3895342460	0.7854351553
H	1.0	-5.8748438427	0.9544808531	-0.1156030445
H	1.0	-3.5329512568	1.8489300517	-0.3245638503
H	1.0	-2.0134646397	-2.9567390858	1.7899828452
H	1.0	1.2760348252	-1.6811190676	-1.3726046294
H	1.0	2.0279877099	-2.9105745104	-0.5357399195

 INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3787480	5.1734148	4.0133588
2 C	5.3787480	0.0000000	1.4016135 *	2.4417005 *
3 C	5.1734148	1.4016135 *	0.0000000	1.4321090 *
4 C	4.0133588	2.4417005 *	1.4321090 *	0.0000000

5 C	2.8169775 *	2.8387569 *	2.4727058 *	1.4075933 *
6 C	3.1379036	2.5317664 *	2.9230088 *	2.5077627 *
7 C	4.5502474	1.4441924 *	2.4797679 *	2.8450992 *
8 C	5.4486868	2.4853113 *	3.7795671	4.2886075
9 C	5.3075665	3.7783969	4.9555908	5.1789119
10 C	4.1672169	4.2919074	5.1846742	5.0062819
11 C	2.8980705 *	3.8352725	4.3838627	3.8927965
12 N	1.9391848 *	5.0515485	5.3235002	4.4916854
13 C	2.8582895 *	6.2333003	6.5857003	5.7609388
14 C	3.2606240	7.5557725	7.7746939	6.8030447
15 C	3.0113248	8.0422104	8.0597205	6.9499075
16 C	4.2830437	9.4357603	9.4099032	8.2557487
17 C	5.4418678	10.3412330	10.4316942	9.3286972
18 C	5.6087295	10.0110506	10.2549053	9.2578930
19 C	4.6942961	8.6969825	9.0165273	8.0988802
20 O	1.9524660 *	7.2702328	7.1177972	5.9481900
21 N	1.9780278 *	4.3428392	3.8154118	2.4749306 *
22 H	6.4389843	1.1051755 *	2.1800360 *	3.4515853
23 H	6.1216811	2.1867448 *	1.1041950 *	2.2014975 *
24 H	4.3401537	3.4391335	2.1942610 *	1.1077901 *
25 H	6.4984653	2.6813841 *	4.0809454	4.8907318
26 H	6.2798771	4.6688880	5.9305909	6.2528532
27 H	4.5235994	5.3916817	6.2677436	6.0075765
28 H	3.8751201	6.4017788	6.9342430	6.2700927
29 H	4.6207143	9.9379213	9.7919754	8.5820135
30 H	6.4226755	11.4201912	11.4769085	10.3440100
31 H	6.6742340	10.8830232	11.1896461	10.2305767
32 H	5.2765242	8.6482903	9.1023382	8.3050861
33 H	2.6575652 *	7.9535148	7.7046463	6.5048372
34 H	2.5030089 *	4.7760824	4.3249370	3.0579519
35 H	2.6187581 *	4.7370739	3.9168113	2.4853766 *

C C C C

1 CO	2.8169775 *	3.1379036	4.5502474	5.4486868
2 C	2.8387569 *	2.5317664 *	1.4441924 *	2.4853113 *
3 C	2.4727058 *	2.9230088 *	2.4797679 *	3.7795671
4 C	1.4075933 *	2.5077627 *	2.8450992 *	4.2886075
5 C	0.0000000	1.4574638 *	2.4752626 *	3.8149373
6 C	1.4574638 *	0.0000000	1.4675565 *	2.5277311 *
7 C	2.4752626 *	1.4675565 *	0.0000000	1.4442854 *
8 C	3.8149373	2.5277311 *	1.4442854 *	0.0000000
9 C	4.3642789	2.9128870 *	2.4781112 *	1.4018053 *
10 C	3.8856971	2.5036907 *	2.8490145 *	2.4446288 *
11 C	2.6243729 *	1.4659279 *	2.4968106 *	2.8593146 *
12 N	3.0924308	2.5293566 *	3.8352819	4.3073620

13	C	4.3540406	3.7342013	4.9343611	5.1564085
14	C	5.4127066	5.0286596	6.3102099	6.5899730
15	C	5.6455158	5.5586764	6.9300300	7.4061753
16	C	6.9881571	6.9615723	8.3345492	8.7893521
17	C	8.0017832	7.8199409	9.1437129	9.4385898
18	C	7.8753432	7.4908554	8.7252784	8.8550528
19	C	6.6980954	6.1973447	7.3845835	7.4767642
20	O	4.7644932	4.9340447	6.3283653	7.0209494
21	N	1.5098155 *	2.5927944 *	3.8873428	5.1111156
22	H	3.9436974	3.5199501	2.1965929 *	2.6801237 *
23	H	3.4666587	4.0270392	3.4865259	4.6709356
24	H	2.1825737 *	3.5068271	3.9524249	5.3955805
25	H	4.6718577	3.5176046	2.1973839 *	1.1051387 *
26	H	5.4684224	4.0170127	3.4842230	2.1850394 *
27	H	4.8015727	3.5045236	3.9503427	3.4311024
28	H	4.8937021	4.0421565	5.0275776	4.9848027
29	H	7.4063803	7.5400069	8.9314806	9.4898809
30	H	9.0394433	8.9040805	10.2360652	10.5350813
31	H	8.8396616	8.3843726	9.5624916	9.5886156
32	H	6.9064195	6.2341472	7.2860936	7.2077849
33	H	5.4364086	5.7302107	7.0990454	7.8386876
34	H	2.1113233 *	2.9622147 *	4.2459598	5.3744562
35	H	2.0881508 *	3.4231014	4.5625882	5.8885413

C C C N

1	CO	5.3075665	4.1672169	2.8980705 *	1.9391848 *
2	C	3.7783969	4.2919074	3.8352725	5.0515485
3	C	4.9555908	5.1846742	4.3838627	5.3235002
4	C	5.1789119	5.0062819	3.8927965	4.4916854
5	C	4.3642789	3.8856971	2.6243729 *	3.0924308
6	C	2.9128870 *	2.5036907 *	1.4659279 *	2.5293566 *
7	C	2.4781112 *	2.8490145 *	2.4968106 *	3.8352819
8	C	1.4018053 *	2.4446288 *	2.8593146 *	4.3073620
9	C	0.0000000	1.4298120 *	2.4827619 *	3.7953115
10	C	1.4298120 *	0.0000000	1.4145339 *	2.4700738 *
11	C	2.4827619 *	1.4145339 *	0.0000000	1.4541214 *
12	N	3.7953115	2.4700738 *	1.4541214 *	0.0000000
13	C	4.3458318	2.9229160 *	2.4459643 *	1.3320287 *
14	C	5.7573142	4.3284876	3.8355950	2.5084540 *
15	C	6.7267485	5.3147451	4.5916972	3.1528756
16	C	8.0566986	6.6395358	5.9879491	4.5540278
17	C	8.5503044	7.1328119	6.6907162	5.3126166
18	C	7.8501316	6.4678482	6.2317959	4.9862213
19	C	6.4746063	5.0960588	4.8980189	3.7425394
20	O	6.5883914	5.2703133	4.2884250	2.9394155 *

21 N	5.3871284	4.5638812	3.1547560	2.8990327 *
22 H	4.0794765	4.8925995	4.6925800	5.9998975
23 H	5.9314326	6.2584913	5.4877795	6.4051261
24 H	6.2661294	6.0066410	4.8008894	5.1732234
25 H	2.1811043 *	3.4534408	3.9643351	5.4115088
26 H	1.1042804 *	2.1970179 *	3.4740271	4.6655055
27 H	2.1815420 *	1.1042205 *	2.1875709 *	2.6889572 *
28 H	3.9908742	2.6552249 *	2.6588348 *	2.0964522 *
29 H	8.8506924	7.4558917	6.7028912	5.2721669
30 H	9.6352241	8.2223919	7.7899324	6.4050322
31 H	8.5055735	7.1740502	7.0782794	5.9183227
32 H	6.1098127	4.8249908	4.8724295	3.9693746
33 H	7.4528397	6.1676101	5.1855743	3.8892093
34 H	5.5550731	4.6833015	3.3336277	3.0059641
35 H	6.3014093	5.5544785	4.1510160	3.8857783

C C C C

1 CO	2.8582895 *	3.2606240	3.0113248	4.2830437
2 C	6.2333003	7.5557725	8.0422104	9.4357603
3 C	6.5857003	7.7746939	8.0597205	9.4099032
4 C	5.7609388	6.8030447	6.9499075	8.2557487
5 C	4.3540406	5.4127066	5.6455158	6.9881571
6 C	3.7342013	5.0286596	5.5586764	6.9615723
7 C	4.9343611	6.3102099	6.9300300	8.3345492
8 C	5.1564085	6.5899730	7.4061753	8.7893521
9 C	4.3458318	5.7573142	6.7267485	8.0566986
10 C	2.9229160 *	4.3284876	5.3147451	6.6395358
11 C	2.4459643 *	3.8355950	4.5916972	5.9879491
12 N	1.3320287 *	2.5084540 *	3.1528756	4.5540278
13 C	0.0000000	1.4668714 *	2.6062847 *	3.8848103
14 C	1.4668714 *	0.0000000	1.4375755 *	2.5012020 *
15 C	2.6062847 *	1.4375755 *	0.0000000	1.4066039 *
16 C	3.8848103	2.5012020 *	1.4066039 *	0.0000000
17 C	4.3437389	2.8822141 *	2.4410150 *	1.4285591 *
18 C	3.7922774	2.4973090 *	2.8243276 *	2.4728743 *
19 C	2.4690002 *	1.4426357 *	2.4454115 *	2.8461939 *
20 O	3.0466977	2.5017476 *	1.4660272 *	2.4608421 *
21 N	3.9875251	4.7133658	4.7056445	5.9471103
22 H	7.1284836	8.4927133	9.0402222	10.4382415
23 H	7.6739224	8.8362617	9.0617755	10.3891708
24 H	6.4093778	7.3003048	7.2784616	8.5006194
25 H	6.2425360	7.6773917	8.5014816	9.8807059
26 H	5.0043287	6.3521406	7.4086204	8.6766767
27 H	2.6406940 *	3.8901076	5.0054950	6.2234861
28 H	1.1082250 *	2.1754694 *	3.5316381	4.6728497

29 H	4.7966048	3.5037678	2.1950205 *	1.1069236 *
30 H	5.4487137	3.9875431	3.4400466	2.1923982 *
31 H	4.6561284	3.4930136	3.9283599	3.4744077
32 H	2.6395775 *	2.1973367 *	3.4502761	3.9521631
33 H	4.0141118	3.3291328	2.0460953 *	2.5110643 *
34 H	3.8592254	4.5667717	4.7161226	5.9217419
35 H	4.9480424	5.5303319	5.3199391	6.4487364

C C C O

1 CO	5.4418678	5.6087295	4.6942961	1.9524660 *
2 C	10.3412330	10.0110506	8.6969825	7.2702328
3 C	10.4316942	10.2549053	9.0165273	7.1177972
4 C	9.3286972	9.2578930	8.0988802	5.9481900
5 C	8.0017832	7.8753432	6.6980954	4.7644932
6 C	7.8199409	7.4908554	6.1973447	4.9340447
7 C	9.1437129	8.7252784	7.3845835	6.3283653
8 C	9.4385898	8.8550528	7.4767642	7.0209494
9 C	8.5503044	7.8501316	6.4746063	6.5883914
10 C	7.1328119	6.4678482	5.0960588	5.2703133
11 C	6.6907162	6.2317959	4.8980189	4.2884250
12 N	5.3126166	4.9862213	3.7425394	2.9394155 *
13 C	4.3437389	3.7922774	2.4690002 *	3.0466977
14 C	2.8822141 *	2.4973090 *	1.4426357 *	2.5017476 *
15 C	2.4410150 *	2.8243276 *	2.4454115 *	1.4660272 *
16 C	1.4285591 *	2.4728743 *	2.8461939 *	2.4608421 *
17 C	0.0000000	1.4232820 *	2.4560714 *	3.7714371
18 C	1.4232820 *	0.0000000	1.4159167 *	4.2901770
19 C	2.4560714 *	1.4159167 *	0.0000000	3.7943223
20 O	3.7714371	4.2901770	3.7943223	0.0000000
21 N	7.0219223	7.0563988	6.0323145	3.7667421
22 H	11.3072540	10.9196073	9.5795584	8.3031502
23 H	11.4495769	11.3145197	10.0930094	8.0545168
24 H	9.6406224	9.6929979	8.6238345	6.1772375
25 H	10.5186125	9.9084113	8.5264206	8.0969290
26 H	9.0411669	8.2364655	6.8874781	7.4073447
27 H	6.5412091	5.7649112	4.4248884	5.2326685
28 H	4.8508290	3.9939456	2.5792386 *	4.1400578
29 H	2.2008442 *	3.4740212	3.9530896	2.6885645 *
30 H	1.1053713 *	2.2008450 *	3.4612453	4.6513431
31 H	2.1972214 *	1.1040337 *	2.1875944 *	5.3941982
32 H	3.4577126	2.1863711 *	1.1059835 *	4.6910633
33 H	3.9315918	4.7314332	4.4871790	0.9916676 *
34 H	6.8597772	6.7841326	5.7502990	4.0361599
35 H	7.6081144	7.7847804	6.8622344	4.2309880

	N	H	H	H
1 CO	1.9780278 *	6.4389843	6.1216811	4.3401537
2 C	4.3428392	1.1051755 *	2.1867448 *	3.4391335
3 C	3.8154118	2.1800360 *	1.1041950 *	2.1942610 *
4 C	2.4749306 *	3.4515853	2.2014975 *	1.1077901 *
5 C	1.5098155 *	3.9436974	3.4666587	2.1825737 *
6 C	2.5927944 *	3.5199501	4.0270392	3.5068271
7 C	3.8873428	2.1965929 *	3.4865259	3.9524249
8 C	5.1111156	2.6801237 *	4.6709356	5.3955805
9 C	5.3871284	4.0794765	5.9314326	6.2661294
10 C	4.5638812	4.8925995	6.2584913	6.0066410
11 C	3.1547560	4.6925800	5.4877795	4.8008894
12 N	2.8990327 *	5.9998975	6.4051261	5.1732234
13 C	3.9875251	7.1284836	7.6739224	6.4093778
14 C	4.7133658	8.4927133	8.8362617	7.3003048
15 C	4.7056445	9.0402222	9.0617755	7.2784616
16 C	5.9471103	10.4382415	10.3891708	8.5006194
17 C	7.0219223	11.3072540	11.4495769	9.6406224
18 C	7.0563988	10.9196073	11.3145197	9.6929979
19 C	6.0323145	9.5795584	10.0930094	8.6238345
20 O	3.7667421	8.3031502	8.0545168	6.1772375
21 N	0.0000000	5.4471515	4.6754215	2.6523918 *
22 H	5.4471515	0.0000000	2.5305806 *	4.3603900
23 H	4.6754215	2.5305806 *	0.0000000	2.5191689 *
24 H	2.6523918 *	4.3603900	2.5191689 *	0.0000000
25 H	6.0565367	2.4001922 *	4.7811371	5.9753602
26 H	6.4705307	4.7783308	6.8523742	7.3473693
27 H	5.2564171	5.9669712	7.3476281	6.9648554
28 H	4.7385868	7.1956683	8.0325405	7.0129163
29 H	6.2789195	10.9625264	10.7157176	8.7140265
30 H	8.0038970	12.3930263	12.4803652	10.6059019
31 H	8.0584838	11.7568282	12.2593379	10.6915749
32 H	6.4165749	9.4574543	10.1924248	8.9206965
33 H	4.3858424	8.9869258	8.5796721	6.6195135
34 H	1.0440567 *	5.8536436	5.1778751	3.2118148
35 H	1.0392808 *	5.8203638	4.5847978	2.2122192 *

	H	H	H	H
1 CO	6.4984653	6.2798771	4.5235994	3.8751201
2 C	2.6813841 *	4.6688880	5.3916817	6.4017788
3 C	4.0809454	5.9305909	6.2677436	6.9342430
4 C	4.8907318	6.2528532	6.0075765	6.2700927
5 C	4.6718577	5.4684224	4.8015727	4.8937021
6 C	3.5176046	4.0170127	3.5045236	4.0421565

7 C	2.1973839 *	3.4842230	3.9503427	5.0275776
8 C	1.1051387 *	2.1850394 *	3.4311024	4.9848027
9 C	2.1811043 *	1.1042804 *	2.1815420 *	3.9908742
10 C	3.4534408	2.1970179 *	1.1042205 *	2.6552249 *
11 C	3.9643351	3.4740271	2.1875709 *	2.6588348 *
12 N	5.4115088	4.6655055	2.6889572 *	2.0964522 *
13 C	6.2425360	5.0043287	2.6406940 *	1.1082250 *
14 C	7.6773917	6.3521406	3.8901076	2.1754694 *
15 C	8.5014816	7.4086204	5.0054950	3.5316381
16 C	9.8807059	8.6766767	6.2234861	4.6728497
17 C	10.5186125	9.0411669	6.5412091	4.8508290
18 C	9.9084113	8.2364655	5.7649112	3.9939456
19 C	8.5264206	6.8874781	4.4248884	2.5792386 *
20 O	8.0969290	7.4073447	5.2326685	4.1400578
21 N	6.0565367	6.4705307	5.2564171	4.7385868
22 H	2.4001922 *	4.7783308	5.9669712	7.1956683
23 H	4.7811371	6.8523742	7.3476281	8.0325405
24 H	5.9753602	7.3473693	6.9648554	7.0129163
25 H	0.0000000	2.5291933 *	4.3486429	6.0144932
26 H	2.5291933 *	0.0000000	2.5001676 *	4.4791899
27 H	4.3486429	2.5001676 *	0.0000000	2.1484447 *
28 H	6.0144932	4.4791899	2.1484447 *	0.0000000
29 H	10.5755219	9.5184176	7.1154322	5.6704909
30 H	11.6128183	10.1010952	7.6030675	5.9304248
31 H	10.6121731	8.7873568	6.3838523	4.6520454
32 H	8.2069693	6.3992601	4.0598584	2.2625459 *
33 H	8.8935615	8.2683727	6.1258529	5.0969027
34 H	6.3319015	6.6045931	5.3122259	4.4928236
35 H	6.7596638	7.3975059	6.2710516	5.7454706

H H H H

1 CO	4.6207143	6.4226755	6.6742340	5.2765242
2 C	9.9379213	11.4201912	10.8830232	8.6482903
3 C	9.7919754	11.4769085	11.1896461	9.1023382
4 C	8.5820135	10.3440100	10.2305767	8.3050861
5 C	7.4063803	9.0394433	8.8396616	6.9064195
6 C	7.5400069	8.9040805	8.3843726	6.2341472
7 C	8.9314806	10.2360652	9.5624916	7.2860936
8 C	9.4898809	10.5350813	9.5886156	7.2077849
9 C	8.8506924	9.6352241	8.5055735	6.1098127
10 C	7.4558917	8.2223919	7.1740502	4.8249908
11 C	6.7028912	7.7899324	7.0782794	4.8724295
12 N	5.2721669	6.4050322	5.9183227	3.9693746
13 C	4.7966048	5.4487137	4.6561284	2.6395775 *
14 C	3.5037678	3.9875431	3.4930136	2.1973367 *

15 C	2.1950205 *	3.4400466	3.9283599	3.4502761
16 C	1.1069236 *	2.1923982 *	3.4744077	3.9521631
17 C	2.2008442 *	1.1053713 *	2.1972214 *	3.4577126
18 C	3.4740212	2.2008450 *	1.1040337 *	2.1863711 *
19 C	3.9530896	3.4612453	2.1875944 *	1.1059835 *
20 O	2.6885645 *	4.6513431	5.3941982	4.6910633
21 N	6.2789195	8.0038970	8.0584838	6.4165749
22 H	10.9625264	12.3930263	11.7568282	9.4574543
23 H	10.7157176	12.4803652	12.2593379	10.1924248
24 H	8.7140265	10.6059019	10.6915749	8.9206965
25 H	10.5755219	11.6128183	10.6121731	8.2069693
26 H	9.5184176	10.1010952	8.7873568	6.3992601
27 H	7.1154322	7.6030675	6.3838523	4.0598584
28 H	5.6704909	5.9304248	4.6520454	2.2625459 *
29 H	0.0000000	2.5211527 *	4.3868452	5.0590616
30 H	2.5211527 *	0.0000000	2.5401734 *	4.3750815
31 H	4.3868452	2.5401734 *	0.0000000	2.5155844 *
32 H	5.0590616	4.3750815	2.5155844 *	0.0000000
33 H	2.3113450 *	4.6340724	5.8171426	5.4657665
34 H	6.3470209	7.8416800	7.7240861	6.0568955
35 H	6.6259887	8.5266394	8.8073784	7.3226717

H H H

1 CO	2.6575652 *	2.5030089 *	2.6187581 *
2 C	7.9535148	4.7760824	4.7370739
3 C	7.7046463	4.3249370	3.9168113
4 C	6.5048372	3.0579519	2.4853766 *
5 C	5.4364086	2.1113233 *	2.0881508 *
6 C	5.7302107	2.9622147 *	3.4231014
7 C	7.0990454	4.2459598	4.5625882
8 C	7.8386876	5.3744562	5.8885413
9 C	7.4528397	5.5550731	6.3014093
10 C	6.1676101	4.6833015	5.5544785
11 C	5.1855743	3.3336277	4.1510160
12 N	3.8892093	3.0059641	3.8857783
13 C	4.0141118	3.8592254	4.9480424
14 C	3.3291328	4.5667717	5.5303319
15 C	2.0460953 *	4.7161226	5.3199391
16 C	2.5110643 *	5.9217419	6.4487364
17 C	3.9315918	6.8597772	7.6081144
18 C	4.7314332	6.7841326	7.7847804
19 C	4.4871790	5.7502990	6.8622344
20 O	0.9916676 *	4.0361599	4.2309880
21 N	4.3858424	1.0440567 *	1.0392808 *
22 H	8.9869258	5.8536436	5.8203638

23 H	8.5796721	5.1778751	4.5847978
24 H	6.6195135	3.2118148	2.2122192 *
25 H	8.8935615	6.3319015	6.7596638
26 H	8.2683727	6.6045931	7.3975059
27 H	6.1258529	5.3122259	6.2710516
28 H	5.0969027	4.4928236	5.7454706
29 H	2.3113450 *	6.3470209	6.6259887
30 H	4.6340724	7.8416800	8.5266394
31 H	5.8171426	7.7240861	8.8073784
32 H	5.4657665	6.0568955	7.3226717
33 H	0.0000000	4.7381402	4.6630950
34 H	4.7381402	0.0000000	1.6665342 *
35 H	4.6630950	1.6665342 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.69 , TOTAL = 7810.3 SECONDS (130.2 MIN)
WALL CLOCK TIME: STEP = 0.69 , TOTAL = 7221.3 SECONDS (120.4 MIN)

CPU UTILIZATION: STEP = 99.43%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.06 , TOTAL = 7811.3 SECONDS (130.2 MIN)
WALL CLOCK TIME: STEP = 1.07 , TOTAL = 7222.4 SECONDS (120.4 MIN)

CPU UTILIZATION: STEP = 99.30%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636916999	-284.636916999	0.004031218	0.000341738	198058292
11335030					
2 1	-284.636927883	-0.000010885	0.001469264	0.000040418	148808086
15498265					
3 2	-284.636927724	0.000000159	0.001006916	0.000095290	133839717
16659685					
4 3	-284.636928087	-0.000000363	0.000557573	0.000015526	127598633
17139527					

5 4	-284.636928049	0.000000038	0.000327472	0.000025687	120091606
17688622					
6 5	-284.636928091	-0.000000043	0.000078464	0.000010774	114590742
18099225					
7 6	-284.636928082	0.000000010	0.000067982	0.000011402	106527405
18703557					
8 7	-284.636928090	-0.000000008	0.000137776	0.000009864	127384757
17277055					
9 8	-284.636928095	-0.000000004	0.000089546	0.000008194	157064158
14889391					
10 9	-284.636928100	-0.000000005	0.000085523	0.000008574	151207285
15384565					
11 10	-284.636928104	-0.000000003	0.000111008	0.000008750	152076620
15296956					
-----DISABLING FDIFF OPTION-----					
12 11	-284.636928129	-0.000000026	0.000110306	0.000007138	198057814
11335073					
13 12	-284.636928132	-0.000000002	0.000062487	0.000003959	198057617
11335073					
14 13	-284.636928132	-0.000000001	0.000032757	0.000002843	198057623
11335072					
15 14	-284.636928133	-0.000000001	0.000018910	0.000002376	198057649
11335070					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 50.1 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 16.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369281329 AFTER 15 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6011470817
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998503355

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 53.21 , TOTAL = 7864.5 SECONDS (131.1 MIN)
 WALL CLOCK TIME: STEP = 48.87 , TOTAL = 7271.2 SECONDS (121.2 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
 END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.67 , TOTAL = 7868.2 SECONDS (131.1 MIN)
 WALL CLOCK TIME: STEP = 3.64 , TOTAL = 7274.9 SECONDS (121.2 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
 USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.89 , TOTAL = 7871.1 SECONDS (131.2 MIN)
 WALL CLOCK TIME: STEP = 2.70 , TOTAL = 7277.6 SECONDS (121.3 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 85 ENERGY= -284.6369281

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000280	0.0000340	-0.0002034
2 C	6.0	-0.0000114	0.0000867	0.0000170
3 C	6.0	0.0000779	-0.0000856	-0.0000084
4 C	6.0	0.0000344	-0.0000454	0.0000344
5 C	6.0	0.0000273	0.0000238	-0.0000298
6 C	6.0	0.0000557	0.0000382	0.0000035
7 C	6.0	0.0000726	-0.0000772	0.0000564
8 C	6.0	0.0000340	-0.0000118	0.0001260
9 C	6.0	-0.0000069	-0.0001091	0.0000011
10 C	6.0	-0.0000118	0.0000336	-0.0001529
11 C	6.0	0.0000779	0.0000831	-0.0000499
12 N	7.0	0.0000310	0.0000038	0.0000805
13 C	6.0	0.0001023	-0.0000614	0.0000500
14 C	6.0	-0.0000122	-0.0000470	-0.0000968

15 C	6.0	-0.0001380	0.0000843	-0.0000195
16 C	6.0	-0.0000761	0.0000210	0.0001282
17 C	6.0	-0.0000904	0.0000100	0.0000175
18 C	6.0	0.0000319	0.0000921	-0.0000180
19 C	6.0	0.0000467	-0.0000045	-0.0000558
20 O	8.0	-0.0000680	-0.0001037	-0.0000233
21 N	7.0	0.0000098	0.0000390	0.0000134
22 H	1.0	0.0000332	0.0000364	0.0001372
23 H	1.0	0.0000481	0.0000589	-0.0000749
24 H	1.0	-0.0000121	0.0000264	-0.0000115
25 H	1.0	0.0000698	0.0000605	-0.0000972
26 H	1.0	-0.0001128	-0.0000197	0.0000182
27 H	1.0	-0.0001169	-0.0001291	-0.0000416
28 H	1.0	-0.0000988	-0.0000494	0.0000399
29 H	1.0	-0.0000838	-0.0000593	0.0000025
30 H	1.0	-0.0001376	0.0000043	0.0001013
31 H	1.0	0.0000459	-0.0000583	0.0001370
32 H	1.0	0.0000853	0.0000215	-0.0000596
33 H	1.0	0.0000541	0.0001127	-0.0000646
34 H	1.0	0.0000984	-0.0001081	-0.0000456
35 H	1.0	-0.0000314	0.0000992	0.0000890

MAXIMUM GRADIENT = 0.0002034 RMS GRADIENT = 0.0000713
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000039964
 PREDICTED ENERGY CHANGE WAS -0.0000031334 RATIO= 1.275
 GDIIS STEP HAS LENGTH = 0.013737
 RADIUS OF STEP TAKEN= 0.01374 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 7871.1 SECONDS (131.2 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7277.6 SECONDS (121.3
 MIN)
 CPU UTILIZATION: STEP = 83.68% , TOTAL = 100.00%

INSERCH= 86

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z

CO	27.0	0.1561274719	-1.7303710282	0.8668343639
C	6.0	4.9817026946	0.6242501257	0.5673928339
C	6.0	5.1844585658	-0.7142116490	0.2046987457
C	6.0	4.0477684327	-1.5333882445	-0.0916652395
C	6.0	2.7396003707	-1.0217297452	-0.0014708071

C	6.0	2.4689986991	0.3433139317	0.4315861412
C	6.0	3.6516520643	1.1750935486	0.6834691212
C	6.0	3.5049746247	2.5619125311	1.0588059669
C	6.0	2.2373371721	3.1390922293	1.2166642309
C	6.0	1.0716738646	2.3310625309	1.0358338830
C	6.0	1.1630588902	0.9766889356	0.6377688285
N	7.0	-0.0501826523	0.1770642060	0.5848097636
C	6.0	-1.2465815502	0.6997641912	0.3206596038
C	6.0	-2.5498696204	0.0364785597	0.4352410634
C	6.0	-2.8211181288	-1.2862370441	0.9285518449
C	6.0	-4.1214206279	-1.8064869691	1.0583827516
C	6.0	-5.2316938782	-0.9900013085	0.6819145359
C	6.0	-5.0171826383	0.3228123964	0.1760540951
C	6.0	-3.6981345503	0.8238313568	0.0577128184
O	8.0	-1.6979099295	-2.1442646947	1.3171307909
N	7.0	1.6325320632	-1.9542007533	-0.4304987186
H	1.0	5.8440954378	1.2840906510	0.7729231233
H	1.0	6.2022315359	-1.1342798307	0.1213872494
H	1.0	4.2112329747	-2.5757928751	-0.4290243469
H	1.0	4.4179160682	3.1598907911	1.2318972548
H	1.0	2.1290586567	4.1954823462	1.5192278565
H	1.0	0.0872675756	2.7751708468	1.2657049702
H	1.0	-1.2923488413	1.7509834009	-0.0271917982
H	1.0	-4.2937217494	-2.8295832958	1.4440099405
H	1.0	-6.2567488598	-1.3904276461	0.7847000691
H	1.0	-5.8747006679	0.9535284918	-0.1173246865
H	1.0	-3.5328867105	1.8482282915	-0.3250343519
H	1.0	-2.0131669450	-2.9569443752	1.7899689563
H	1.0	1.2754885194	-1.6796155268	-1.3724367914
H	1.0	2.0264886675	-2.9100993762	-0.5357970626

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3777395	5.1725349	4.0127787
2 C	5.3777395	0.0000000	1.4014767 *	2.4417195 *
3 C	5.1725349	1.4014767 *	0.0000000	1.4321126 *
4 C	4.0127787	2.4417195 *	1.4321126 *	0.0000000
5 C	2.8161070 *	2.8389925 *	2.4727323 *	1.4075628 *
6 C	3.1367154	2.5320051 *	2.9229370 *	2.5076517 *
7 C	4.5490702	1.4442773 *	2.4795546 *	2.8449280 *
8 C	5.4475066	2.4853065 *	3.7793062	4.2883211
9 C	5.3071167	3.7785614	4.9555574	5.1789440
10 C	4.1667768	4.2919659	5.1845423	5.0062334

11 C	2.8973359 *	3.8355191	4.3838738	3.8928281
12 N	1.9391779 *	5.0517471	5.3235633	4.4918225
13 C	2.8585760 *	6.2336269	6.5856702	5.7608266
14 C	3.2604372	7.5556284	7.7740927	6.8022746
15 C	3.0108230	8.0414184	8.0585628	6.9486351
16 C	4.2825112	9.4348507	9.4085721	8.2542621
17 C	5.4415955	10.3408120	10.4307251	9.3274925
18 C	5.6085539	10.0110798	10.2542539	9.2569159
19 C	4.6940349	8.6970789	9.0159659	8.0980128
20 O	1.9523139 *	7.2693883	7.1168499	5.9473268
21 N	1.9781161 *	4.3429414	3.8153939	2.4749259 *
22 H	6.4380725	1.1051486 *	2.1797275 *	3.4514477
23 H	6.1209795	2.1865588 *	1.1042010 *	2.2014518 *
24 H	4.3402613	3.4390036	2.1941417 *	1.1077632 *
25 H	6.4969819	2.6812115 *	4.0806120	4.8903676
26 H	6.2796348	4.6687544	5.9303078	6.2527100
27 H	4.5236873	5.3916227	6.2676056	6.0076370
28 H	3.8752026	6.4020920	6.9339739	6.2696177
29 H	4.6198006	9.9363435	9.7901272	8.5801444
30 H	6.4224053	11.4196735	11.4758397	10.3427042
31 H	6.6740373	10.8829571	11.1888364	10.2294089
32 H	5.2759596	8.6482820	9.1015836	8.3039824
33 H	2.6575361 *	7.9528515	7.7038136	6.5039985
34 H	2.5039730 *	4.7756423	4.3242812	3.0573345
35 H	2.6186609 *	4.7372929	3.9170181	2.4855902 *

C C C C

1 CO	2.8161070 *	3.1367154	4.5490702	5.4475066
2 C	2.8389925 *	2.5320051 *	1.4442773 *	2.4853065 *
3 C	2.4727323 *	2.9229370 *	2.4795546 *	3.7793062
4 C	1.4075628 *	2.5076517 *	2.8449280 *	4.2883211
5 C	0.0000000	1.4574319 *	2.4752805 *	3.8147708
6 C	1.4574319 *	0.0000000	1.4676414 *	2.5276136 *
7 C	2.4752805 *	1.4676414 *	0.0000000	1.4441811 *
8 C	3.8147708	2.5276136 *	1.4441811 *	0.0000000
9 C	4.3644657	2.9131411 *	2.4782805 *	1.4017704 *
10 C	3.8857684	2.5037525 *	2.8489845 *	2.4443347 *
11 C	2.6244595 *	1.4659993 *	2.4969079 *	2.8591564 *
12 N	3.0925267	2.5293065 *	3.8352805	4.3071240
13 C	4.3539586	3.7342868	4.9345984	5.1565243
14 C	5.4119326	5.0282403	6.3100660	6.5899764
15 C	5.6441560	5.5576746	6.9292834	7.4057188
16 C	6.9866117	6.9604702	8.3337292	8.7889032
17 C	8.0005971	7.8192749	9.1433841	9.4386183
18 C	7.8744518	7.4905693	8.7253967	8.8555059

19 C	6.6973151	6.1971131	7.3847356	7.4771582
20 O	4.7634329	4.9330887	6.3275177	7.0203165
21 N	1.5096911 *	2.5925741 *	3.8871909	5.1107092
22 H	3.9439046	3.5203480	2.1969730 *	2.6806798 *
23 H	3.4666376	4.0269758	3.4863444	4.6707373
24 H	2.1825711 *	3.5067385	3.9522046	5.3952254
25 H	4.6716047	3.5173686	2.1971240 *	1.1049890 *
26 H	5.4685087	4.0171788	3.4841831	2.1848761 *
27 H	4.8017765	3.5046149	3.9502003	3.4305987
28 H	4.8933847	4.0422451	5.0279054	4.9851088
29 H	7.4044155	7.5383464	8.9299957	9.4887446
30 H	9.0381581	8.9033263	10.2356512	10.5350545
31 H	8.8386226	8.3839719	9.5625184	9.5889776
32 H	6.9054650	6.2337685	7.2861366	7.2080407
33 H	5.4353573	5.7294605	7.0984684	7.8385118
34 H	2.1109204 *	2.9616227 *	4.2452640	5.3732774
35 H	2.0880548 *	3.4229145	4.5625177	5.8882590

C C C N

1 CO	5.3071167	4.1667768	2.8973359 *	1.9391779 *
2 C	3.7785614	4.2919659	3.8355191	5.0517471
3 C	4.9555574	5.1845423	4.3838738	5.3235633
4 C	5.1789440	5.0062334	3.8928281	4.4918225
5 C	4.3644657	3.8857684	2.6244595 *	3.0925267
6 C	2.9131411 *	2.5037525 *	1.4659993 *	2.5293065 *
7 C	2.4782805 *	2.8489845 *	2.4969079 *	3.8352805
8 C	1.4017704 *	2.4443347 *	2.8591564 *	4.3071240
9 C	0.0000000	1.4298191 *	2.4829784 *	3.7954706
10 C	1.4298191 *	0.0000000	1.4146147 *	2.4701606 *
11 C	2.4829784 *	1.4146147 *	0.0000000	1.4540149 *
12 N	3.7954706	2.4701606 *	1.4540149 *	0.0000000
13 C	4.3463588	2.9235110 *	2.4461424 *	1.3320514 *
14 C	5.7579669	4.3291344	3.8354727	2.5081009 *
15 C	6.7271478	5.3150913	4.5911932	3.1523789
16 C	8.0571464	6.6398836	5.9873791	4.5534301
17 C	8.5511283	7.1335243	6.6904919	5.3122057
18 C	7.8512648	6.4688842	6.2318633	4.9859214
19 C	6.4756024	5.0970127	4.8980641	3.7421507
20 O	6.5886359	5.2705100	4.2880097	2.9393651 *
21 N	5.3870742	4.5637895	3.1546339	2.8990810 *
22 H	4.0800297	4.8929827	4.6930657	6.0002840
23 H	5.9314187	6.2583890	5.4878138	6.4052374
24 H	6.2661366	6.0066522	4.8009936	5.1735621
25 H	2.1807313 *	3.4529312	3.9640200	5.4110889
26 H	1.1041871 *	2.1972241 *	3.4742994	4.6658241

27 H	2.1812022 *	1.1041416 *	2.1877312 *	2.6893622 *
28 H	3.9915795	2.6561474 *	2.6590847 *	2.0963646 *
29 H	8.8505087	7.4556249	6.7018048	5.2712217
30 H	9.6360075	8.2230370	7.7896326	6.4045649
31 H	8.5065488	7.1749212	7.0781892	5.9178459
32 H	6.1105358	4.8256678	4.8722147	3.9686060
33 H	7.4536653	6.1683044	5.1855035	3.8894377
34 H	5.5541463	4.6826111	3.3330947	3.0059071
35 H	6.3014520	5.5544103	4.1508904	3.8857306

C C C C

1 CO	2.8585760 *	3.2604372	3.0108230	4.2825112
2 C	6.2336269	7.5556284	8.0414184	9.4348507
3 C	6.5856702	7.7740927	8.0585628	9.4085721
4 C	5.7608266	6.8022746	6.9486351	8.2542621
5 C	4.3539586	5.4119326	5.6441560	6.9866117
6 C	3.7342868	5.0282403	5.5576746	6.9604702
7 C	4.9345984	6.3100660	6.9292834	8.3337292
8 C	5.1565243	6.5899764	7.4057188	8.7889032
9 C	4.3463588	5.7579669	6.7271478	8.0571464
10 C	2.9235110 *	4.3291344	5.3150913	6.6398836
11 C	2.4461424 *	3.8354727	4.5911932	5.9873791
12 N	1.3320514 *	2.5081009 *	3.1523789	4.5534301
13 C	0.0000000	1.4668458 *	2.6063191 *	3.8846145
14 C	1.4668458 *	0.0000000	1.4375353 *	2.5009198 *
15 C	2.6063191 *	1.4375353 *	0.0000000	1.4065215 *
16 C	3.8846145	2.5009198 *	1.4065215 *	0.0000000
17 C	4.3436083	2.8821329 *	2.4412007 *	1.4286651 *
18 C	3.7921545	2.4973583 *	2.8245340 *	2.4728140 *
19 C	2.4687336 *	1.4425548 *	2.4453849 *	2.8458893 *
20 O	3.0471548	2.5018405 *	1.4658792 *	2.4605789 *
21 N	3.9871122	4.7121962	4.7040614	5.9452972
22 H	7.1290729	8.4928920	9.0397307	10.4376562
23 H	7.6738676	8.8356355	9.0606537	10.3878591
24 H	6.4092932	7.2995496	7.2773573	8.4992545
25 H	6.2425243	7.6772653	8.5008051	9.8800449
26 H	5.0051532	6.3533227	7.4096151	8.6778168
27 H	2.6418889 *	3.8916061	5.0067368	6.2247592
28 H	1.1082225 *	2.1759434 *	3.5320376	4.6730841
29 H	4.7961728	3.5032764	2.1945788 *	1.1068523 *
30 H	5.4484871	3.9873721	3.4402191	2.1926318 *
31 H	4.6557183	3.4929659	3.9287115	3.4747610
32 H	2.6387652 *	2.1969930 *	3.4500675	3.9518551
33 H	4.0147280	3.3292519	2.0459930 *	2.5106780 *
34 H	3.8586086	4.5657467	4.7150272	5.9204399

35 H 4.9474864 5.5288599 5.3179449 6.4464066

C C C O

1 CO 5.4415955 5.6085539 4.6940349 1.9523139 *
2 C 10.3408120 10.0110798 8.6970789 7.2693883
3 C 10.4307251 10.2542539 9.0159659 7.1168499
4 C 9.3274925 9.2569159 8.0980128 5.9473268
5 C 8.0005971 7.8744518 6.6973151 4.7634329
6 C 7.8192749 7.4905693 6.1971131 4.9330887
7 C 9.1433841 8.7253967 7.3847356 6.3275177
8 C 9.4386183 8.8555059 7.4771582 7.0203165
9 C 8.5511283 7.8512648 6.4756024 6.5886359
10 C 7.1335243 6.4688842 5.0970127 5.2705100
11 C 6.6904919 6.2318633 4.8980641 4.2880097
12 N 5.3122057 4.9859214 3.7421507 2.9393651 *
13 C 4.3436083 3.7921545 2.4687336 * 3.0471548
14 C 2.8821329 * 2.4973583 * 1.4425548 * 2.5018405 *
15 C 2.4412007 * 2.8245340 * 2.4453849 * 1.4658792 *
16 C 1.4286651 * 2.4728140 * 2.8458893 * 2.4605789 *
17 C 0.0000000 1.4231619 * 2.4558951 * 3.7713993
18 C 1.4231619 * 0.0000000 1.4159493 * 4.2902327
19 C 2.4558951 * 1.4159493 * 0.0000000 3.7942886
20 O 3.7713993 4.2902327 3.7942886 0.0000000
21 N 7.0203092 7.0548849 6.0309054 3.7659231
22 H 11.3072050 10.9200581 9.5800583 8.3025073
23 H 11.4485657 11.3137686 10.0923487 8.0537015
24 H 9.6393873 9.6918361 8.6227868 6.1768312
25 H 10.5185102 9.9088297 8.5267907 8.0959655
26 H 9.0427326 8.2383526 6.8891391 7.4080311
27 H 6.5428345 5.7668720 4.4267641 5.2335790
28 H 4.8512131 3.9944171 2.5796559 * 4.1406087
29 H 2.2010550 * 3.4740044 3.9527184 2.6877498 *
30 H 1.1052800 * 2.2004922 * 3.4609190 4.6513186
31 H 2.1976235 * 1.1041789 * 2.1874413 * 5.3944014
32 H 3.4576638 2.1865767 * 1.1059798 * 4.6908258
33 H 3.9313567 4.7313461 4.4871029 0.9916709 *
34 H 6.8585239 6.7827171 5.7488695 4.0361827
35 H 7.6059721 7.7827859 6.8604521 4.2297741

N H H H

1 CO 1.9781161 * 6.4380725 6.1209795 4.3402613
2 C 4.3429414 1.1051486 * 2.1865588 * 3.4390036
3 C 3.8153939 2.1797275 * 1.1042010 * 2.1941417 *
4 C 2.4749259 * 3.4514477 2.2014518 * 1.1077632 *

5 C	1.5096911 *	3.9439046	3.4666376	2.1825711 *
6 C	2.5925741 *	3.5203480	4.0269758	3.5067385
7 C	3.8871909	2.1969730 *	3.4863444	3.9522046
8 C	5.1107092	2.6806798 *	4.6707373	5.3952254
9 C	5.3870742	4.0800297	5.9314187	6.2661366
10 C	4.5637895	4.8929827	6.2583890	6.0066522
11 C	3.1546339	4.6930657	5.4878138	4.8009936
12 N	2.8990810 *	6.0002840	6.4052374	5.1735621
13 C	3.9871122	7.1290729	7.6738676	6.4092932
14 C	4.7121962	8.4928920	8.8356355	7.2995496
15 C	4.7040614	9.0397307	9.0606537	7.2773573
16 C	5.9452972	10.4376562	10.3878591	8.4992545
17 C	7.0203092	11.3072050	11.4485657	9.6393873
18 C	7.0548849	10.9200581	11.3137686	9.6918361
19 C	6.0309054	9.5800583	10.0923487	8.6227868
20 O	3.7659231	8.3025073	8.0537015	6.1768312
21 N	0.0000000	5.4472031	4.6753611	2.6525605 *
22 H	5.4472031	0.0000000	2.5300744 *	4.3600021
23 H	4.6753611	2.5300744 *	0.0000000	2.5189260 *
24 H	2.6525605 *	4.3600021	2.5189260 *	0.0000000
25 H	6.0560595	2.4006814 *	4.7808907	5.9749013
26 H	6.4704385	4.7785637	6.8520844	7.3471971
27 H	5.2566058	5.9671787	7.3475201	6.9650564
28 H	4.7377183	7.1963192	8.0321575	7.0122660
29 H	6.2769867	10.9612047	10.7139358	8.7124579
30 H	8.0022061	12.3928858	12.4792543	10.6045679
31 H	8.0567680	11.7572103	12.2583938	10.6901508
32 H	6.4149155	9.4578833	10.1915246	8.9193143
33 H	4.3848709	8.9865084	8.5789885	6.6190907
34 H	1.0440903 *	5.8530584	5.1770356	3.2111924
35 H	1.0392457 *	5.8204897	4.5850032	2.2127514 *

H H H H

1 CO	6.4969819	6.2796348	4.5236873	3.8752026
2 C	2.6812115 *	4.6687544	5.3916227	6.4020920
3 C	4.0806120	5.9303078	6.2676056	6.9339739
4 C	4.8903676	6.2527100	6.0076370	6.2696177
5 C	4.6716047	5.4685087	4.8017765	4.8933847
6 C	3.5173686	4.0171788	3.5046149	4.0422451
7 C	2.1971240 *	3.4841831	3.9502003	5.0279054
8 C	1.1049890 *	2.1848761 *	3.4305987	4.9851088
9 C	2.1807313 *	1.1041871 *	2.1812022 *	3.9915795
10 C	3.4529312	2.1972241 *	1.1041416 *	2.6561474 *
11 C	3.9640200	3.4742994	2.1877312 *	2.6590847 *
12 N	5.4110889	4.6658241	2.6893622 *	2.0963646 *

13 C	6.2425243	5.0051532	2.6418889 *	1.1082225 *
14 C	7.6772653	6.3533227	3.8916061	2.1759434 *
15 C	8.5008051	7.4096151	5.0067368	3.5320376
16 C	9.8800449	8.6778168	6.2247592	4.6730841
17 C	10.5185102	9.0427326	6.5428345	4.8512131
18 C	9.9088297	8.2383526	5.7668720	3.9944171
19 C	8.5267907	6.8891391	4.4267641	2.5796559 *
20 O	8.0959655	7.4080311	5.2335790	4.1406087
21 N	6.0560595	6.4704385	5.2566058	4.7377183
22 H	2.4006814 *	4.7785637	5.9671787	7.1963192
23 H	4.7808907	6.8520844	7.3475201	8.0321575
24 H	5.9749013	7.3471971	6.9650564	7.0122660
25 H	0.0000000	2.5286117 *	4.3478350	6.0147694
26 H	2.5286117 *	0.0000000	2.5000939 *	4.4802922
27 H	4.3478350	2.5000939 *	0.0000000	2.1503217 *
28 H	6.0147694	4.4802922	2.1503217 *	0.0000000
29 H	10.5740922	9.5188924	7.1160473	5.6704731
30 H	11.6126592	10.1026575	7.6046118	5.9306744
31 H	10.6125583	8.7891258	6.3856258	4.6520970
32 H	8.2072992	6.4006664	4.0614272	2.2623388 *
33 H	8.8930279	8.2697365	6.1273014	5.0976697
34 H	6.3307368	6.6035658	5.3119472	4.4913786
35 H	6.7593231	7.3974955	6.2712268	5.7444803

H H H H

1 CO	4.6198006	6.4224053	6.6740373	5.2759596
2 C	9.9363435	11.4196735	10.8829571	8.6482820
3 C	9.7901272	11.4758397	11.1888364	9.1015836
4 C	8.5801444	10.3427042	10.2294089	8.3039824
5 C	7.4044155	9.0381581	8.8386226	6.9054650
6 C	7.5383464	8.9033263	8.3839719	6.2337685
7 C	8.9299957	10.2356512	9.5625184	7.2861366
8 C	9.4887446	10.5350545	9.5889776	7.2080407
9 C	8.8505087	9.6360075	8.5065488	6.1105358
10 C	7.4556249	8.2230370	7.1749212	4.8256678
11 C	6.7018048	7.7896326	7.0781892	4.8722147
12 N	5.2712217	6.4045649	5.9178459	3.9686060
13 C	4.7961728	5.4484871	4.6557183	2.6387652 *
14 C	3.5032764	3.9873721	3.4929659	2.1969930 *
15 C	2.1945788 *	3.4402191	3.9287115	3.4500675
16 C	1.1068523 *	2.1926318 *	3.4747610	3.9518551
17 C	2.2010550 *	1.1052800 *	2.1976235 *	3.4576638
18 C	3.4740044	2.2004922 *	1.1041789 *	2.1865767 *
19 C	3.9527184	3.4609190	2.1874413 *	1.1059798 *
20 O	2.6877498 *	4.6513186	5.3944014	4.6908258

21 N	6.2769867	8.0022061	8.0567680	6.4149155
22 H	10.9612047	12.3928858	11.7572103	9.4578833
23 H	10.7139358	12.4792543	12.2583938	10.1915246
24 H	8.7124579	10.6045679	10.6901508	8.9193143
25 H	10.5740922	11.6126592	10.6125583	8.2072992
26 H	9.5188924	10.1026575	8.7891258	6.4006664
27 H	7.1160473	7.6046118	6.3856258	4.0614272
28 H	5.6704731	5.9306744	4.6520970	2.2623388 *
29 H	0.0000000	2.5217720 *	4.3873904	5.0586865
30 H	2.5217720 *	0.0000000	2.5404212 *	4.3749089
31 H	4.3873904	2.5404212 *	0.0000000	2.5154967 *
32 H	5.0586865	4.3749089	2.5154967 *	0.0000000
33 H	2.3101599 *	4.6338459	5.8173026	5.4655715
34 H	6.3459358	7.8403743	7.7223027	6.0550150
35 H	6.6235322	8.5243850	8.8051992	7.3207075

H H H

1 CO	2.6575361 *	2.5039730 *	2.6186609 *
2 C	7.9528515	4.7756423	4.7372929
3 C	7.7038136	4.3242812	3.9170181
4 C	6.5039985	3.0573345	2.4855902 *
5 C	5.4353573	2.1109204 *	2.0880548 *
6 C	5.7294605	2.9616227 *	3.4229145
7 C	7.0984684	4.2452640	4.5625177
8 C	7.8385118	5.3732774	5.8882590
9 C	7.4536653	5.5541463	6.3014520
10 C	6.1683044	4.6826111	5.5544103
11 C	5.1855035	3.3330947	4.1508904
12 N	3.8894377	3.0059071	3.8857306
13 C	4.0147280	3.8586086	4.9474864
14 C	3.3292519	4.5657467	5.5288599
15 C	2.0459930 *	4.7150272	5.3179449
16 C	2.5106780 *	5.9204399	6.4464066
17 C	3.9313567	6.8585239	7.6059721
18 C	4.7313461	6.7827171	7.7827859
19 C	4.4871029	5.7488695	6.8604521
20 O	0.9916709 *	4.0361827	4.2297741
21 N	4.3848709	1.0440903 *	1.0392457 *
22 H	8.9865084	5.8530584	5.8204897
23 H	8.5789885	5.1770356	4.5850032
24 H	6.6190907	3.2111924	2.2127514 *
25 H	8.8930279	6.3307368	6.7593231
26 H	8.2697365	6.6035658	7.3974955
27 H	6.1273014	5.3119472	6.2712268
28 H	5.0976697	4.4913786	5.7444803

29 H	2.3101599 *	6.3459358	6.6235322
30 H	4.6338459	7.8403743	8.5243850
31 H	5.8173026	7.7223027	8.8051992
32 H	5.4655715	6.0550150	7.3207075
33 H	0.0000000	4.7378934	4.6615662
34 H	4.7378934	0.0000000	1.6667507 *
35 H	4.6615662	1.6667507 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.50 , TOTAL = 7871.6 SECONDS (131.2 MIN)
WALL CLOCK TIME: STEP = 0.49 , TOTAL = 7278.1 SECONDS (121.3 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.35 , TOTAL = 7873.0 SECONDS (131.2 MIN)
WALL CLOCK TIME: STEP = 1.36 , TOTAL = 7279.4 SECONDS (121.3 MIN)

CPU UTILIZATION: STEP = 99.46%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636925926	-284.636925926	0.001641942	0.000238307	198075845
11333865					
2 1	-284.636930716	-0.000004790	0.000749717	0.000022022	145509292
15742384					
3 2	-284.636930663	0.000000054	0.000449300	0.000039321	130333520
16892630					
4 3	-284.636930808	-0.000000146	0.000105364	0.000011949	124307160
17345174					
5 4	-284.636930766	0.000000042	0.000113457	0.000026666	114381742
18073114					
6 5	-284.636930796	-0.000000029	0.000050394	0.000006437	107702428
18617328					
7 6	-284.636930798	-0.000000002	0.000036793	0.000006987	106915840
18620348					

8	7	-284.636930779	0.000000019	0.000070007	0.000005399	100850618
19099599						
9	8	-284.636930779	0.000000000	0.000092601	0.000004789	130530418
16957809						
10	9	-284.636930781	-0.000000002	0.000088589	0.000004501	151398860
15391552						
11	10	-284.636930783	-0.000000002	0.000124767	0.000006326	151279433
15380141						
-----DISABLING FDIFF OPTION-----						
12	11	-284.636930823	-0.000000039	0.000132147	0.000006509	198076762
11333751						
13	12	-284.636930824	-0.000000002	0.000059056	0.000004285	198076799
11333748						
14	13	-284.636930825	-0.000000001	0.000051246	0.000001888	198076790
11333750						
15	14	-284.636930826	0.000000000	0.000012404	0.000001126	198076721
11333759						
16	15	-284.636930826	0.000000000	0.000015405	0.000000961	198076740
11333756						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 52.1 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 17.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369308258 AFTER 16 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6014996604
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998492469

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 54.74 , TOTAL = 7927.7 SECONDS (132.1 MIN)

WALL CLOCK TIME: STEP = 50.65 , TOTAL = 7330.1 SECONDS (122.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.95 , TOTAL = 7931.6 SECONDS (132.2 MIN)

WALL CLOCK TIME: STEP = 3.93 , TOTAL = 7334.0 SECONDS (122.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.89 , TOTAL = 7934.5 SECONDS (132.2 MIN)

WALL CLOCK TIME: STEP = 2.71 , TOTAL = 7336.7 SECONDS (122.3 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 86 ENERGY= -284.6369308

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000372	0.0000331	-0.0001367
2 C	6.0	0.0000948	0.0000122	0.0000735
3 C	6.0	0.0000337	0.0000396	0.0000237
4 C	6.0	0.0000068	-0.0000386	0.0000230
5 C	6.0	-0.0000224	-0.0000146	-0.0000126
6 C	6.0	0.0000238	-0.0000488	0.0000104
7 C	6.0	0.0000845	-0.0000445	0.0000821
8 C	6.0	0.0000086	-0.0000426	0.0000262
9 C	6.0	-0.0000146	0.0000753	-0.0000047
10 C	6.0	-0.0000104	0.0000146	-0.0001064
11 C	6.0	0.0000182	-0.0000146	-0.0000553
12 N	7.0	0.0000054	0.0000390	0.0000353
13 C	6.0	-0.0000165	0.0000322	0.0000416
14 C	6.0	-0.0000505	-0.0001194	-0.0000416
15 C	6.0	-0.0000834	0.0000280	-0.0000381
16 C	6.0	0.0000184	-0.0000462	0.0000322
17 C	6.0	-0.0001509	0.0000894	0.0000576

18 C	6.0	0.0000049	-0.0000834	0.0000673
19 C	6.0	0.0000469	-0.0000203	-0.0000483
20 O	8.0	-0.0000881	-0.0000641	-0.0000098
21 N	7.0	0.0000130	0.0000046	0.0000002
22 H	1.0	0.0000571	-0.0000071	0.0000977
23 H	1.0	0.0000528	0.0000715	-0.0000957
24 H	1.0	0.0000007	0.0000532	-0.0000278
25 H	1.0	-0.0000311	0.0000015	-0.0000570
26 H	1.0	-0.0000756	-0.0000686	-0.0000016
27 H	1.0	-0.0000230	-0.0001097	-0.0000211
28 H	1.0	-0.0000509	-0.0000623	0.0000068
29 H	1.0	-0.0000252	0.0000025	0.0000386
30 H	1.0	-0.0000953	0.0000610	0.0000673
31 H	1.0	0.0000088	0.0000374	0.0000718
32 H	1.0	0.0001294	0.0000171	-0.0000534
33 H	1.0	0.0000502	0.0000991	-0.0000764
34 H	1.0	0.0001500	-0.0000453	-0.0000928
35 H	1.0	-0.0000329	0.0001193	0.0001244

MAXIMUM GRADIENT = 0.0001509 RMS GRADIENT = 0.0000602
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000026929
 PREDICTED ENERGY CHANGE WAS -0.0000020889 RATIO= 1.289
 GDIIS STEP HAS LENGTH = 0.017581
 RADIUS OF STEP TAKEN= 0.01758 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 7934.6 SECONDS (132.2 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7336.7 SECONDS (122.3
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 87

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1567507493	-1.7296828904	0.8681134022
C	6.0	4.9811434487	0.6234478232	0.5681291320
C	6.0	5.1835200494	-0.7146856865	0.2042446569
C	6.0	4.0466987374	-1.5333343875	-0.0927084734
C	6.0	2.7386709372	-1.0214908434	-0.0016755689
C	6.0	2.4684012395	0.3434272652	0.4320399924
C	6.0	3.6512243580	1.1747717163	0.6842292617
C	6.0	3.5049692366	2.5615222595	1.0596130089

C	6.0	2.2376598802	3.1393393799	1.2169186734
C	6.0	1.0717804172	2.3315662045	1.0365186518
C	6.0	1.1627005549	0.9771669153	0.6383010696
N	7.0	-0.0505253790	0.1776107775	0.5848473341
C	6.0	-1.2467224970	0.7004151188	0.3201294892
C	6.0	-2.5495459160	0.0367580501	0.4350810824
C	6.0	-2.8200511037	-1.2860001162	0.9291835782
C	6.0	-4.1202829949	-1.8065194651	1.0586766194
C	6.0	-5.2307494089	-0.9908200139	0.6816605876
C	6.0	-5.0170385227	0.3217589643	0.1747372205
C	6.0	-3.6982293269	0.8232008698	0.0565756155
O	8.0	-1.6969872290	-2.1434304465	1.3194492333
N	7.0	1.6315977752	-1.9537016840	-0.4312989192
H	1.0	5.8440500078	1.2827410127	0.7735912818
H	1.0	6.2010328030	-1.1351443720	0.1202619047
H	1.0	4.2099073011	-2.5754897604	-0.4309720466
H	1.0	4.4180166035	3.1588658989	1.2340533759
H	1.0	2.1302585790	4.1960114126	1.5191289068
H	1.0	0.0877885211	2.7766557009	1.2662110429
H	1.0	-1.2920613610	1.7515174551	-0.0283041726
H	1.0	-4.2920045290	-2.8291189514	1.4458085196
H	1.0	-6.2556504424	-1.3914655826	0.7848259590
H	1.0	-5.8745736410	0.9520871503	-0.1195882158
H	1.0	-3.5332141345	1.8472462733	-0.3269017562
H	1.0	-2.0125621624	-2.9562649870	1.7920488267
H	1.0	1.2743727816	-1.6782046775	-1.3728625497
H	1.0	2.0256516673	-2.9096513837	-0.5371797241

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3760561	5.1710106	4.0116613
2 C	5.3760561	0.0000000	1.4014170 *	2.4416394 *
3 C	5.1710106	1.4014170 *	0.0000000	1.4320369 *
4 C	4.0116613	2.4416394 *	1.4320369 *	0.0000000
5 C	2.8150277 *	2.8388701 *	2.4726139 *	1.4075537 *
6 C	3.1355500	2.5319568 *	2.9229033 *	2.5077118 *
7 C	4.5476385	1.4443414 *	2.4795896 *	2.8449729 *
8 C	5.4462538	2.4853127 *	3.7792494	4.2882592
9 C	5.3065267	3.7785368	4.9555131	5.1789598
10 C	4.1664594	4.2918733	5.1844704	5.0062710
11 C	2.8968577 *	3.8354331	4.3838065	3.8928701
12 N	1.9393226 *	5.0514098	5.3231835	4.4915098
13 C	2.8592656 *	6.2332770	6.5851316	5.7602413

14 C	3.2606552	7.5546799	7.7729185	6.8010437
15 C	3.0103045	8.0395888	8.0566176	6.9467756
16 C	4.2819664	9.4329922	9.4065353	8.2522669
17 C	5.4411250	10.3393184	10.4288630	9.3255034
18 C	5.6086790	10.0104653	10.2531207	9.2554974
19 C	4.6943243	8.6967293	9.0151191	8.0968793
20 O	1.9522386 *	7.2675668	7.1152212	5.9461193
21 N	1.9783404 *	4.3428116	3.8151315	2.4746848 *
22 H	6.4365367	1.1052104 *	2.1794882 *	3.4512646
23 H	6.1193221	2.1866325 *	1.1041607 *	2.2011513 *
24 H	4.3394804	3.4389257	2.1940861 *	1.1077667 *
25 H	6.4953990	2.6812146 *	4.0805519	4.8902881
26 H	6.2795229	4.6685282	5.9301157	6.2526927
27 H	4.5244143	5.3915253	6.2676724	6.0079653
28 H	3.8757421	6.4016695	6.9332093	6.2687127
29 H	4.6188651	9.9338719	9.7876389	8.5778823
30 H	6.4218546	11.4180721	11.4738715	10.3406282
31 H	6.6741531	10.8824424	11.1876912	10.2278878
32 H	5.2762036	8.6482974	9.1009377	8.3029062
33 H	2.6578335 *	7.9513673	7.7025580	6.5032057
34 H	2.5047360 *	4.7754792	4.3240107	3.0570530
35 H	2.6191535 *	4.7370275	3.9165951	2.4852433 *

C C C C

1 CO	2.8150277 *	3.1355500	4.5476385	5.4462538
2 C	2.8388701 *	2.5319568 *	1.4443414 *	2.4853127 *
3 C	2.4726139 *	2.9229033 *	2.4795896 *	3.7792494
4 C	1.4075537 *	2.5077118 *	2.8449729 *	4.2882592
5 C	0.0000000	1.4574486 *	2.4752350 *	3.8146467
6 C	1.4574486 *	0.0000000	1.4675843 *	2.5275020 *
7 C	2.4752350 *	1.4675843 *	0.0000000	1.4440847 *
8 C	3.8146467	2.5275020 *	1.4440847 *	0.0000000
9 C	4.3644578	2.9131427 *	2.4781946 *	1.4016742 *
10 C	3.8857899	2.5037253 *	2.8488265 *	2.4441401 *
11 C	2.6244782 *	1.4659549 *	2.4967795 *	2.8590048 *
12 N	3.0921627	2.5289991 *	3.8349912	4.3069686
13 C	4.3533756	3.7339133	4.9343152	5.1564649
14 C	5.4107194	5.0273103	6.3092553	6.5895089
15 C	5.6423271	5.5560700	6.9276841	7.4044799
16 C	6.9846879	6.9588580	8.3321446	8.7877336
17 C	7.9987218	7.8178927	9.1421689	9.4379428
18 C	7.8731487	7.4898920	8.7250212	8.8557417
19 C	6.6962651	6.1966514	7.3845799	7.4775608
20 O	4.7622665	4.9317763	6.3259258	7.0188636
21 N	1.5097034 *	2.5927583 *	3.8872407	5.1107325

22 H	3.9438436	3.5205074	2.1973000 *	2.6811171 *
23 H	3.4663721	4.0268993	3.4864444	4.6708119
24 H	2.1826004 *	3.5068091	3.9522477	5.3951528
25 H	4.6714677	3.5172319	2.1970222 *	1.1049454 *
26 H	5.4685777	4.0172761	3.4840040	2.1846142 *
27 H	4.8021486	3.5048194	3.9500392	3.4301733
28 H	4.8925542	4.0417464	5.0275653	4.9850952
29 H	7.4022380	7.5363030	8.9278233	9.4868836
30 H	9.0362206	8.9018756	10.2343472	10.5342924
31 H	8.8372448	8.3833162	9.5622455	9.5894015
32 H	6.9044889	6.2335264	7.2863409	7.2089277
33 H	5.4346126	5.7285798	7.0972675	7.8374480
34 H	2.1108282 *	2.9614815 *	4.2450588	5.3728747
35 H	2.0881359 *	3.4231469	4.5625474	5.8882823

C C C N

1 CO	5.3065267	4.1664594	2.8968577 *	1.9393226 *
2 C	3.7785368	4.2918733	3.8354331	5.0514098
3 C	4.9555131	5.1844704	4.3838065	5.3231835
4 C	5.1789598	5.0062710	3.8928701	4.4915098
5 C	4.3644578	3.8857899	2.6244782 *	3.0921627
6 C	2.9131427 *	2.5037253 *	1.4659549 *	2.5289991 *
7 C	2.4781946 *	2.8488265 *	2.4967795 *	3.8349912
8 C	1.4016742 *	2.4441401 *	2.8590048 *	4.3069686
9 C	0.0000000	1.4297960 *	2.4830074 *	3.7956742
10 C	1.4297960 *	0.0000000	1.4146523 *	2.4704456 *
11 C	2.4830074 *	1.4146523 *	0.0000000	1.4539823 *
12 N	3.7956742	2.4704456 *	1.4539823 *	0.0000000
13 C	4.3466657	2.9239225 *	2.4460466 *	1.3320238 *
14 C	5.7580049	4.3291888	3.8348978	2.5074635 *
15 C	6.7265787	5.3145705	4.5900815	3.1513484
16 C	8.0566741	6.6394101	5.9862794	4.5523855
17 C	8.5511318	7.1334463	6.6896229	5.3112451
18 C	7.8521048	6.4695988	6.2316632	4.9855012
19 C	6.4765480	5.0978866	4.8980353	3.7418714
20 O	6.5878386	5.2698880	4.2871791	2.9389979 *
21 N	5.3872999	4.5641434	3.1549801	2.8990661 *
22 H	4.0803856	4.8932323	4.6932624	6.0002463
23 H	5.9314579	6.2583415	5.4877150	6.4047752
24 H	6.2661452	6.0067102	4.8010607	5.1732715
25 H	2.1805115 *	3.4526427	3.9638130	5.4108426
26 H	1.1042744 *	2.1975997 *	3.4746203	4.6665024
27 H	2.1808063 *	1.1041301 *	2.1881194 *	2.6904315 *
28 H	3.9919371	2.6566995 *	2.6589166 *	2.0963179 *
29 H	8.8493730	7.4545542	6.7002752	5.2698978

30 H	9.6359337	8.2228680	7.7886983	6.4035591
31 H	8.5075646	7.1757495	7.0780120	5.9173965
32 H	6.1119451	4.8269510	4.8723987	3.9683863
33 H	7.4532915	6.1680754	5.1851050	3.8894860
34 H	5.5537032	4.6823524	3.3329039	3.0053343
35 H	6.3017536	5.5548860	4.1513608	3.8859546

C C C C

1 CO	2.8592656 *	3.2606552	3.0103045	4.2819664
2 C	6.2332770	7.5546799	8.0395888	9.4329922
3 C	6.5851316	7.7729185	8.0566176	9.4065353
4 C	5.7602413	6.8010437	6.9467756	8.2522669
5 C	4.3533756	5.4107194	5.6423271	6.9846879
6 C	3.7339133	5.0273103	5.5560700	6.9588580
7 C	4.9343152	6.3092553	6.9276841	8.3321446
8 C	5.1564649	6.5895089	7.4044799	8.7877336
9 C	4.3466657	5.7580049	6.7265787	8.0566741
10 C	2.9239225 *	4.3291888	5.3145705	6.6394101
11 C	2.4460466 *	3.8348978	4.5900815	5.9862794
12 N	1.3320238 *	2.5074635 *	3.1513484	4.5523855
13 C	0.0000000	1.4666300 *	2.6061764 *	3.8842661
14 C	1.4666300 *	0.0000000	1.4377063 *	2.5007516 *
15 C	2.6061764 *	1.4377063 *	0.0000000	1.4065247 *
16 C	3.8842661	2.5007516 *	1.4065247 *	0.0000000
17 C	4.3432075	2.8819386 *	2.4412835 *	1.4285105 *
18 C	3.7920710	2.4975036 *	2.8250367 *	2.4728705 *
19 C	2.4686885 *	1.4426477 *	2.4456840 *	2.8456572 *
20 O	3.0477592	2.5024359 *	1.4658672 *	2.4604621 *
21 N	3.9866914	4.7111046	4.7025435	5.9435530
22 H	7.1290803	8.4923210	9.0382127	10.4361265
23 H	7.6732187	8.8343135	9.0585356	10.3856115
24 H	6.4086282	7.2982254	7.2755152	8.4972018
25 H	6.2424760	7.6767729	8.4993767	9.8786825
26 H	5.0060757	6.3541418	7.4098618	8.6782293
27 H	2.6432489 *	3.8927303	5.0074236	6.2254663
28 H	1.1082769 *	2.1763256 *	3.5324281	4.6733277
29 H	4.7956758	3.5029963	2.1942570 *	1.1068284 *
30 H	5.4480517	3.9871487	3.4402478	2.1925004 *
31 H	4.6555018	3.4930352	3.9292575	3.4750186
32 H	2.6385441 *	2.1968360 *	3.4501572	3.9515163
33 H	4.0155157	3.3298498	2.0460595 *	2.5104256 *
34 H	3.8574571	4.5642208	4.7135494	5.9187126
35 H	4.9473217	5.5280243	5.3167001	6.4448561

C C C O

1 CO	5.4411250	5.6086790	4.6943243	1.9522386 *
2 C	10.3393184	10.0104653	8.6967293	7.2675668
3 C	10.4288630	10.2531207	9.0151191	7.1152212
4 C	9.3255034	9.2554974	8.0968793	5.9461193
5 C	7.9987218	7.8731487	6.6962651	4.7622665
6 C	7.8178927	7.4898920	6.1966514	4.9317763
7 C	9.1421689	8.7250212	7.3845799	6.3259258
8 C	9.4379428	8.8557417	7.4775608	7.0188636
9 C	8.5511318	7.8521048	6.4765480	6.5878386
10 C	7.1334463	6.4695988	5.0978866	5.2698880
11 C	6.6896229	6.2316632	4.8980353	4.2871791
12 N	5.3112451	4.9855012	3.7418714	2.9389979 *
13 C	4.3432075	3.7920710	2.4686885 *	3.0477592
14 C	2.8819386 *	2.4975036 *	1.4426477 *	2.5024359 *
15 C	2.4412835 *	2.8250367 *	2.4456840 *	1.4658672 *
16 C	1.4285105 *	2.4728705 *	2.8456572 *	2.4604621 *
17 C	0.0000000	1.4232032 *	2.4556101 *	3.7713075
18 C	1.4232032 *	0.0000000	1.4158615 *	4.2907185
19 C	2.4556101 *	1.4158615 *	0.0000000	3.7948282
20 O	3.7713075	4.2907185	3.7948282	0.0000000
21 N	7.0183779	7.0533230	6.0296158	3.7657130
22 H	11.3061361	10.9199522	9.5802079	8.3008346
23 H	11.4464686	11.3124117	10.0913113	8.0519197
24 H	9.6371743	9.6900703	8.6213355	6.1759253
25 H	10.5177810	9.9091671	8.5273227	8.0941282
26 H	9.0437278	8.2402110	6.8910220	7.4078476
27 H	6.5438840	5.7686300	4.4286719	5.2340717
28 H	4.8515697	3.9951083	2.5804303 *	4.1413794
29 H	2.2010241 *	3.4740939	3.9524647	2.6870523 *
30 H	1.1052521 *	2.2003423 *	3.4605634	4.6510949
31 H	2.1980440 *	1.1042226 *	2.1872631 *	5.3949315
32 H	3.4573753	2.1864327 *	1.1058725 *	4.6912367
33 H	3.9309878	4.7315976	4.4875052	0.9917852 *
34 H	6.8563968	6.7806177	5.7469205	4.0365775
35 H	7.6041332	7.7812803	6.8592671	4.2299180

N H H H

1 CO	1.9783404 *	6.4365367	6.1193221	4.3394804
2 C	4.3428116	1.1052104 *	2.1866325 *	3.4389257
3 C	3.8151315	2.1794882 *	1.1041607 *	2.1940861 *
4 C	2.4746848 *	3.4512646	2.2011513 *	1.1077667 *
5 C	1.5097034 *	3.9438436	3.4663721	2.1826004 *
6 C	2.5927583 *	3.5205074	4.0268993	3.5068091
7 C	3.8872407	2.1973000 *	3.4864444	3.9522477

8 C	5.1107325	2.6811171 *	4.6708119	5.3951528
9 C	5.3872999	4.0803856	5.9314579	6.2661452
10 C	4.5641434	4.8932323	6.2583415	6.0067102
11 C	3.1549801	4.6932624	5.4877150	4.8010607
12 N	2.8990661 *	6.0002463	6.4047752	5.1732715
13 C	3.9866914	7.1290803	7.6732187	6.4086282
14 C	4.7111046	8.4923210	8.8343135	7.2982254
15 C	4.7025435	9.0382127	9.0585356	7.2755152
16 C	5.9435530	10.4361265	10.3856115	8.4972018
17 C	7.0183779	11.3061361	11.4464686	9.6371743
18 C	7.0533230	10.9199522	11.3124117	9.6900703
19 C	6.0296158	9.5802079	10.0913113	8.6213355
20 O	3.7657130	8.3008346	8.0519197	6.1759253
21 N	0.0000000	5.4471163	4.6748253	2.6522256 *
22 H	5.4471163	0.0000000	2.5299102 *	4.3597408
23 H	4.6748253	2.5299102 *	0.0000000	2.5185382 *
24 H	2.6522256 *	4.3597408	2.5185382 *	0.0000000
25 H	6.0560611	2.4011333 *	4.7810252	5.9748183
26 H	6.4708425	4.7786209	6.8519525	7.3471805
27 H	5.2574869	5.9673278	7.3475938	6.9654687
28 H	4.7369649	7.1963097	8.0312732	7.0111905
29 H	6.2752651	10.9589630	10.7112304	8.7102892
30 H	8.0002346	12.3917012	12.4770310	10.6022628
31 H	8.0550221	11.7572634	12.2570116	10.6881951
32 H	6.4135315	9.4584795	10.1906905	8.9178111
33 H	4.3850097	8.9851423	8.5775576	6.6186054
34 H	1.0440548 *	5.8528979	5.1765156	3.2108630
35 H	1.0393888 *	5.8201753	4.5842025	2.2122199 *

H H H H

1 CO	6.4953990	6.2795229	4.5244143	3.8757421
2 C	2.6812146 *	4.6685282	5.3915253	6.4016695
3 C	4.0805519	5.9301157	6.2676724	6.9332093
4 C	4.8902881	6.2526927	6.0079653	6.2687127
5 C	4.6714677	5.4685777	4.8021486	4.8925542
6 C	3.5172319	4.0172761	3.5048194	4.0417464
7 C	2.1970222 *	3.4840040	3.9500392	5.0275653
8 C	1.1049454 *	2.1846142 *	3.4301733	4.9850952
9 C	2.1805115 *	1.1042744 *	2.1808063 *	3.9919371
10 C	3.4526427	2.1975997 *	1.1041301 *	2.6566995 *
11 C	3.9638130	3.4746203	2.1881194 *	2.6589166 *
12 N	5.4108426	4.6665024	2.6904315 *	2.0963179 *
13 C	6.2424760	5.0060757	2.6432489 *	1.1082769 *
14 C	7.6767729	6.3541418	3.8927303	2.1763256 *
15 C	8.4993767	7.4098618	5.0074236	3.5324281

16 C	9.8786825	8.6782293	6.2254663	4.6733277
17 C	10.5177810	9.0437278	6.5438840	4.8515697
18 C	9.9091671	8.2402110	5.7686300	3.9951083
19 C	8.5273227	6.8910220	4.4286719	2.5804303 *
20 O	8.0941282	7.4078476	5.2340717	4.1413794
21 N	6.0560611	6.4708425	5.2574869	4.7369649
22 H	2.4011333 *	4.7786209	5.9673278	7.1963097
23 H	4.7810252	6.8519525	7.3475938	8.0312732
24 H	5.9748183	7.3471805	6.9654687	7.0111905
25 H	0.0000000	2.5279983 *	4.3471823	6.0149120
26 H	2.5279983 *	0.0000000	2.5000444 *	4.4813361
27 H	4.3471823	2.5000444 *	0.0000000	2.1518977 *
28 H	6.0149120	4.4813361	2.1518977 *	0.0000000
29 H	10.5719095	9.5185764	7.1161473	5.6705288
30 H	11.6118254	10.1035919	7.6055364	5.9309982
31 H	10.6131820	8.7912330	6.3874293	4.6526165
32 H	8.2084711	6.4030813	4.0636770	2.2629826 *
33 H	8.8914863	8.2699762	6.1281611	5.0986294
34 H	6.3305418	6.6032242	5.3121062	4.4897010
35 H	6.7592587	7.3979586	6.2722899	5.7439245

H H H H

1 CO	4.6188651	6.4218546	6.6741531	5.2762036
2 C	9.9338719	11.4180721	10.8824424	8.6482974
3 C	9.7876389	11.4738715	11.1876912	9.1009377
4 C	8.5778823	10.3406282	10.2278878	8.3029062
5 C	7.4022380	9.0362206	8.8372448	6.9044889
6 C	7.5363030	8.9018756	8.3833162	6.2335264
7 C	8.9278233	10.2343472	9.5622455	7.2863409
8 C	9.4868836	10.5342924	9.5894015	7.2089277
9 C	8.8493730	9.6359337	8.5075646	6.1119451
10 C	7.4545542	8.2228680	7.1757495	4.8269510
11 C	6.7002752	7.7886983	7.0780120	4.8723987
12 N	5.2698978	6.4035591	5.9173965	3.9683863
13 C	4.7956758	5.4480517	4.6555018	2.6385441 *
14 C	3.5029963	3.9871487	3.4930352	2.1968360 *
15 C	2.1942570 *	3.4402478	3.9292575	3.4501572
16 C	1.1068284 *	2.1925004 *	3.4750186	3.9515163
17 C	2.2010241 *	1.1052521 *	2.1980440 *	3.4573753
18 C	3.4740939	2.2003423 *	1.1042226 *	2.1864327 *
19 C	3.9524647	3.4605634	2.1872631 *	1.1058725 *
20 O	2.6870523 *	4.6510949	5.3949315	4.6912367
21 N	6.2752651	8.0002346	8.0550221	6.4135315
22 H	10.9589630	12.3917012	11.7572634	9.4584795
23 H	10.7112304	12.4770310	12.2570116	10.1906905

24 H	8.7102892	10.6022628	10.6881951	8.9178111
25 H	10.5719095	11.6118254	10.6131820	8.2084711
26 H	9.5185764	10.1035919	8.7912330	6.4030813
27 H	7.1161473	7.6055364	6.3874293	4.0636770
28 H	5.6705288	5.9309982	4.6526165	2.2629826 *
29 H	0.0000000	2.5218347 *	4.3877684	5.0583254
30 H	2.5218347 *	0.0000000	2.5407526 *	4.3745688
31 H	4.3877684	2.5407526 *	0.0000000	2.5152044 *
32 H	5.0583254	4.3745688	2.5152044 *	0.0000000
33 H	2.3090920 *	4.6332379	5.8176202	5.4658992
34 H	6.3446093	7.8383090	7.7198813	6.0527457
35 H	6.6220471	8.5224733	8.8034634	7.3193771

H H H

1 CO	2.6578335 *	2.5047360 *	2.6191535 *
2 C	7.9513673	4.7754792	4.7370275
3 C	7.7025580	4.3240107	3.9165951
4 C	6.5032057	3.0570530	2.4852433 *
5 C	5.4346126	2.1108282 *	2.0881359 *
6 C	5.7285798	2.9614815 *	3.4231469
7 C	7.0972675	4.2450588	4.5625474
8 C	7.8374480	5.3728747	5.8882823
9 C	7.4532915	5.5537032	6.3017536
10 C	6.1680754	4.6823524	5.5548860
11 C	5.1851050	3.3329039	4.1513608
12 N	3.8894860	3.0053343	3.8859546
13 C	4.0155157	3.8574571	4.9473217
14 C	3.3298498	4.5642208	5.5280243
15 C	2.0460595 *	4.7135494	5.3167001
16 C	2.5104256 *	5.9187126	6.4448561
17 C	3.9309878	6.8563968	7.6041332
18 C	4.7315976	6.7806177	7.7812803
19 C	4.4875052	5.7469205	6.8592671
20 O	0.9917852 *	4.0365775	4.2299180
21 N	4.3850097	1.0440548 *	1.0393888 *
22 H	8.9851423	5.8528979	5.8201753
23 H	8.5775576	5.1765156	4.5842025
24 H	6.6186054	3.2108630	2.2122199 *
25 H	8.8914863	6.3305418	6.7592587
26 H	8.2699762	6.6032242	7.3979586
27 H	6.1281611	5.3121062	6.2722899
28 H	5.0986294	4.4897010	5.7439245
29 H	2.3090920 *	6.3446093	6.6220471
30 H	4.6332379	7.8383090	8.5224733
31 H	5.8176202	7.7198813	8.8034634

32 H	5.4658992	6.0527457	7.3193771
33 H	0.0000000	4.7385698	4.6620435
34 H	4.7385698	0.0000000	1.6671073 *
35 H	4.6620435	1.6671073 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.73 , TOTAL = 7935.3 SECONDS (132.3 MIN)
WALL CLOCK TIME: STEP = 0.73 , TOTAL = 7337.5 SECONDS (122.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.89 , TOTAL = 7936.2 SECONDS (132.3 MIN)
WALL CLOCK TIME: STEP = 0.89 , TOTAL = 7338.4 SECONDS (122.3 MIN)
CPU UTILIZATION: STEP = 99.66%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
INTEGRALS	SKIPPED				

-----START SECOND ORDER SCF-----

1	0	-284.636927009	-284.636927009	0.001573274	0.000277131	198221319
11326918						
2	1	-284.636932890	-0.000005881	0.000924402	0.000024851	146164899
15717655						
3	2	-284.636932836	0.000000054	0.000557444	0.000043185	130813227
16883016						
4	3	-284.636933027	-0.000000191	0.000097111	0.000018520	124708100
17330503						
5	4	-284.636932967	0.000000059	0.000063825	0.000038484	117250053
17912729						
6	5	-284.636932978	-0.000000010	0.000073031	0.000010757	110750671
18427299						
7	6	-284.636932982	-0.000000004	0.000052846	0.000010832	134183243
16625776						
8	7	-284.636932988	-0.000000007	0.000102368	0.000007664	127273539
17204724						
9	8	-284.636932994	-0.000000006	0.000166205	0.000006145	152766778
15253176						

-----DISABLING FDIFF OPTION-----

10	9	-284.636933026	-0.000000032	0.000149704	0.000009903	198221902
11326836						
11	10	-284.636933032	-0.000000006	0.000229578	0.000011260	198221957
11326832						
12	11	-284.636933040	-0.000000008	0.000199159	0.000008963	198221995
11326836						
13	12	-284.636933043	-0.000000003	0.000079841	0.000007851	198222113
11326833						
14	13	-284.636933046	-0.000000003	0.000038430	0.000002147	198222100
11326835						
15	14	-284.636933046	0.000000000	0.000017582	0.000001887	198222144
11326833						
16	15	-284.636933046	0.000000000	0.000019197	0.000001882	198222090
11326834						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 53.0 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 17.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 1.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369330461 AFTER 16 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6016484094
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998479234

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 55.59 , TOTAL = 7991.8 SECONDS (133.2 MIN)
WALL CLOCK TIME: STEP = 51.08 , TOTAL = 7389.4 SECONDS (123.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.72 , TOTAL = 7995.5 SECONDS (133.3 MIN)
 WALL CLOCK TIME: STEP = 3.68 , TOTAL = 7393.1 SECONDS (123.2 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
 USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.16 , TOTAL = 7998.7 SECONDS (133.3 MIN)
 WALL CLOCK TIME: STEP = 2.99 , TOTAL = 7396.1 SECONDS (123.3 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 87 ENERGY= -284.6369330

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000542	0.0000146	-0.0000506
2 C	6.0	0.0000594	-0.0000765	0.0001256
3 C	6.0	0.0000261	0.0001033	0.0000254
4 C	6.0	0.0000260	-0.0000416	-0.0000235
5 C	6.0	-0.0000371	0.0000428	0.0000514
6 C	6.0	0.0000088	-0.0000569	0.0000260
7 C	6.0	-0.0000215	0.0000268	0.0000811
8 C	6.0	-0.0000710	-0.0000386	-0.0000600
9 C	6.0	-0.0000270	0.0000312	-0.0000622
10 C	6.0	0.0000343	-0.0000459	-0.0000236
11 C	6.0	0.0000194	-0.0000263	-0.0000310
12 N	7.0	-0.0000757	-0.0000058	-0.0000293
13 C	6.0	-0.0001258	0.0000256	0.0000070
14 C	6.0	0.0000769	-0.0000050	-0.0000172
15 C	6.0	-0.0000043	-0.0001149	-0.0000102
16 C	6.0	-0.0000823	-0.0000052	-0.0001018
17 C	6.0	-0.0000026	0.0000123	0.0001256
18 C	6.0	-0.0000232	-0.0000513	0.0000491
19 C	6.0	-0.0000669	0.0000370	-0.0000611
20 O	8.0	-0.0000382	-0.0000183	0.0000182
21 N	7.0	-0.0000013	0.0000339	-0.0001100
22 H	1.0	0.0001190	-0.0000120	0.0000695

23 H	1.0	0.0000123	0.0000495	-0.0001083
24 H	1.0	0.0000066	0.0000483	-0.0000276
25 H	1.0	-0.0000654	-0.0000228	0.0000094
26 H	1.0	-0.0000245	0.0000019	-0.0000002
27 H	1.0	0.0000330	-0.0000405	-0.0000162
28 H	1.0	-0.0000120	-0.0000318	-0.0000133
29 H	1.0	0.0000204	0.0000319	0.0000712
30 H	1.0	-0.0000810	0.0000907	0.0000714
31 H	1.0	0.0000142	0.0000905	0.0000386
32 H	1.0	0.0001205	-0.0000536	-0.0000299
33 H	1.0	0.0000154	0.0000064	-0.0000458
34 H	1.0	0.0001875	-0.0000056	-0.0000878
35 H	1.0	0.0000344	0.0000059	0.0001400

MAXIMUM GRADIENT = 0.0001875 RMS GRADIENT = 0.0000584
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000022204
 PREDICTED ENERGY CHANGE WAS -0.0000016989 RATIO= 1.307
 GDIIS STEP HAS LENGTH = 0.009779
 RADIUS OF STEP TAKEN= 0.00978 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 7998.7 SECONDS (133.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7396.1 SECONDS (123.3
 MIN)
 CPU UTILIZATION: STEP = 82.33% , TOTAL = 100.00%

INSERCH= 88

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1572466360	-1.7292512540	0.8696237593
C	6.0	4.9806929531	0.6230583640	0.5679491168
C	6.0	5.1828884199	-0.7150608963	0.2039266247
C	6.0	4.0460050878	-1.5333334190	-0.0930302118
C	6.0	2.7381388697	-1.0214229919	-0.0015149192
C	6.0	2.4679826638	0.3435909383	0.4323244173
C	6.0	3.6509780871	1.1746788427	0.6841913025
C	6.0	3.5051592459	2.5614882147	1.0595974445
C	6.0	2.2380336575	3.1396665055	1.2167407888
C	6.0	1.0718923586	2.3320898318	1.0369972862
C	6.0	1.1624403183	0.9775658464	0.6388954599
N	7.0	-0.0506412281	0.1779843493	0.5852680846
C	6.0	-1.2467026925	0.7008827242	0.3201668390

C	6.0	-2.5494487896	0.0371329701	0.4353834051
C	6.0	-2.8193688053	-1.2857887204	0.9292415755
C	6.0	-4.1194277634	-1.8067273454	1.0581376841
C	6.0	-5.2301322237	-0.9913871246	0.6809040658
C	6.0	-5.0169661766	0.3213331833	0.1744334022
C	6.0	-3.6983078349	0.8230559369	0.0567823204
O	8.0	-1.6964847418	-2.1431085636	1.3202236165
N	7.0	1.6310892805	-1.9536873358	-0.4308722611
H	1.0	5.8437241094	1.2820787698	0.7732986810
H	1.0	6.2002785547	-1.1358447432	0.1199010708
H	1.0	4.2090010754	-2.5754779449	-0.4315795970
H	1.0	4.4183710458	3.1584165600	1.2346349534
H	1.0	2.1312873717	4.1965632936	1.5183600447
H	1.0	0.0882046483	2.7778925042	1.2666752898
H	1.0	-1.2918308268	1.7520112191	-0.0284933900
H	1.0	-4.2909296008	-2.8293357409	1.4451725391
H	1.0	-6.2547879936	-1.3924671718	0.7840040072
H	1.0	-5.8747044477	0.9513030806	-0.1201154366
H	1.0	-3.5338859020	1.8470416803	-0.3268761354
H	1.0	-2.0124657125	-2.9563539585	1.7920407929
H	1.0	1.2733860711	-1.6778758573	-1.3722155926
H	1.0	2.0252812847	-2.9096067473	-0.5372900283

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3749421	5.1699913	4.0109262
2 C	5.3749421	0.0000000	1.4014130 *	2.4414259 *
3 C	5.1699913	1.4014130 *	0.0000000	1.4318719 *
4 C	4.0109262	2.4414259 *	1.4318719 *	0.0000000
5 C	2.8144108 *	2.8386012 *	2.4724207 *	1.4074592 *
6 C	3.1348694	2.5318391 *	2.9229476 *	2.5077873 *
7 C	4.5467961	1.4442780 *	2.4796209 *	2.8448989 *
8 C	5.4456454	2.4852421 *	3.7792488	4.2881965
9 C	5.3062722	3.7784160	4.9554904	5.1789177
10 C	4.1664232	4.2917965	5.1845369	5.0063765
11 C	2.8966375 *	3.8353308	4.3838552	3.8929778
12 N	1.9394904 *	5.0510112	5.3228548	4.4912368
13 C	2.8598125 *	6.2328091	6.5846830	5.7597925
14 C	3.2611161	7.5540662	7.7722845	6.8004116
15 C	3.0100586	8.0383576	8.0553046	6.9454789
16 C	4.2815282	9.4316669	9.4050252	8.2507106
17 C	5.4409475	10.3382853	10.4276010	9.3241302
18 C	5.6089807	10.0099491	10.2524151	9.2546622

19 C	4.6947080	8.6963409	9.0146049	8.0962582
20 O	1.9520856 *	7.2665190	7.1141559	5.9451915
21 N	1.9783512 *	4.3424771	3.8147663	2.4743995 *
22 H	6.4353254	1.1051240 *	2.1793245 *	3.4509224
23 H	6.1182065	2.1867502 *	1.1041748 *	2.2009614 *
24 H	4.3388874	3.4387789	2.1939636 *	1.1078125 *
25 H	6.4945909	2.6811783 *	4.0805238	4.8901809
26 H	6.2795680	4.6682256	5.9299289	6.2525546
27 H	4.5251256	5.3914720	6.2678514	6.0082986
28 H	3.8762905	6.4011587	6.9327089	6.2681853
29 H	4.6181938	9.9323477	9.7859122	8.5761396
30 H	6.4214439	11.4168759	11.4723934	10.3390217
31 H	6.6745329	10.8821335	11.1871414	10.2271516
32 H	5.2769255	8.6485201	9.1010041	8.3027927
33 H	2.6578724 *	7.9507774	7.7018584	6.5025801
34 H	2.5048454 *	4.7752133	4.3238230	3.0568978
35 H	2.6195799 *	4.7366375	3.9161099	2.4849185 *

C C C C

1 CO	2.8144108 *	3.1348694	4.5467961	5.4456454
2 C	2.8386012 *	2.5318391 *	1.4442780 *	2.4852421 *
3 C	2.4724207 *	2.9229476 *	2.4796209 *	3.7792488
4 C	1.4074592 *	2.5077873 *	2.8448989 *	4.2881965
5 C	0.0000000	1.4575541 *	2.4751428 *	3.8146471
6 C	1.4575541 *	0.0000000	1.4675225 *	2.5275037 *
7 C	2.4751428 *	1.4675225 *	0.0000000	1.4441029 *
8 C	3.8146471	2.5275037 *	1.4441029 *	0.0000000
9 C	4.3645066	2.9131125 *	2.4781439 *	1.4016388 *
10 C	3.8859919	2.5037622 *	2.8488165 *	2.4441608 *
11 C	2.6246729 *	1.4659593 *	2.4967430 *	2.8590439 *
12 N	3.0919552	2.5286921 *	3.8347322	4.3069474
13 C	4.3530195	3.7335136	4.9339916	5.1564331
14 C	5.4101760	5.0267827	6.3088200	6.5894075
15 C	5.6411070	5.5549879	6.9267120	7.4039305
16 C	6.9832504	6.9576927	8.3311359	8.7872428
17 C	7.9974960	7.8169643	9.1414426	9.4377778
18 C	7.8724587	7.4894234	8.7247527	8.8559828
19 C	6.6957708	6.1962938	7.3843946	7.4778154
20 O	4.7614134	4.9310068	6.3251568	7.0184227
21 N	1.5096434 *	2.5928723 *	3.8871574	5.1108168
22 H	3.9434904	3.5203200	2.1971823 *	2.6809963 *
23 H	3.4661571	4.0269555	3.4865277	4.6708638
24 H	2.1825394 *	3.5069129	3.9522159	5.3951296
25 H	4.6714350	3.5172376	2.1970652 *	1.1049513 *
26 H	5.4686076	4.0172420	3.4838317	2.1843666 *

27 H	4.8026301	3.5050405	3.9500552	3.4300570
28 H	4.8921693	4.0413114	5.0271853	4.9850084
29 H	7.4006254	7.5349997	8.9266524	9.4862349
30 H	9.0347909	8.9008036	10.2334942	10.5340536
31 H	8.8366727	8.3830145	9.5621877	9.5899041
32 H	6.9045090	6.2337128	7.2867414	7.2097780
33 H	5.4340633	5.7282530	7.0969964	7.8375532
34 H	2.1107467 *	2.9613770 *	4.2448582	5.3727771
35 H	2.0881712 *	3.4233656	4.5624879	5.8883757

C C C N

1 CO	5.3062722	4.1664232	2.8966375 *	1.9394904 *
2 C	3.7784160	4.2917965	3.8353308	5.0510112
3 C	4.9554904	5.1845369	4.3838552	5.3228548
4 C	5.1789177	5.0063765	3.8929778	4.4912368
5 C	4.3645066	3.8859919	2.6246729 *	3.0919552
6 C	2.9131125 *	2.5037622 *	1.4659593 *	2.5286921 *
7 C	2.4781439 *	2.8488165 *	2.4967430 *	3.8347322
8 C	1.4016388 *	2.4441608 *	2.8590439 *	4.3069474
9 C	0.0000000	1.4298158 *	2.4830396 *	3.7958335
10 C	1.4298158 *	0.0000000	1.4147152 *	2.4706905 *
11 C	2.4830396 *	1.4147152 *	0.0000000	1.4538821 *
12 N	3.7958335	2.4706905 *	1.4538821 *	0.0000000
13 C	4.3468263	2.9241350 *	2.4458355 *	1.3320152 *
14 C	5.7581440	4.3293046	3.8345732	2.5072582 *
15 C	6.7264128	5.3143739	4.5893222	3.1506827
16 C	8.0566297	6.6392815	5.9854977	4.5516711
17 C	8.5513874	7.1335696	6.6890600	5.3107159
18 C	7.8526702	6.4700353	6.2314871	4.9853503
19 C	6.4770625	5.0983149	4.8979181	3.7417758
20 O	6.5877808	5.2698700	4.2867551	2.9387808 *
21 N	5.3875100	4.5645622	3.1553574	2.8991004 *
22 H	4.0802300	4.8931011	4.6931024	5.9998269
23 H	5.9314786	6.2584328	5.4877749	6.4044291
24 H	6.2661431	6.0068620	4.8012050	5.1730152
25 H	2.1804914 *	3.4526506	3.9638492	5.4107970
26 H	1.1042644 *	2.1977919 *	3.4747758	4.6669529
27 H	2.1806280 *	1.1041438 *	2.1884391 *	2.6913038 *
28 H	3.9920093	2.6568682 *	2.6586877 *	2.0963815 *
29 H	8.8492107	7.4543129	6.6993900	5.2691038
30 H	9.6361567	8.2229299	7.7880286	6.4029096
31 H	8.5083864	7.1763981	7.0780078	5.9173727
32 H	6.1129933	4.8278997	4.8728003	3.9687218
33 H	7.4538031	6.1685487	5.1851227	3.8896185
34 H	5.5535533	4.6823852	3.3329037	3.0048307

35 H 6.3020310 5.5554220 4.1518692 3.8862334

C C C C

1 CO 2.8598125 * 3.2611161 3.0100586 4.2815282
2 C 6.2328091 7.5540662 8.0383576 9.4316669
3 C 6.5846830 7.7722845 8.0553046 9.4050252
4 C 5.7597925 6.8004116 6.9454789 8.2507106
5 C 4.3530195 5.4101760 5.6411070 6.9832504
6 C 3.7335136 5.0267827 5.5549879 6.9576927
7 C 4.9339916 6.3088200 6.9267120 8.3311359
8 C 5.1564331 6.5894075 7.4039305 8.7872428
9 C 4.3468263 5.7581440 6.7264128 8.0566297
10 C 2.9241350 * 4.3293046 5.3143739 6.6392815
11 C 2.4458355 * 3.8345732 4.5893222 5.9854977
12 N 1.3320152 * 2.5072582 * 3.1506827 4.5516711
13 C 0.0000000 1.4666240 * 2.6059766 * 3.8839746
14 C 1.4666240 * 0.0000000 1.4376629 * 2.5004955 *
15 C 2.6059766 * 1.4376629 * 0.0000000 1.4064653 *
16 C 3.8839746 2.5004955 * 1.4064653 * 0.0000000
17 C 4.3429966 2.8817005 * 2.4413365 * 1.4285480 *
18 C 3.7921212 2.4975001 * 2.8252452 * 2.4728829 *
19 C 2.4687376 * 1.4425293 * 2.4455970 * 2.8453145 *
20 O 3.0480656 2.5027870 * 1.4658557 * 2.4601818 *
21 N 3.9865384 4.7106966 4.7013376 5.9419857
22 H 7.1286233 8.4917270 9.0370040 10.4348575
23 H 7.6727573 8.8336365 9.0571272 10.3839641
24 H 6.4081484 7.2975342 7.2741402 8.4954671
25 H 6.2424983 7.6767003 8.4987707 9.8781483
26 H 5.0066223 6.3547612 7.4102794 8.6788676
27 H 2.6442060 * 3.8935876 5.0081284 6.2262667
28 H 1.1083644 * 2.1766010 * 3.5325426 4.6734026
29 H 4.7953517 3.5027236 2.1941316 * 1.1067686 *
30 H 5.4477681 3.9868323 3.4401423 2.1923786 *
31 H 4.6556373 3.4930805 3.9294791 3.4750552
32 H 2.6388543 * 2.1967989 * 3.4500714 3.9510949
33 H 4.0159913 3.3301403 2.0460458 * 2.5098893 *
34 H 3.8566174 4.5631936 4.7118022 5.9165582
35 H 4.9473979 5.5278860 5.3158381 6.4435380

C C C O

1 CO 5.4409475 5.6089807 4.6947080 1.9520856 *
2 C 10.3382853 10.0099491 8.6963409 7.2665190
3 C 10.4276010 10.2524151 9.0146049 7.1141559
4 C 9.3241302 9.2546622 8.0962582 5.9451915

5 C	7.9974960	7.8724587	6.6957708	4.7614134
6 C	7.8169643	7.4894234	6.1962938	4.9310068
7 C	9.1414426	8.7247527	7.3843946	6.3251568
8 C	9.4377778	8.8559828	7.4778154	7.0184227
9 C	8.5513874	7.8526702	6.4770625	6.5877808
10 C	7.1335696	6.4700353	5.0983149	5.2698700
11 C	6.6890600	6.2314871	4.8979181	4.2867551
12 N	5.3107159	4.9853503	3.7417758	2.9387808 *
13 C	4.3429966	3.7921212	2.4687376 *	3.0480656
14 C	2.8817005 *	2.4975001 *	1.4425293 *	2.5027870 *
15 C	2.4413365 *	2.8252452 *	2.4455970 *	1.4658557 *
16 C	1.4285480 *	2.4728829 *	2.8453145 *	2.4601818 *
17 C	0.0000000	1.4230906 *	2.4552429 *	3.7711876
18 C	1.4230906 *	0.0000000	1.4157780 *	4.2909096
19 C	2.4552429 *	1.4157780 *	0.0000000	3.7949587
20 O	3.7711876	4.2909096	3.7949587	0.0000000
21 N	7.0170100	7.0525708	6.0291445	3.7649656
22 H	11.3051969	10.9195359	9.5798993	8.2997461
23 H	11.4450812	11.3116277	10.0907526	8.0507282
24 H	9.6355696	9.6890267	8.6205605	6.1749915
25 H	10.5176568	9.9095236	8.5277032	8.0935132
26 H	9.0447035	8.2414244	6.8920927	7.4082749
27 H	6.5448685	5.7697873	4.4297747	5.2349055
28 H	4.8517726	3.9955791	2.5809613 *	4.1418282
29 H	2.2009686 *	3.4739922	3.9520619	2.6865711 *
30 H	1.1051761 *	2.2002025 *	3.4602001	4.6507120
31 H	2.1979879 *	1.1042355 *	2.1873368 *	5.3951348
32 H	3.4568122	2.1860066 *	1.1057917 *	4.6915114
33 H	3.9305340	4.7314807	4.4874408	0.9918788 *
34 H	6.8543648	6.7791955	5.7458189	4.0355672
35 H	7.6029329	7.7806666	6.8589478	4.2295885

N H H H

1 CO	1.9783512 *	6.4353254	6.1182065	4.3388874
2 C	4.3424771	1.1051240 *	2.1867502 *	3.4387789
3 C	3.8147663	2.1793245 *	1.1041748 *	2.1939636 *
4 C	2.4743995 *	3.4509224	2.2009614 *	1.1078125 *
5 C	1.5096434 *	3.9434904	3.4661571	2.1825394 *
6 C	2.5928723 *	3.5203200	4.0269555	3.5069129
7 C	3.8871574	2.1971823 *	3.4865277	3.9522159
8 C	5.1108168	2.6809963 *	4.6708638	5.3951296
9 C	5.3875100	4.0802300	5.9314786	6.2661431
10 C	4.5645622	4.8931011	6.2584328	6.0068620
11 C	3.1553574	4.6931024	5.4877749	4.8012050
12 N	2.8991004 *	5.9998269	6.4044291	5.1730152

13 C	3.9865384	7.1286233	7.6727573	6.4081484
14 C	4.7106966	8.4917270	8.8336365	7.2975342
15 C	4.7013376	9.0370040	9.0571272	7.2741402
16 C	5.9419857	10.4348575	10.3839641	8.4954671
17 C	7.0170100	11.3051969	11.4450812	9.6355696
18 C	7.0525708	10.9195359	11.3116277	9.6890267
19 C	6.0291445	9.5798993	10.0907526	8.6205605
20 O	3.7649656	8.2997461	8.0507282	6.1749915
21 N	0.0000000	5.4466964	4.6743672	2.6518396 *
22 H	5.4466964	0.0000000	2.5299039 *	4.3594489
23 H	4.6743672	2.5299039 *	0.0000000	2.5183051 *
24 H	2.6518396 *	4.3594489	2.5183051 *	0.0000000
25 H	6.0561093	2.4010635 *	4.7810570	5.9747513
26 H	6.4711118	4.7782343	6.8517846	7.3470880
27 H	5.2583275	5.9671504	7.3477805	6.9658889
28 H	4.7368315	7.1958218	8.0307805	7.0106200
29 H	6.2734848	10.9574792	10.7093279	8.7083560
30 H	7.9986219	12.3906136	12.4753986	10.6003792
31 H	8.0543453	11.7570902	12.2563864	10.6872032
32 H	6.4135267	9.4588127	10.1907399	8.9175076
33 H	4.3843102	8.9845348	8.5766820	6.6178700
34 H	1.0441029 *	5.8525680	5.1763384	3.2106574
35 H	1.0394681 *	5.8196543	4.5835286	2.2116620 *

H H H H

1 CO	6.4945909	6.2795680	4.5251256	3.8762905
2 C	2.6811783 *	4.6682256	5.3914720	6.4011587
3 C	4.0805238	5.9299289	6.2678514	6.9327089
4 C	4.8901809	6.2525546	6.0082986	6.2681853
5 C	4.6714350	5.4686076	4.8026301	4.8921693
6 C	3.5172376	4.0172420	3.5050405	4.0413114
7 C	2.1970652 *	3.4838317	3.9500552	5.0271853
8 C	1.1049513 *	2.1843666 *	3.4300570	4.9850084
9 C	2.1804914 *	1.1042644 *	2.1806280 *	3.9920093
10 C	3.4526506	2.1977919 *	1.1041438 *	2.6568682 *
11 C	3.9638492	3.4747758	2.1884391 *	2.6586877 *
12 N	5.4107970	4.6669529	2.6913038 *	2.0963815 *
13 C	6.2424983	5.0066223	2.6442060 *	1.1083644 *
14 C	7.6767003	6.3547612	3.8935876	2.1766010 *
15 C	8.4987707	7.4102794	5.0081284	3.5325426
16 C	9.8781483	8.6788676	6.2262667	4.6734026
17 C	10.5176568	9.0447035	6.5448685	4.8517726
18 C	9.9095236	8.2414244	5.7697873	3.9955791
19 C	8.5277032	6.8920927	4.4297747	2.5809613 *
20 O	8.0935132	7.4082749	5.2349055	4.1418282

21 N	6.0561093	6.4711118	5.2583275	4.7368315
22 H	2.4010635 *	4.7782343	5.9671504	7.1958218
23 H	4.7810570	6.8517846	7.3477805	8.0307805
24 H	5.9747513	7.3470880	6.9658889	7.0106200
25 H	0.0000000	2.5276472 *	4.3469721	6.0149709
26 H	2.5276472 *	0.0000000	2.5000318 *	4.4817774
27 H	4.3469721	2.5000318 *	0.0000000	2.1527639 *
28 H	6.0149709	4.4817774	2.1527639 *	0.0000000
29 H	10.5711599	9.5191115	7.1168593	5.6705401
30 H	11.6116293	10.1045930	7.6064727	5.9311753
31 H	10.6138637	8.7927368	6.3887325	4.6531988
32 H	8.2095317	6.4046340	4.0651481	2.2638185 *
33 H	8.8913880	8.2710227	6.1294704	5.0992511
34 H	6.3305864	6.6030643	5.3124638	4.4888810
35 H	6.7592532	7.3982827	6.2732930	5.7439350

H H H H

1 CO	4.6181938	6.4214439	6.6745329	5.2769255
2 C	9.9323477	11.4168759	10.8821335	8.6485201
3 C	9.7859122	11.4723934	11.1871414	9.1010041
4 C	8.5761396	10.3390217	10.2271516	8.3027927
5 C	7.4006254	9.0347909	8.8366727	6.9045090
6 C	7.5349997	8.9008036	8.3830145	6.2337128
7 C	8.9266524	10.2334942	9.5621877	7.2867414
8 C	9.4862349	10.5340536	9.5899041	7.2097780
9 C	8.8492107	9.6361567	8.5083864	6.1129933
10 C	7.4543129	8.2229299	7.1763981	4.8278997
11 C	6.6993900	7.7880286	7.0780078	4.8728003
12 N	5.2691038	6.4029096	5.9173727	3.9687218
13 C	4.7953517	5.4477681	4.6556373	2.6388543 *
14 C	3.5027236	3.9868323	3.4930805	2.1967989 *
15 C	2.1941316 *	3.4401423	3.9294791	3.4500714
16 C	1.1067686 *	2.1923786 *	3.4750552	3.9510949
17 C	2.2009686 *	1.1051761 *	2.1979879 *	3.4568122
18 C	3.4739922	2.2002025 *	1.1042355 *	2.1860066 *
19 C	3.9520619	3.4602001	2.1873368 *	1.1057917 *
20 O	2.6865711 *	4.6507120	5.3951348	4.6915114
21 N	6.2734848	7.9986219	8.0543453	6.4135267
22 H	10.9574792	12.3906136	11.7570902	9.4588127
23 H	10.7093279	12.4753986	12.2563864	10.1907399
24 H	8.7083560	10.6003792	10.6872032	8.9175076
25 H	10.5711599	11.6116293	10.6138637	8.2095317
26 H	9.5191115	10.1045930	8.7927368	6.4046340
27 H	7.1168593	7.6064727	6.3887325	4.0651481
28 H	5.6705401	5.9311753	4.6531988	2.2638185 *

29 H	0.0000000	2.5216017 *	4.3876758	5.0578432
30 H	2.5216017 *	0.0000000	2.5406996 *	4.3739891
31 H	4.3876758	2.5406996 *	0.0000000	2.5148616 *
32 H	5.0578432	4.3739891	2.5148616 *	0.0000000
33 H	2.3082134 *	4.6324052	5.8174748	5.4659984
34 H	6.3423296	7.8360797	7.7185189	6.0520775
35 H	6.6205076	8.5209787	8.8028651	7.3194479

H H H

1 CO	2.6578724 *	2.5048454 *	2.6195799 *
2 C	7.9507774	4.7752133	4.7366375
3 C	7.7018584	4.3238230	3.9161099
4 C	6.5025801	3.0568978	2.4849185 *
5 C	5.4340633	2.1107467 *	2.0881712 *
6 C	5.7282530	2.9613770 *	3.4233656
7 C	7.0969964	4.2448582	4.5624879
8 C	7.8375532	5.3727771	5.8883757
9 C	7.4538031	5.5535533	6.3020310
10 C	6.1685487	4.6823852	5.5554220
11 C	5.1851227	3.3329037	4.1518692
12 N	3.8896185	3.0048307	3.8862334
13 C	4.0159913	3.8566174	4.9473979
14 C	3.3301403	4.5631936	5.5278860
15 C	2.0460458 *	4.7118022	5.3158381
16 C	2.5098893 *	5.9165582	6.4435380
17 C	3.9305340	6.8543648	7.6029329
18 C	4.7314807	6.7791955	7.7806666
19 C	4.4874408	5.7458189	6.8589478
20 O	0.9918788 *	4.0355672	4.2295885
21 N	4.3843102	1.0441029 *	1.0394681 *
22 H	8.9845348	5.8525680	5.8196543
23 H	8.5766820	5.1763384	4.5835286
24 H	6.6178700	3.2106574	2.2116620 *
25 H	8.8913880	6.3305864	6.7592532
26 H	8.2710227	6.6030643	7.3982827
27 H	6.1294704	5.3124638	6.2732930
28 H	5.0992511	4.4888810	5.7439350
29 H	2.3082134 *	6.3423296	6.6205076
30 H	4.6324052	7.8360797	8.5209787
31 H	5.8174748	7.7185189	8.8028651
32 H	5.4659984	6.0520775	7.3194479
33 H	0.0000000	4.7374937	4.6616916
34 H	4.7374937	0.0000000	1.6672157 *
35 H	4.6616916	1.6672157 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80 , TOTAL = 7999.5 SECONDS (133.3 MIN)
WALL CLOCK TIME: STEP = 0.81 , TOTAL = 7396.9 SECONDS (123.3 MIN)
CPU UTILIZATION: STEP = 99.13%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.16 , TOTAL = 8000.6 SECONDS (133.3 MIN)
WALL CLOCK TIME: STEP = 1.16 , TOTAL = 7398.1 SECONDS (123.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636932816	-284.636932816	0.001012767	0.000146537	198238552
11325698						
2	1	-284.636934878	-0.000002062	0.000410960	0.000011553	142970864
15953874						
3	2	-284.636934876	0.000000002	0.000241434	0.000018362	125038275
17294558						
4	3	-284.636934927	-0.000000051	0.000061500	0.000008468	117937165
17813560						
5	4	-284.636934907	0.000000020	0.000029153	0.000019491	110986840
18369657						
6	5	-284.636934871	0.000000036	0.000052928	0.000004671	103304695
18974950						
7	6	-284.636934873	-0.000000002	0.000042983	0.000004312	130563115
16915844						
8	7	-284.636934873	0.000000000	0.000056736	0.000004003	123854240
17456123						
9	8	-284.636934874	-0.000000001	0.000071077	0.000003434	148212272
15592703						

-----DISABLING FDIFF OPTION-----

10	9	-284.636934914	-0.000000040	0.000096059	0.000005480	198239556
11325575						
11	10	-284.636934915	-0.000000001	0.000126558	0.000007156	198239569
11325576						

12 11 -284.636934917 -0.000000002 0.000141807 0.000007006 198239616
11325574
13 12 -284.636934919 -0.000000001 0.000077402 0.000004474 198239476
11325577
14 13 -284.636934919 -0.000000001 0.000025842 0.000003227 198239540
11325573
15 14 -284.636934920 0.000000000 0.000023627 0.000002782 198239552
11325573

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 49.2 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 16.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.6 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369349197 AFTER 15 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6019382279
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998477627

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 51.77 , TOTAL = 8052.4 SECONDS (134.2 MIN)
WALL CLOCK TIME: STEP = 47.44 , TOTAL = 7445.5 SECONDS (124.1
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.99 , TOTAL = 8056.4 SECONDS (134.3 MIN)
WALL CLOCK TIME: STEP = 3.97 , TOTAL = 7449.5 SECONDS (124.2
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.

USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.85 , TOTAL = 8059.3 SECONDS (134.3 MIN)

WALL CLOCK TIME: STEP = 2.68 , TOTAL = 7452.2 SECONDS (124.2 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 88 ENERGY= -284.6369349

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000607	-0.0000156	-0.0000043
2 C	6.0	0.0000144	-0.0000526	0.0001334
3 C	6.0	-0.0000574	0.0000642	0.0000100
4 C	6.0	0.0000232	0.0000754	-0.0000132
5 C	6.0	0.0000473	-0.0000110	0.0000509
6 C	6.0	-0.0000182	-0.0000172	0.0000462
7 C	6.0	-0.0000294	0.0000081	0.0000458
8 C	6.0	-0.0000895	0.0000035	-0.0000848
9 C	6.0	-0.0000478	0.0000284	-0.0000787
10 C	6.0	0.0000363	-0.0000547	0.0000351
11 C	6.0	-0.0000430	-0.0000478	-0.0000009
12 N	7.0	-0.0000553	-0.0000281	-0.0000611
13 C	6.0	-0.0001083	-0.0000042	-0.0000335
14 C	6.0	-0.0000391	0.0000187	0.0000164
15 C	6.0	0.0000602	-0.0000686	-0.0000435
16 C	6.0	-0.0000114	-0.0000513	-0.0000988
17 C	6.0	-0.0000107	0.0000956	0.0000543
18 C	6.0	-0.0000035	-0.0000249	0.0000551
19 C	6.0	-0.0000388	-0.0000473	0.0000110
20 O	8.0	-0.0000092	0.0000280	0.0000060
21 N	7.0	0.0000178	0.0000458	-0.0000690
22 H	1.0	0.0000776	-0.0000536	0.0000528
23 H	1.0	0.0000131	0.0000219	-0.0001048
24 H	1.0	0.0000148	0.0000219	-0.0000408
25 H	1.0	-0.0000636	-0.0000312	0.0000568
26 H	1.0	0.0000163	0.0000058	-0.0000260
27 H	1.0	0.0000533	0.0000080	-0.0000121
28 H	1.0	-0.0000004	0.0000213	-0.0000309
29 H	1.0	0.0000327	0.0000717	0.0000612

30 H	1.0	-0.0000319	0.0001146	0.0000842
31 H	1.0	-0.0000046	0.0000869	0.0000299
32 H	1.0	0.0000653	-0.0001093	-0.0000300
33 H	1.0	-0.0000144	-0.0000689	-0.0000162
34 H	1.0	0.0001934	0.0000188	-0.0001230
35 H	1.0	0.0000713	-0.0000525	0.0001225

MAXIMUM GRADIENT = 0.0001934 RMS GRADIENT = 0.0000564
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000018735
 PREDICTED ENERGY CHANGE WAS -0.0000013558 RATIO= 1.382
 GDIIS STEP HAS LENGTH = 0.020772
 RADIUS OF STEP TAKEN= 0.02077 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.04 , TOTAL = 8059.3 SECONDS (134.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7452.2 SECONDS (124.2
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 89

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1581657306	-1.7285252805	0.8730536087
C	6.0	4.9802078377	0.6226228725	0.5665048063
C	6.0	5.1823515969	-0.7156766194	0.2036161889
C	6.0	4.0451822206	-1.5336218336	-0.0931283989
C	6.0	2.7373837185	-1.0213120532	-0.0010774693
C	6.0	2.4675486411	0.3439748164	0.4325861726
C	6.0	3.6508183418	1.1748074535	0.6832965521
C	6.0	3.5060187955	2.5616865043	1.0588698543
C	6.0	2.2390552314	3.1403277550	1.2161268424
C	6.0	1.0723012414	2.3332624668	1.0377454915
C	6.0	1.1623985838	0.9783735054	0.6401818089
N	7.0	-0.0506470900	0.1785916090	0.5869660411
C	6.0	-1.2464630209	0.7015630898	0.3209989454
C	6.0	-2.5492177955	0.0377678551	0.4363475325
C	6.0	-2.8187270631	-1.2855889663	0.9293865657
C	6.0	-4.1185610924	-1.8073080602	1.0567799673
C	6.0	-5.2293634192	-0.9925772711	0.6792492976
C	6.0	-5.0169391272	0.3208825548	0.1744517025
C	6.0	-3.6984642457	0.8233743296	0.0577884842
O	8.0	-1.6961476665	-2.1432128892	1.3207298091

N	7.0	1.6302108281	-1.9537456812	-0.4290887686
H	1.0	5.8429977337	1.2816848696	0.7718531533
H	1.0	6.1995283510	-1.1369991677	0.1205432642
H	1.0	4.2079064506	-2.5756888778	-0.4319981140
H	1.0	4.4196287969	3.1581311644	1.2339686983
H	1.0	2.1332581883	4.1977533221	1.5164103048
H	1.0	0.0889844347	2.7798599138	1.2681713945
H	1.0	-1.2914351929	1.7525641873	-0.0280817121
H	1.0	-4.2898214025	-2.8307019105	1.4420275529
H	1.0	-6.2536384580	-1.3945693140	0.7815301426
H	1.0	-5.8751514757	0.9502751332	-0.1202542227
H	1.0	-3.5353272518	1.8475038521	-0.3261446506
H	1.0	-2.0130002600	-2.9575218152	1.7903741686
H	1.0	1.2706209120	-1.6773572188	-1.3695489512
H	1.0	2.0243339268	-2.9094952960	-0.5373490627

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3734495	5.1687960	4.0100364
2 C	5.3734495	0.0000000	1.4012836 *	2.4410613 *
3 C	5.1687960	1.4012836 *	0.0000000	1.4318680 *
4 C	4.0100364	2.4410613 *	1.4318680 *	0.0000000
5 C	2.8136491 *	2.8381212 *	2.4724847 *	1.4075765 *
6 C	3.1340896	2.5316072 *	2.9232591 *	2.5081213 *
7 C	4.5457641	1.4442384 *	2.4798422 *	2.8449864 *
8 C	5.4450496	2.4850804 *	3.7792406	4.2882803
9 C	5.3059900	3.7781959	4.9554960	5.1790007
10 C	4.1666398	4.2918632	5.1850087	5.0069643
11 C	2.8965521 *	3.8350560	4.3841097	3.8933669
12 N	1.9397277 *	5.0504538	5.3226824	4.4911047
13 C	2.8606076 *	6.2320089	6.5842239	5.7592588
14 C	3.2619671	7.5532276	7.7716799	6.7996854
15 C	3.0101921	8.0371849	8.0541171	6.9440844
16 C	4.2813963	9.4304046	9.4035379	8.2488725
17 C	5.4410155	10.3371625	10.4262510	9.3223652
18 C	5.6097974	10.0093806	10.2518699	9.2538008
19 C	4.6957900	8.6958865	9.0143682	8.0958179
20 O	1.9521419 *	7.2658396	7.1133364	5.9441959
21 N	1.9781850 *	4.3418155	3.8145556	2.4741585 *
22 H	6.4334222	1.1049602 *	2.1791740 *	3.4505486
23 H	6.1167179	2.1867542 *	1.1041116 *	2.2009481 *
24 H	4.3383460	3.4384089	2.1938994 *	1.1077976 *
25 H	6.4938231	2.6811489 *	4.0804116	4.8901885

26 H	6.2797831	4.6678689	5.9297717	6.2525778
27 H	4.5261950	5.3916671	6.2685279	6.0092231
28 H	3.8770313	6.4002974	6.9322299	6.2675940
29 H	4.6176958	9.9310339	9.7841226	8.5738793
30 H	6.4211476	11.4155422	11.4706908	10.3368308
31 H	6.6755935	10.8819952	11.1869863	10.2266075
32 H	5.2790104	8.6493638	9.1021132	8.3036396
33 H	2.6581707 *	7.9511164	7.7017374	6.5020495
34 H	2.5038852 *	4.7748558	4.3245017	3.0574662
35 H	2.6204026 *	4.7361950	3.9159859	2.4847913 *

C C C C

1 CO	2.8136491 *	3.1340896	4.5457641	5.4450496
2 C	2.8381212 *	2.5316072 *	1.4442384 *	2.4850804 *
3 C	2.4724847 *	2.9232591 *	2.4798422 *	3.7792406
4 C	1.4075765 *	2.5081213 *	2.8449864 *	4.2882803
5 C	0.0000000	1.4576980 *	2.4750094 *	3.8147302
6 C	1.4576980 *	0.0000000	1.4674010 *	2.5276267 *
7 C	2.4750094 *	1.4674010 *	0.0000000	1.4441107 *
8 C	3.8147302	2.5276267 *	1.4441107 *	0.0000000
9 C	4.3645347	2.9130285 *	2.4779534 *	1.4016962 *
10 C	3.8864924	2.5040364 *	2.8489301 *	2.4445050 *
11 C	2.6249827 *	1.4659380 *	2.4965332 *	2.8591494 *
12 N	3.0917115	2.5283383 *	3.8343933	4.3071692
13 C	4.3523634	3.7328546	4.9334151	5.1566070
14 C	5.4093573	5.0261041	6.3082716	6.5896578
15 C	5.6396784	5.5540075	6.9259749	7.4041005
16 C	6.9814634	6.9566139	8.3304117	8.7876240
17 C	7.9957945	7.8159881	9.1408534	9.4384218
18 C	7.8715830	7.4889735	8.7245705	8.8568736
19 C	6.6952574	6.1959674	7.3842210	7.4785339
20 O	4.7604660	4.9306459	6.3250001	7.0190587
21 N	1.5094562 *	2.5929014 *	3.8869140	5.1109494
22 H	3.9428486	3.5196674	2.1965690 *	2.6799726 *
23 H	3.4662113	4.0271984	3.4866981	4.6707308
24 H	2.1827086 *	3.5072478	3.9522718	5.3951793
25 H	4.6715129	3.5174290	2.1972442 *	1.1050290 *
26 H	5.4686726	4.0172171	3.4835713	2.1841542 *
27 H	4.8035320	3.5056107	3.9503079	3.4303834
28 H	4.8914722	4.0405814	5.0265029	4.9851487
29 H	7.3985171	7.5338963	8.9260034	9.4868218
30 H	9.0327336	8.8996293	10.2327714	10.5346944
31 H	8.8361259	8.3829516	9.5624374	9.5913156
32 H	6.9052644	6.2346444	7.2878104	7.2117180
33 H	5.4336319	5.7287683	7.0979298	7.8394088

34 H	2.1105693 *	2.9607618 *	4.2443324	5.3724960
35 H	2.0883638 *	3.4237817	4.5625603	5.8887295

	C	C	C	N
--	---	---	---	---

1 CO	5.3059900	4.1666398	2.8965521 *	1.9397277 *
2 C	3.7781959	4.2918632	3.8350560	5.0504538
3 C	4.9554960	5.1850087	4.3841097	5.3226824
4 C	5.1790007	5.0069643	3.8933669	4.4911047
5 C	4.3645347	3.8864924	2.6249827 *	3.0917115
6 C	2.9130285 *	2.5040364 *	1.4659380 *	2.5283383 *
7 C	2.4779534 *	2.8489301 *	2.4965332 *	3.8343933
8 C	1.4016962 *	2.4445050 *	2.8591494 *	4.3071692
9 C	0.0000000	1.4298563 *	2.4829314 *	3.7961113
10 C	1.4298563 *	0.0000000	1.4148846 *	2.4711984 *
11 C	2.4829314 *	1.4148846 *	0.0000000	1.4539473 *
12 N	3.7961113	2.4711984 *	1.4539473 *	0.0000000
13 C	4.3471444	2.9245232 *	2.4456320 *	1.3319960 *
14 C	5.7586016	4.3297084	3.8343687	2.5070646 *
15 C	6.7269696	5.3148780	4.5889571	3.1501339
16 C	8.0575292	6.6400104	5.9851576	4.5510929
17 C	8.5525680	7.1344731	6.6888560	5.3102971
18 C	7.8539043	6.4709966	6.2316461	4.9854259
19 C	6.4779749	5.0990471	4.8980807	3.7419706
20 O	6.5888212	5.2709791	4.2870426	2.9388531 *
21 N	5.3876720	4.5652278	3.1558693	2.8990538 *
22 H	4.0792566	4.8924492	4.6922642	5.9988372
23 H	5.9313722	6.2587885	5.4879415	6.4041410
24 H	6.2662219	6.0074928	4.8016713	5.1729708
25 H	2.1807192 *	3.4530441	3.9640226	5.4110660
26 H	1.1043152 *	2.1979708 *	3.4748743	4.6676514
27 H	2.1806995 *	1.1042904 *	2.1890505 *	2.6926074 *
28 H	3.9922807	2.6571504 *	2.6584295 *	2.0964800 *
29 H	8.8504495	7.4553559	6.6991578	5.2685460
30 H	9.6374277	8.2238536	7.7877110	6.4023271
31 H	8.5101466	7.1777933	7.0785707	5.9178127
32 H	6.1150215	4.8297410	4.8741976	3.9701429
33 H	7.4561052	6.1707320	5.1862677	3.8902736
34 H	5.5528077	4.6818231	3.3322118	3.0030395
35 H	6.3024711	5.5564195	4.1527142	3.8866324

	C	C	C	C
--	---	---	---	---

1 CO	2.8606076 *	3.2619671	3.0101921	4.2813963
2 C	6.2320089	7.5532276	8.0371849	9.4304046
3 C	6.5842239	7.7716799	8.0541171	9.4035379

4 C	5.7592588	6.7996854	6.9440844	8.2488725
5 C	4.3523634	5.4093573	5.6396784	6.9814634
6 C	3.7328546	5.0261041	5.5540075	6.9566139
7 C	4.9334151	6.3082716	6.9259749	8.3304117
8 C	5.1566070	6.5896578	7.4041005	8.7876240
9 C	4.3471444	5.7586016	6.7269696	8.0575292
10 C	2.9245232 *	4.3297084	5.3148780	6.6400104
11 C	2.4456320 *	3.8343687	4.5889571	5.9851576
12 N	1.3319960 *	2.5070646 *	3.1501339	4.5510929
13 C	0.0000000	1.4666627 *	2.6059399 *	3.8839098
14 C	1.4666627 *	0.0000000	1.4377051 *	2.5004159 *
15 C	2.6059399 *	1.4377051 *	0.0000000	1.4064098 *
16 C	3.8839098	2.5004159 *	1.4064098 *	0.0000000
17 C	4.3430347	2.8816303 *	2.4412276 *	1.4283548 *
18 C	3.7924773	2.4976773 *	2.8253873 *	2.4728084 *
19 C	2.4690945 *	1.4426545 *	2.4456792 *	2.8451635 *
20 O	3.0486765	2.5033053 *	1.4658966 *	2.4597944 *
21 N	3.9860442	4.7098545	4.6994614	5.9394973
22 H	7.1274304	8.4905344	9.0355513	10.4333942
23 H	7.6722409	8.8329140	9.0556743	10.3821396
24 H	6.4076151	7.2967738	7.2726408	8.4933463
25 H	6.2428228	7.6770886	8.4990126	9.8786471
26 H	5.0074814	6.3559103	7.4117338	8.6808563
27 H	2.6457274 *	3.8950110	5.0097341	6.2281808
28 H	1.1083696 *	2.1767494 *	3.5326676	4.6735700
29 H	4.7953760	3.5027435	2.1941498 *	1.1068337 *
30 H	5.4477212	3.9866619	3.4398190	2.1919560 *
31 H	4.6563203	3.4934667	3.9297028	3.4749510
32 H	2.6402414 *	2.1974873 *	3.4505282	3.9509862
33 H	4.0169074	3.3305672	2.0459362 *	2.5088919 *
34 H	3.8539493	4.5600531	4.7075847	5.9116192
35 H	4.9471827	5.5273701	5.3144732	6.4413681

C C C O

1 CO	5.4410155	5.6097974	4.6957900	1.9521419 *
2 C	10.3371625	10.0093806	8.6958865	7.2658396
3 C	10.4262510	10.2518699	9.0143682	7.1133364
4 C	9.3223652	9.2538008	8.0958179	5.9441959
5 C	7.9957945	7.8715830	6.6952574	4.7604660
6 C	7.8159881	7.4889735	6.1959674	4.9306459
7 C	9.1408534	8.7245705	7.3842210	6.3250001
8 C	9.4384218	8.8568736	7.4785339	7.0190587
9 C	8.5525680	7.8539043	6.4779749	6.5888212
10 C	7.1344731	6.4709966	5.0990471	5.2709791
11 C	6.6888560	6.2316461	4.8980807	4.2870426

12 N	5.3102971	4.9854259	3.7419706	2.9388531 *
13 C	4.3430347	3.7924773	2.4690945 *	3.0486765
14 C	2.8816303 *	2.4976773 *	1.4426545 *	2.5033053 *
15 C	2.4412276 *	2.8253873 *	2.4456792 *	1.4658966 *
16 C	1.4283548 *	2.4728084 *	2.8451635 *	2.4597944 *
17 C	0.0000000	1.4230676 *	2.4551061 *	3.7708186
18 C	1.4230676 *	0.0000000	1.4157981 *	4.2910810
19 C	2.4551061 *	1.4157981 *	0.0000000	3.7953830
20 O	3.7708186	4.2910810	3.7953830	0.0000000
21 N	7.0147001	7.0514394	6.0286170	3.7632996
22 H	11.3038943	10.9187114	9.5791144	8.2987893
23 H	11.4434513	11.3109446	10.0904539	8.0495101
24 H	9.6334405	9.6879143	8.6199895	6.1738923
25 H	10.5185144	9.9106695	8.5286531	8.0941027
26 H	9.0470198	8.2435612	6.8936926	7.4101614
27 H	6.5469791	5.7717630	4.4314366	5.2369939
28 H	4.8521539	3.9962622	2.5815802 *	4.1424828
29 H	2.2007435 *	3.4738931	3.9519735	2.6859817 *
30 H	1.1050784 *	2.2001692 *	3.4600565	4.6499383
31 H	2.1979362 *	1.1043165 *	2.1876404 *	5.3953847
32 H	3.4563906	2.1854846 *	1.1058298 *	4.6926109
33 H	3.9294526	4.7310453	4.4875180	0.9919982 *
34 H	6.8495470	6.7757148	5.7430617	4.0319148
35 H	7.6007112	7.7795583	6.8584928	4.2286675

N H H H

1 CO	1.9781850 *	6.4334222	6.1167179	4.3383460
2 C	4.3418155	1.1049602 *	2.1867542 *	3.4384089
3 C	3.8145556	2.1791740 *	1.1041116 *	2.1938994 *
4 C	2.4741585 *	3.4505486	2.2009481 *	1.1077976 *
5 C	1.5094562 *	3.9428486	3.4662113	2.1827086 *
6 C	2.5929014 *	3.5196674	4.0271984	3.5072478
7 C	3.8869140	2.1965690 *	3.4866981	3.9522718
8 C	5.1109494	2.6799726 *	4.6707308	5.3951793
9 C	5.3876720	4.0792566	5.9313722	6.2662219
10 C	4.5652278	4.8924492	6.2587885	6.0074928
11 C	3.1558693	4.6922642	5.4879415	4.8016713
12 N	2.8990538 *	5.9988372	6.4041410	5.1729708
13 C	3.9860442	7.1274304	7.6722409	6.4076151
14 C	4.7098545	8.4905344	8.8329140	7.2967738
15 C	4.6994614	9.0355513	9.0556743	7.2726408
16 C	5.9394973	10.4333942	10.3821396	8.4933463
17 C	7.0147001	11.3038943	11.4434513	9.6334405
18 C	7.0514394	10.9187114	11.3109446	9.6879143
19 C	6.0286170	9.5791144	10.0904539	8.6199895

20	O	3.7632996	8.2987893	8.0495101	6.1738923
21	N	0.0000000	5.4459017	4.6741665	2.6516667 *
22	H	5.4459017	0.0000000	2.5300892 *	4.3591414
23	H	4.6741665	2.5300892 *	0.0000000	2.5182708 *
24	H	2.6516667 *	4.3591414	2.5182708 *	0.0000000
25	H	6.0562280	2.4001210 *	4.7807848	5.9746936
26	H	6.4713958	4.7770271	6.8514657	7.3471069
27	H	5.2595715	5.9665341	7.3483047	6.9669217
28	H	4.7364074	7.1945644	8.0303300	7.0099702
29	H	6.2703198	10.9560432	10.7070728	8.7056523
30	H	7.9958337	12.3891500	12.4733560	10.5977175
31	H	8.0535197	11.7567304	12.2561246	10.6863307
32	H	6.4142715	9.4593197	10.1918694	8.9181560
33	H	4.3825300	8.9847072	8.5760285	6.6169793
34	H	1.0441077 *	5.8521930	5.1774984	3.2114868
35	H	1.0394761 *	5.8191232	4.5833190	2.2114508 *

H H H H

1	CO	6.4938231	6.2797831	4.5261950	3.8770313
2	C	2.6811489 *	4.6678689	5.3916671	6.4002974
3	C	4.0804116	5.9297717	6.2685279	6.9322299
4	C	4.8901885	6.2525778	6.0092231	6.2675940
5	C	4.6715129	5.4686726	4.8035320	4.8914722
6	C	3.5174290	4.0172171	3.5056107	4.0405814
7	C	2.1972442 *	3.4835713	3.9503079	5.0265029
8	C	1.1050290 *	2.1841542 *	3.4303834	4.9851487
9	C	2.1807192 *	1.1043152 *	2.1806995 *	3.9922807
10	C	3.4530441	2.1979708 *	1.1042904 *	2.6571504 *
11	C	3.9640226	3.4748743	2.1890505 *	2.6584295 *
12	N	5.4110660	4.6676514	2.6926074 *	2.0964800 *
13	C	6.2428228	5.0074814	2.6457274 *	1.1083696 *
14	C	7.6770886	6.3559103	3.8950110	2.1767494 *
15	C	8.4990126	7.4117338	5.0097341	3.5326676
16	C	9.8786471	8.6808563	6.2281808	4.6735700
17	C	10.5185144	9.0470198	6.5469791	4.8521539
18	C	9.9106695	8.2435612	5.7717630	3.9962622
19	C	8.5286531	6.8936926	4.4314366	2.5815802 *
20	O	8.0941027	7.4101614	5.2369939	4.1424828
21	N	6.0562280	6.4713958	5.2595715	4.7364074
22	H	2.4001210 *	4.7770271	5.9665341	7.1945644
23	H	4.7807848	6.8514657	7.3483047	8.0303300
24	H	5.9746936	7.3471069	6.9669217	7.0099702
25	H	0.0000000	2.5274647 *	4.3472681	6.0153671
26	H	2.5274647 *	0.0000000	2.5002199 *	4.4825138
27	H	4.3472681	2.5002199 *	0.0000000	2.1543368 *

28 H	6.0153671	4.4825138	2.1543368 *	0.0000000
29 H	10.5718462	9.5215895	7.1191692	5.6707909
30 H	11.6125112	10.1071339	7.6086493	5.9315581
31 H	10.6156040	8.7954199	6.3910894	4.6543118
32 H	8.2117613	6.4071477	4.0677717	2.2655919 *
33 H	8.8932286	8.2743264	6.1325838	5.1002302
34 H	6.3306005	6.6022593	5.3123082	4.4864269
35 H	6.7595188	7.3988361	6.2748900	5.7435596

H H H H

1 CO	4.6176958	6.4211476	6.6755935	5.2790104
2 C	9.9310339	11.4155422	10.8819952	8.6493638
3 C	9.7841226	11.4706908	11.1869863	9.1021132
4 C	8.5738793	10.3368308	10.2266075	8.3036396
5 C	7.3985171	9.0327336	8.8361259	6.9052644
6 C	7.5338963	8.8996293	8.3829516	6.2346444
7 C	8.9260034	10.2327714	9.5624374	7.2878104
8 C	9.4868218	10.5346944	9.5913156	7.2117180
9 C	8.8504495	9.6374277	8.5101466	6.1150215
10 C	7.4553559	8.2238536	7.1777933	4.8297410
11 C	6.6991578	7.7877110	7.0785707	4.8741976
12 N	5.2685460	6.4023271	5.9178127	3.9701429
13 C	4.7953760	5.4477212	4.6563203	2.6402414 *
14 C	3.5027435	3.9866619	3.4934667	2.1974873 *
15 C	2.1941498 *	3.4398190	3.9297028	3.4505282
16 C	1.1068337 *	2.1919560 *	3.4749510	3.9509862
17 C	2.2007435 *	1.1050784 *	2.1979362 *	3.4563906
18 C	3.4738931	2.2001692 *	1.1043165 *	2.1854846 *
19 C	3.9519735	3.4600565	2.1876404 *	1.1058298 *
20 O	2.6859817 *	4.6499383	5.3953847	4.6926109
21 N	6.2703198	7.9958337	8.0535197	6.4142715
22 H	10.9560432	12.3891500	11.7567304	9.4593197
23 H	10.7070728	12.4733560	12.2561246	10.1918694
24 H	8.7056523	10.5977175	10.6863307	8.9181560
25 H	10.5718462	11.6125112	10.6156040	8.2117613
26 H	9.5215895	10.1071339	8.7954199	6.4071477
27 H	7.1191692	7.6086493	6.3910894	4.0677717
28 H	5.6707909	5.9315581	4.6543118	2.2655919 *
29 H	0.0000000	2.5209742 *	4.3874575	5.0577963
30 H	2.5209742 *	0.0000000	2.5406225 *	4.3734652
31 H	4.3874575	2.5406225 *	0.0000000	2.5143961 *
32 H	5.0577963	4.3734652	2.5143961 *	0.0000000
33 H	2.3068037 *	4.6307234	5.8170087	5.4667543
34 H	6.3366936	7.8308103	7.7153906	6.0506591
35 H	6.6176051	8.5181729	8.8019126	7.3200738

	H	H	H
1 CO	2.6581707 *	2.5038852 *	2.6204026 *
2 C	7.9511164	4.7748558	4.7361950
3 C	7.7017374	4.3245017	3.9159859
4 C	6.5020495	3.0574662	2.4847913 *
5 C	5.4336319	2.1105693 *	2.0883638 *
6 C	5.7287683	2.9607618 *	3.4237817
7 C	7.0979298	4.2443324	4.5625603
8 C	7.8394088	5.3724960	5.8887295
9 C	7.4561052	5.5528077	6.3024711
10 C	6.1707320	4.6818231	5.5564195
11 C	5.1862677	3.3322118	4.1527142
12 N	3.8902736	3.0030395	3.8866324
13 C	4.0169074	3.8539493	4.9471827
14 C	3.3305672	4.5600531	5.5273701
15 C	2.0459362 *	4.7075847	5.3144732
16 C	2.5088919 *	5.9116192	6.4413681
17 C	3.9294526	6.8495470	7.6007112
18 C	4.7310453	6.7757148	7.7795583
19 C	4.4875180	5.7430617	6.8584928
20 O	0.9919982 *	4.0319148	4.2286675
21 N	4.3825300	1.0441077 *	1.0394761 *
22 H	8.9847072	5.8521930	5.8191232
23 H	8.5760285	5.1774984	4.5833190
24 H	6.6169793	3.2114868	2.2114508 *
25 H	8.8932286	6.3306005	6.7595188
26 H	8.2743264	6.6022593	7.3988361
27 H	6.1325838	5.3123082	6.2748900
28 H	5.1002302	4.4864269	5.7435596
29 H	2.3068037 *	6.3366936	6.6176051
30 H	4.6307234	7.8308103	8.5181729
31 H	5.8170087	7.7153906	8.8019126
32 H	5.4667543	6.0506591	7.3200738
33 H	0.0000000	4.7335086	4.6605439
34 H	4.7335086	0.0000000	1.6669746 *
35 H	4.6605439	1.6669746 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.73 , TOTAL = 8060.0 SECONDS (134.3 MIN)

WALL CLOCK TIME: STEP = 0.73 , TOTAL = 7452.9 SECONDS (124.2 MIN)

CPU UTILIZATION: STEP = 99.57%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.02 , TOTAL = 8061.0 SECONDS (134.4 MIN)

WALL CLOCK TIME: STEP = 1.01 , TOTAL = 7454.0 SECONDS (124.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.636928679 -284.636928679 0.003871016 0.000317424 198250935
11324864

2 1 -284.636938363 -0.000009684 0.000890843 0.000030104 149315352
15446682

3 2 -284.636938253 0.000000110 0.000511012 0.000065887 132585929
16750563

4 3 -284.636938519 -0.000000266 0.000226753 0.000024431 126118234
17241554

5 4 -284.636938471 0.000000047 0.000130606 0.000044311 119592188
17725325

6 5 -284.636938502 -0.000000030 0.000066892 0.000007153 113333259
18211996

7 6 -284.636938516 -0.000000014 0.000040972 0.000006939 108560292
18517910

8 7 -284.636938511 0.000000005 0.000044297 0.000004566 101744673
18997856

9 8 -284.636938514 -0.000000003 0.000069877 0.000003774 126229418
17273742

10 9 -284.636938516 -0.000000002 0.000052171 0.000003187 148558340
15610559

11 10 -284.636938516 -0.000000001 0.000046663 0.000003884 147069610
15687637

12 11 -284.636938517 -0.000000001 0.000050929 0.000004747 148385432
15580860

-----DISABLING FDIFF OPTION-----

13 12 -284.636938557 -0.000000040 0.000149759 0.000004468 198250409
11324937

14 13 -284.636938558 -0.000000001 0.000043034 0.000003545 198250557
11324928

15 14	-284.636938559	-0.000000001	0.000074803	0.000003756	198250495
11324933					
16 15	-284.636938559	0.000000000	0.000060978	0.000002968	198250426
11324933					
17 16	-284.636938560	0.000000000	0.000063328	0.000001491	198250374
11324938					
18 17	-284.636938560	0.000000000	0.000064721	0.000000923	198250416
11324935					
19 18	-284.636938560	0.000000000	0.000015542	0.000000831	198250496
11324932					
20 19	-284.636938560	0.000000000	0.000034971	0.000000692	198250497
11324931					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 66.2 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 21.8 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.8 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369385599 AFTER 20 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6018588528
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998486594

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 69.27 , TOTAL = 8130.3 SECONDS (135.5 MIN)
WALL CLOCK TIME: STEP = 63.52 , TOTAL = 7517.5 SECONDS (125.3 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 4.03 , TOTAL = 8134.3 SECONDS (135.6 MIN)

WALL CLOCK TIME: STEP = 4.02 , TOTAL = 7521.5 SECONDS (125.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.87 , TOTAL = 8137.2 SECONDS (135.6 MIN)

WALL CLOCK TIME: STEP = 2.69 , TOTAL = 7524.2 SECONDS (125.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 89 ENERGY= -284.6369386

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000023	-0.0000476	-0.0000015
2 C	6.0	-0.0000043	-0.0001393	-0.0000207
3 C	6.0	0.0000328	0.0001173	0.0000643
4 C	6.0	0.0000874	0.0000042	-0.0000385
5 C	6.0	-0.0000707	0.0000164	0.0000339
6 C	6.0	-0.0000400	-0.0000106	0.0000397
7 C	6.0	-0.0001074	0.0000373	0.0000005
8 C	6.0	0.0000097	0.0000405	-0.0000377
9 C	6.0	-0.0001149	-0.0000713	-0.0000890
10 C	6.0	0.0000081	0.0000474	0.0000638
11 C	6.0	-0.0000016	-0.0000607	0.0000516
12 N	7.0	-0.0001005	-0.0000991	-0.0000713
13 C	6.0	-0.0000120	0.0000396	-0.0001287
14 C	6.0	-0.0000247	-0.0000121	0.0000506
15 C	6.0	0.0000468	-0.0000484	-0.0000243
16 C	6.0	-0.0000381	0.0000836	-0.0000816
17 C	6.0	0.0000783	0.0000198	-0.0000261
18 C	6.0	-0.0000061	0.0000173	0.0000854
19 C	6.0	0.0000085	-0.0000448	0.0000946
20 O	8.0	0.0000255	0.0000557	-0.0000214
21 N	7.0	0.0000995	0.0000135	0.0000673
22 H	1.0	-0.0000473	-0.0000933	0.0000642
23 H	1.0	-0.0000287	0.0000089	-0.0000575
24 H	1.0	0.0000392	0.0000451	-0.0000715

25 H	1.0	-0.0000097	-0.0000140	0.0001078
26 H	1.0	0.0000539	0.0000519	-0.0000773
27 H	1.0	-0.0000090	0.0000878	0.0000377
28 H	1.0	-0.0000080	0.0000230	-0.0000285
29 H	1.0	0.0000195	0.0000201	0.0000317
30 H	1.0	0.0000413	0.0001291	0.0001124
31 H	1.0	-0.0000720	0.0000912	0.0000106
32 H	1.0	-0.0000473	-0.0000932	-0.0000936
33 H	1.0	-0.0000682	-0.0001613	0.0000165
34 H	1.0	0.0001917	0.0000099	-0.0001058
35 H	1.0	0.0000657	-0.0000639	0.0000423

MAXIMUM GRADIENT = 0.0001917 RMS GRADIENT = 0.0000650
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000036402
 PREDICTED ENERGY CHANGE WAS -0.0000022993 RATIO= 1.583
 GDIIS STEP HAS LENGTH = 0.019007
 RADIUS OF STEP TAKEN= 0.01901 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 8137.2 SECONDS (135.6 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7524.2 SECONDS (125.4
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 90

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1587489497	-1.7277658358	0.8760926866
C	6.0	4.9801065268	0.6225652237	0.5653327600
C	6.0	5.1820488281	-0.7161631175	0.2032935277
C	6.0	4.0446354895	-1.5339002721	-0.0929896677
C	6.0	2.7369868596	-1.0213277501	-0.0004065662
C	6.0	2.4674870720	0.3441585778	0.4330810251
C	6.0	3.6510342881	1.1748289738	0.6826840071
C	6.0	3.5068820781	2.5618982766	1.0580983804
C	6.0	2.2401546104	3.1409815011	1.2155112330
C	6.0	1.0728468007	2.3341741404	1.0382076790
C	6.0	1.1625311324	0.9790371750	0.6414066129
N	7.0	-0.0504644016	0.1792273083	0.5889196740
C	6.0	-1.2462603068	0.7019159841	0.3223000514
C	6.0	-2.5491315219	0.0380670828	0.4371941286
C	6.0	-2.8186057915	-1.2855906715	0.9295103520

C	6.0	-4.1182569303	-1.8079959001	1.0559014764
C	6.0	-5.2291351144	-0.9935435542	0.6779147563
C	6.0	-5.0168978571	0.3205247163	0.1742266621
C	6.0	-3.6985562917	0.8236927520	0.0586413354
O	8.0	-1.6961426191	-2.1436437421	1.3204975083
N	7.0	1.6292860964	-1.9536482981	-0.4273398616
H	1.0	5.8427511249	1.2817591895	0.7704512399
H	1.0	6.1992777296	-1.1376452678	0.1210605372
H	1.0	4.2072840236	-2.5758026705	-0.4323313114
H	1.0	4.4207710529	3.1581515134	1.2323808569
H	1.0	2.1347566015	4.1987796112	1.5144020797
H	1.0	0.0897811462	2.7811163546	1.2693018866
H	1.0	-1.2912405317	1.7528115011	-0.0273573580
H	1.0	-4.2895164538	-2.8320320781	1.4395399927
H	1.0	-6.2532034588	-1.3963009526	0.7790608752
H	1.0	-5.8752252966	0.9495240891	-0.1206884495
H	1.0	-3.5360910077	1.8480635892	-0.3247444082
H	1.0	-2.0135949335	-2.9589373936	1.7879573738
H	1.0	1.2680069848	-1.6765321538	-1.3668364412
H	1.0	2.0229421211	-2.9093429021	-0.5373876344

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3727197	5.1681274	4.0095908
2 C	5.3727197	0.0000000	1.4014445 *	2.4410731 *
3 C	5.1681274	1.4014445 *	0.0000000	1.4318474 *
4 C	4.0095908	2.4410731 *	1.4318474 *	0.0000000
5 C	2.8132928 *	2.8379625 *	2.4724375 *	1.4075678 *
6 C	3.1335925	2.5314536 *	2.9233423 *	2.5082369 *
7 C	4.5451645	1.4440220 *	2.4798532 *	2.8449615 *
8 C	5.4446616	2.4847980 *	3.7792276	4.2883270
9 C	5.3058604	3.7778948	4.9554910	5.1790777
10 C	4.1666788	4.2918404	5.1852850	5.0073082
11 C	2.8964528 *	3.8349369	4.3843095	3.8936767
12 N	1.9398096 *	5.0501236	5.3225582	4.4910633
13 C	2.8607850 *	6.2316134	6.5839403	5.7588990
14 C	3.2624246	7.5529784	7.7714041	6.7992602
15 C	3.0104839	8.0370143	8.0537018	6.9434318
16 C	4.2815356	9.4301910	9.4029105	8.2479023
17 C	5.4412913	10.3369772	10.4256873	9.3214323
18 C	5.6102968	10.0092102	10.2515404	9.2531985
19 C	4.6964850	8.6957678	9.0142791	8.0955701
20 O	1.9521969 *	7.2659816	7.1130418	5.9435904

21 N	1.9779886 *	4.3416901	3.8146023	2.4742456 *
22 H	6.4324398	1.1048828 *	2.1794240 *	3.4506069
23 H	6.1160693	2.1868007 *	1.1041576 *	2.2012085 *
24 H	4.3384071	3.4383347	2.1937285 *	1.1077761 *
25 H	6.4933783	2.6808594 *	4.0803037	4.8901365
26 H	6.2798078	4.6675538	5.9297266	6.2525966
27 H	4.5265206	5.3916786	6.2688538	6.0096655
28 H	3.8772555	6.3998853	6.9319918	6.2672446
29 H	4.6177854	9.9309814	9.7834429	8.5727406
30 H	6.4212474	11.4152860	11.4699211	10.3356128
31 H	6.6760991	10.8819004	11.1867238	10.2260355
32 H	5.2801902	8.6498384	9.1027493	8.3041438
33 H	2.6582623 *	7.9519703	7.7018495	6.5016035
34 H	2.5027603 *	4.7748099	4.3251983	3.0582177
35 H	2.6209287 *	4.7365798	3.9164526	2.4852718 *

C C C C

1 CO	2.8132928 *	3.1335925	4.5451645	5.4446616
2 C	2.8379625 *	2.5314536 *	1.4440220 *	2.4847980 *
3 C	2.4724375 *	2.9233423 *	2.4798532 *	3.7792276
4 C	1.4075678 *	2.5082369 *	2.8449615 *	4.2883270
5 C	0.0000000	1.4577704 *	2.4749141 *	3.8147975
6 C	1.4577704 *	0.0000000	1.4673442 *	2.5277180 *
7 C	2.4749141 *	1.4673442 *	0.0000000	1.4441873 *
8 C	3.8147975	2.5277180 *	1.4441873 *	0.0000000
9 C	4.3646439	2.9130904 *	2.4779512 *	1.4016828 *
10 C	3.8868335	2.5042687 *	2.8491278 *	2.4447457 *
11 C	2.6253180 *	1.4660765 *	2.4965348 *	2.8592066 *
12 N	3.0916860	2.5281550 *	3.8342023	4.3071990
13 C	4.3520072	3.7325839	4.9332563	5.1568688
14 C	5.4089610	5.0259498	6.3082921	6.5901856
15 C	5.6390771	5.5538547	6.9260978	7.4048297
16 C	6.9806161	6.9564142	8.3305715	8.7885565
17 C	7.9949979	7.8158418	9.1410760	9.4394758
18 C	7.8710732	7.4888972	8.7247586	8.8577542
19 C	6.6950581	6.1959865	7.3843895	7.4792122
20 O	4.7599388	4.9307688	6.3254540	7.0201457
21 N	1.5094683 *	2.5928404 *	3.8867710	5.1109739
22 H	3.9426137	3.5192785	2.1960783 *	2.6791381 *
23 H	3.4663730	4.0273268	3.4866177	4.6705093
24 H	2.1828250 *	3.5074215	3.9522033	5.3951751
25 H	4.6715031	3.5174927	2.1973233 *	1.1050273 *
26 H	5.4687153	4.0172214	3.4835514	2.1841067 *
27 H	4.8040024	3.5059256	3.9505447	3.4306329
28 H	4.8911339	4.0403391	5.0263608	4.9854605

29 H	7.3975567	7.5338067	8.9263717	9.4880879
30 H	9.0317051	8.8994014	10.2329821	10.5358660
31 H	8.8356620	8.3829576	9.5627293	9.5923526
32 H	6.9058025	6.2353011	7.2885477	7.2128555
33 H	5.4332867	5.7294178	7.0991322	7.8414276
34 H	2.1105273 *	2.9600078 *	4.2437735	5.3718864
35 H	2.0887340 *	3.4241351	4.5628630	5.8891539

C C C N

1 CO	5.3058604	4.1666788	2.8964528 *	1.9398096 *
2 C	3.7778948	4.2918404	3.8349369	5.0501236
3 C	4.9554910	5.1852850	4.3843095	5.3225582
4 C	5.1790777	5.0073082	3.8936767	4.4910633
5 C	4.3646439	3.8868335	2.6253180 *	3.0916860
6 C	2.9130904 *	2.5042687 *	1.4660765 *	2.5281550 *
7 C	2.4779512 *	2.8491278 *	2.4965348 *	3.8342023
8 C	1.4016828 *	2.4447457 *	2.8592066 *	4.3071990
9 C	0.0000000	1.4300287 *	2.4829160 *	3.7962535
10 C	1.4300287 *	0.0000000	1.4148818 *	2.4713324 *
11 C	2.4829160 *	1.4148818 *	0.0000000	1.4538944 *
12 N	3.7962535	2.4713324 *	1.4538944 *	0.0000000
13 C	4.3476380	2.9249014 *	2.4455881 *	1.3319975 *
14 C	5.7594372	4.3303639	3.8345231	2.5072463 *
15 C	6.7281048	5.3158175	4.5892259	3.1502858
16 C	8.0589857	6.6411929	5.9854893	4.5512706
17 C	8.5541567	7.1357195	6.6892305	5.3105501
18 C	7.8551932	6.4719578	6.2319530	4.9857193
19 C	6.4789245	5.0997443	4.8983587	3.7423395
20 O	6.5903507	5.2723660	4.2876936	2.9392504 *
21 N	5.3877057	4.5653998	3.1560614	2.8988797 *
22 H	4.0784173	4.8919585	4.6917750	5.9982097
23 H	5.9311993	6.2589922	5.4881619	6.4040864
24 H	6.2663071	6.0079159	4.8021162	5.1731582
25 H	2.1807493 *	3.4532939	3.9640784	5.4110977
26 H	1.1042560 *	2.1979916 *	3.4747784	4.6678163
27 H	2.1809407 *	1.1043459 *	2.1891858 *	2.6930309 *
28 H	3.9928048	2.6575026 *	2.6583768 *	2.0965424 *
29 H	8.8523265	7.4569226	6.6997081	5.2688519
30 H	9.6392195	8.2252425	7.7880870	6.4025319
31 H	8.5115983	7.1788580	7.0789601	5.9181704
32 H	6.1162928	4.8307608	4.8750082	3.9710691
33 H	7.4586252	6.1729472	5.1874849	3.8909704
34 H	5.5517590	4.6806078	3.3310980	3.0011984
35 H	6.3028772	5.5569463	4.1532352	3.8867530

	C	C	C	C
1 CO	2.8607850 *	3.2624246	3.0104839	4.2815356
2 C	6.2316134	7.5529784	8.0370143	9.4301910
3 C	6.5839403	7.7714041	8.0537018	9.4029105
4 C	5.7588990	6.7992602	6.9434318	8.2479023
5 C	4.3520072	5.4089610	5.6390771	6.9806161
6 C	3.7325839	5.0259498	5.5538547	6.9564142
7 C	4.9332563	6.3082921	6.9260978	8.3305715
8 C	5.1568688	6.5901856	7.4048297	8.7885565
9 C	4.3476380	5.7594372	6.7281048	8.0589857
10 C	2.9249014 *	4.3303639	5.3158175	6.6411929
11 C	2.4455881 *	3.8345231	4.5892259	5.9854893
12 N	1.3319975 *	2.5072463 *	3.1502858	4.5512706
13 C	0.0000000	1.4667547 *	2.6059849 *	3.8840949
14 C	1.4667547 *	0.0000000	1.4377279 *	2.5005803 *
15 C	2.6059849 *	1.4377279 *	0.0000000	1.4064050 *
16 C	3.8840949	2.5005803 *	1.4064050 *	0.0000000
17 C	4.3433094	2.8817679 *	2.4411562 *	1.4283756 *
18 C	3.7927685	2.4977600 *	2.8253404 *	2.4729549 *
19 C	2.4694334 *	1.4428053 *	2.4457723 *	2.8454282 *
20 O	3.0489346	2.5035329 *	1.4659637 *	2.4595342 *
21 N	3.9853166	4.7088770	4.6979874	5.9376317
22 H	7.1267904	8.4900839	9.0352470	10.4331083
23 H	7.6720610	8.8327178	9.0552583	10.3814652
24 H	6.4073437	7.2964060	7.2720277	8.4922904
25 H	6.2431230	7.6776813	8.4998325	9.8797148
26 H	5.0080373	6.3569422	7.4132459	8.6828425
27 H	2.6466759 *	3.8962267	5.0112153	6.2300141
28 H	1.1084516 *	2.1767972 *	3.5327508	4.6738443
29 H	4.7956670	3.5030139	2.1943540 *	1.1068687 *
30 H	5.4479927	3.9867823	3.4396734	2.1918326 *
31 H	4.6567011	3.4935493	3.9295774	3.4749415
32 H	2.6411447 *	2.1978914 *	3.4507578	3.9511861
33 H	4.0173127	3.3306751	2.0457427 *	2.5080220 *
34 H	3.8511995	4.5568545	4.7038758	5.9075190
35 H	4.9465077	5.5263815	5.3130921	6.4393991

	C	C	C	O
1 CO	5.4412913	5.6102968	4.6964850	1.9521969 *
2 C	10.3369772	10.0092102	8.6957678	7.2659816
3 C	10.4256873	10.2515404	9.0142791	7.1130418
4 C	9.3214323	9.2531985	8.0955701	5.9435904
5 C	7.9949979	7.8710732	6.6950581	4.7599388
6 C	7.8158418	7.4888972	6.1959865	4.9307688

7 C	9.1410760	8.7247586	7.3843895	6.3254540
8 C	9.4394758	8.8577542	7.4792122	7.0201457
9 C	8.5541567	7.8551932	6.4789245	6.5903507
10 C	7.1357195	6.4719578	5.0997443	5.2723660
11 C	6.6892305	6.2319530	4.8983587	4.2876936
12 N	5.3105501	4.9857193	3.7423395	2.9392504 *
13 C	4.3433094	3.7927685	2.4694334 *	3.0489346
14 C	2.8817679 *	2.4977600 *	1.4428053 *	2.5035329 *
15 C	2.4411562 *	2.8253404 *	2.4457723 *	1.4659637 *
16 C	1.4283756 *	2.4729549 *	2.8454282 *	2.4595342 *
17 C	0.0000000	1.4232083 *	2.4553042 *	3.7706338
18 C	1.4232083 *	0.0000000	1.4158257 *	4.2910929
19 C	2.4553042 *	1.4158257 *	0.0000000	3.7956590
20 O	3.7706338	4.2910929	3.7956590	0.0000000
21 N	7.0129402	7.0502132	6.0279105	3.7615834
22 H	11.3036379	10.9183988	9.5787810	8.2988466
23 H	11.4428787	11.3106888	10.0904837	8.0491207
24 H	9.6323516	9.6872161	8.6197410	6.1732987
25 H	10.5197288	9.9116805	8.5294102	8.0952721
26 H	9.0491343	8.2451860	6.8947799	7.4121334
27 H	6.5489439	5.7733761	4.4326862	5.2388364
28 H	4.8525136	3.9965740	2.5818262 *	4.1428278
29 H	2.2006809 *	3.4740057	3.9522701	2.6858216 *
30 H	1.1050611 *	2.2004014 *	3.4602888	4.6495675
31 H	2.1978880 *	1.1042378 *	2.1876656 *	5.3953161
32 H	3.4563644	2.1852085 *	1.1057645 *	4.6931821
33 H	3.9286978	4.7306265	4.4875293	0.9919670 *
34 H	6.8454610	6.7722331	5.7401971	4.0281683
35 H	7.5986756	7.7780323	6.8575761	4.2272478

N H H H

1 CO	1.9779886 *	6.4324398	6.1160693	4.3384071
2 C	4.3416901	1.1048828 *	2.1868007 *	3.4383347
3 C	3.8146023	2.1794240 *	1.1041576 *	2.1937285 *
4 C	2.4742456 *	3.4506069	2.2012085 *	1.1077761 *
5 C	1.5094683 *	3.9426137	3.4663730	2.1828250 *
6 C	2.5928404 *	3.5192785	4.0273268	3.5074215
7 C	3.8867710	2.1960783 *	3.4866177	3.9522033
8 C	5.1109739	2.6791381 *	4.6705093	5.3951751
9 C	5.3877057	4.0784173	5.9311993	6.2663071
10 C	4.5653998	4.8919585	6.2589922	6.0079159
11 C	3.1560614	4.6917750	5.4881619	4.8021162
12 N	2.8988797 *	5.9982097	6.4040864	5.1731582
13 C	3.9853166	7.1267904	7.6720610	6.4073437
14 C	4.7088770	8.4900839	8.8327178	7.2964060

15 C	4.6979874	9.0352470	9.0552583	7.2720277
16 C	5.9376317	10.4331083	10.3814652	8.4922904
17 C	7.0129402	11.3036379	11.4428787	9.6323516
18 C	7.0502132	10.9183988	11.3106888	9.6872161
19 C	6.0279105	9.5787810	10.0904837	8.6197410
20 O	3.7615834	8.2988466	8.0491207	6.1732987
21 N	0.0000000	5.4457187	4.6745510	2.6520133 *
22 H	5.4457187	0.0000000	2.5302841 *	4.3591538
23 H	4.6745510	2.5302841 *	0.0000000	2.5184476 *
24 H	2.6520133 *	4.3591538	2.5184476 *	0.0000000
25 H	6.0562000	2.3992196 *	4.7803754	5.9745355
26 H	6.4713392	4.7761590	6.8512162	7.3471155
27 H	5.2599111	5.9660362	7.3485440	6.9674936
28 H	4.7357477	7.1939020	8.0302324	7.0096132
29 H	6.2680956	10.9559940	10.7062663	8.7043193
30 H	7.9937276	12.3888739	12.4725360	10.5962490
31 H	8.0523373	11.7565080	12.2559513	10.6855999
32 H	6.4144103	9.4595367	10.1926740	8.9186336
33 H	4.3804943	8.9855996	8.5759505	6.6163290
34 H	1.0440162 *	5.8521595	5.1789640	3.2126837
35 H	1.0394363 *	5.8195120	4.5841298	2.2121563 *

H H H H

1 CO	6.4933783	6.2798078	4.5265206	3.8772555
2 C	2.6808594 *	4.6675538	5.3916786	6.3998853
3 C	4.0803037	5.9297266	6.2688538	6.9319918
4 C	4.8901365	6.2525966	6.0096655	6.2672446
5 C	4.6715031	5.4687153	4.8040024	4.8911339
6 C	3.5174927	4.0172214	3.5059256	4.0403391
7 C	2.1973233 *	3.4835514	3.9505447	5.0263608
8 C	1.1050273 *	2.1841067 *	3.4306329	4.9854605
9 C	2.1807493 *	1.1042560 *	2.1809407 *	3.9928048
10 C	3.4532939	2.1979916 *	1.1043459 *	2.6575026 *
11 C	3.9640784	3.4747784	2.1891858 *	2.6583768 *
12 N	5.4110977	4.6678163	2.6930309 *	2.0965424 *
13 C	6.2431230	5.0080373	2.6466759 *	1.1084516 *
14 C	7.6776813	6.3569422	3.8962267	2.1767972 *
15 C	8.4998325	7.4132459	5.0112153	3.5327508
16 C	9.8797148	8.6828425	6.2300141	4.6738443
17 C	10.5197288	9.0491343	6.5489439	4.8525136
18 C	9.9116805	8.2451860	5.7733761	3.9965740
19 C	8.5294102	6.8947799	4.4326862	2.5818262 *
20 O	8.0952721	7.4121334	5.2388364	4.1428278
21 N	6.0562000	6.4713392	5.2599111	4.7357477
22 H	2.3992196 *	4.7761590	5.9660362	7.1939020

23 H	4.7803754	6.8512162	7.3485440	8.0302324
24 H	5.9745355	7.3471155	6.9674936	7.0096132
25 H	0.0000000	2.5275096 *	4.3475271	6.0157292
26 H	2.5275096 *	0.0000000	2.5003535 *	4.4829944
27 H	4.3475271	2.5003535 *	0.0000000	2.1554482 *
28 H	6.0157292	4.4829944	2.1554482 *	0.0000000
29 H	10.5732834	9.5241378	7.1214229	5.6711760
30 H	11.6138826	10.1095760	7.6108216	5.9319723
31 H	10.6167967	8.7972150	6.3928167	4.6547715
32 H	8.2129546	6.4083413	4.0692161	2.2664655 *
33 H	8.8954206	8.2774734	6.1352597	5.1007589
34 H	6.3300883	6.6009150	5.3111272	4.4837875
35 H	6.7598929	7.3991722	6.2755530	5.7427886

H H H H

1 CO	4.6177854	6.4212474	6.6760991	5.2801902
2 C	9.9309814	11.4152860	10.8819004	8.6498384
3 C	9.7834429	11.4699211	11.1867238	9.1027493
4 C	8.5727406	10.3356128	10.2260355	8.3041438
5 C	7.3975567	9.0317051	8.8356620	6.9058025
6 C	7.5338067	8.8994014	8.3829576	6.2353011
7 C	8.9263717	10.2329821	9.5627293	7.2885477
8 C	9.4880879	10.5358660	9.5923526	7.2128555
9 C	8.8523265	9.6392195	8.5115983	6.1162928
10 C	7.4569226	8.2252425	7.1788580	4.8307608
11 C	6.6997081	7.7880870	7.0789601	4.8750082
12 N	5.2688519	6.4025319	5.9181704	3.9710691
13 C	4.7956670	5.4479927	4.6567011	2.6411447 *
14 C	3.5030139	3.9867823	3.4935493	2.1978914 *
15 C	2.1943540 *	3.4396734	3.9295774	3.4507578
16 C	1.1068687 *	2.1918326 *	3.4749415	3.9511861
17 C	2.2006809 *	1.1050611 *	2.1978880 *	3.4563644
18 C	3.4740057	2.2004014 *	1.1042378 *	2.1852085 *
19 C	3.9522701	3.4602888	2.1876656 *	1.1057645 *
20 O	2.6858216 *	4.6495675	5.3953161	4.6931821
21 N	6.2680956	7.9937276	8.0523373	6.4144103
22 H	10.9559940	12.3888739	11.7565080	9.4595367
23 H	10.7062663	12.4725360	12.2559513	10.1926740
24 H	8.7043193	10.5962490	10.6855999	8.9186336
25 H	10.5732834	11.6138826	10.6167967	8.2129546
26 H	9.5241378	10.1095760	8.7972150	6.4083413
27 H	7.1214229	7.6108216	6.3928167	4.0692161
28 H	5.6711760	5.9319723	4.6547715	2.2664655 *
29 H	0.0000000	2.5206394 *	4.3873628	5.0580278
30 H	2.5206394 *	0.0000000	2.5407305 *	4.3734411

31 H	4.3873628	2.5407305 *	0.0000000	2.5140726 *
32 H	5.0580278	4.3734411	2.5140726 *	0.0000000
33 H	2.3059311 *	4.6296852	5.8164585	5.4670615
34 H	6.3322188	7.8263664	7.7119922	6.0488088
35 H	6.6152364	8.5156866	8.8003148	7.3199032

H H H

1 CO	2.6582623 *	2.5027603 *	2.6209287 *
2 C	7.9519703	4.7748099	4.7365798
3 C	7.7018495	4.3251983	3.9164526
4 C	6.5016035	3.0582177	2.4852718 *
5 C	5.4332867	2.1105273 *	2.0887340 *
6 C	5.7294178	2.9600078 *	3.4241351
7 C	7.0991322	4.2437735	4.5628630
8 C	7.8414276	5.3718864	5.8891539
9 C	7.4586252	5.5517590	6.3028772
10 C	6.1729472	4.6806078	5.5569463
11 C	5.1874849	3.3310980	4.1532352
12 N	3.8909704	3.0011984	3.8867530
13 C	4.0173127	3.8511995	4.9465077
14 C	3.3306751	4.5568545	5.5263815
15 C	2.0457427 *	4.7038758	5.3130921
16 C	2.5080220 *	5.9075190	6.4393991
17 C	3.9286978	6.8454610	7.5986756
18 C	4.7306265	6.7722331	7.7780323
19 C	4.4875293	5.7401971	6.8575761
20 O	0.9919670 *	4.0281683	4.2272478
21 N	4.3804943	1.0440162 *	1.0394363 *
22 H	8.9855996	5.8521595	5.8195120
23 H	8.5759505	5.1789640	4.5841298
24 H	6.6163290	3.2126837	2.2121563 *
25 H	8.8954206	6.3300883	6.7598929
26 H	8.2774734	6.6009150	7.3991722
27 H	6.1352597	5.3111272	6.2755530
28 H	5.1007589	4.4837875	5.7427886
29 H	2.3059311 *	6.3322188	6.6152364
30 H	4.6296852	7.8263664	8.5156866
31 H	5.8164585	7.7119922	8.8003148
32 H	5.4670615	6.0488088	7.3199032
33 H	0.0000000	4.7292915	4.6586823
34 H	4.7292915	0.0000000	1.6666538 *
35 H	4.6586823	1.6666538 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.74 , TOTAL = 8138.0 SECONDS (135.6 MIN)
WALL CLOCK TIME: STEP = 0.75 , TOTAL = 7525.0 SECONDS (125.4 MIN)

CPU UTILIZATION: STEP = 98.84%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.93 , TOTAL = 8138.9 SECONDS (135.6 MIN)
WALL CLOCK TIME: STEP = 0.92 , TOTAL = 7525.9 SECONDS (125.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636933457	-284.636933457	0.004689974	0.000249592	198253646
11324874						
2	1	-284.636940707	-0.000007250	0.000787887	0.000027958	146757100
15649430						
3	2	-284.636940611	0.000000097	0.000590745	0.000063758	131096100
16861608						
4	3	-284.636940853	-0.000000242	0.000340388	0.000011830	125118217
17313662						
5	4	-284.636940842	0.000000010	0.000205614	0.000017623	117270274
17862295						
6	5	-284.636940863	-0.000000020	0.000041045	0.000007384	109670851
18401682						
7	6	-284.636940835	0.000000027	0.000041145	0.000006568	103811902
18887858						
8	7	-284.636940843	-0.000000008	0.000046025	0.000003910	123223885
17513916						
9	8	-284.636940843	0.000000000	0.000028883	0.000005006	150114399
15417226						
10	9	-284.636940844	-0.000000001	0.000017707	0.000001699	143319809
15966214						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 32.4 SECONDS (3.2 SEC/ITER)

OF THE ABOVE TIME, DFT PART= 10.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.3
TIME TO SOLVE SCF EQUATIONS= 0.8 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369408444 AFTER 10 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6016643818
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998502320

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 34.14 , TOTAL = 8173.0 SECONDS (136.2 MIN)
WALL CLOCK TIME: STEP = 31.46 , TOTAL = 7557.3 SECONDS (126.0
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.95 , TOTAL = 8177.0 SECONDS (136.3 MIN)
WALL CLOCK TIME: STEP = 3.92 , TOTAL = 7561.3 SECONDS (126.0
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.85 , TOTAL = 8179.8 SECONDS (136.3 MIN)
WALL CLOCK TIME: STEP = 2.67 , TOTAL = 7563.9 SECONDS (126.1
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 90 ENERGY= -284.6369408

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000479	-0.0000458	-0.0000210
2 C	6.0	-0.0000944	0.0000630	-0.0000705
3 C	6.0	0.0000158	-0.0000461	0.0000186
4 C	6.0	0.0000307	-0.0000027	-0.0000167
5 C	6.0	0.0000040	0.0000122	0.0000303
6 C	6.0	-0.0000200	-0.0000393	0.0000315
7 C	6.0	-0.0000178	-0.0000464	-0.0000464
8 C	6.0	0.0000785	0.0000556	0.0000370
9 C	6.0	-0.0000345	-0.0000247	-0.0000396
10 C	6.0	-0.0000971	0.0000463	0.0000250
11 C	6.0	-0.0000696	-0.0000094	0.0000950
12 N	7.0	-0.0000506	-0.0000576	-0.0000717
13 C	6.0	0.0000713	-0.0000150	-0.0001143
14 C	6.0	-0.0000134	-0.0000599	0.0000251
15 C	6.0	0.0000076	0.0000174	-0.0000014
16 C	6.0	0.0000287	0.0000490	0.0000212
17 C	6.0	0.0000188	-0.0000530	-0.0000424
18 C	6.0	-0.0000391	0.0001606	0.0000333
19 C	6.0	0.0000163	0.0000809	0.0000767
20 O	8.0	0.0000355	-0.0000102	-0.0000277
21 N	7.0	0.0000821	-0.0000386	0.0001072
22 H	1.0	-0.0001193	-0.0000915	0.0000813
23 H	1.0	0.0000126	0.0000101	-0.0000030
24 H	1.0	0.0000698	0.0000748	-0.0001066
25 H	1.0	-0.0000064	-0.0000156	0.0001051
26 H	1.0	0.0000530	0.0000236	-0.0001382
27 H	1.0	-0.0000349	0.0001021	0.0000717
28 H	1.0	-0.0000171	0.0000625	-0.0000531
29 H	1.0	-0.0000066	-0.0000157	-0.0000022
30 H	1.0	0.0000634	0.0001077	0.0001202
31 H	1.0	-0.0000384	0.0000463	0.0000224
32 H	1.0	-0.0001128	-0.0001299	-0.0000902
33 H	1.0	-0.0000837	-0.0001409	-0.0000078
34 H	1.0	0.0001927	-0.0000263	-0.0000233
35 H	1.0	0.0000273	-0.0000436	-0.0000257

MAXIMUM GRADIENT = 0.0001927 RMS GRADIENT = 0.0000641

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0000022845

PREDICTED ENERGY CHANGE WAS -0.0000015778 RATIO= 1.448

GDIIS STEP HAS LENGTH = 0.016317

RADIUS OF STEP TAKEN= 0.01632 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8179.9 SECONDS (136.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7564.0 SECONDS (126.1 MIN)
 CPU UTILIZATION: STEP = 81.98% , TOTAL = 100.00%

INSERCH= 91

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1591816631	-1.7267897409	0.8786105140
C	6.0	4.9801803119	0.6222600524	0.5646148837
C	6.0	5.1817406156	-0.7166419845	0.2028994962
C	6.0	4.0440110106	-1.5342085325	-0.0930253864
C	6.0	2.7364685046	-1.0213436304	0.0000326719
C	6.0	2.4674150137	0.3443566568	0.4335137840
C	6.0	3.6512264100	1.1747558665	0.6824850678
C	6.0	3.5076236913	2.5619508591	1.0577647775
C	6.0	2.2411715908	3.1415392665	1.2152427279
C	6.0	1.0735608927	2.3350058580	1.0385611303
C	6.0	1.1628178394	0.9796798219	0.6422348614
N	7.0	-0.0503389848	0.1800542717	0.5906492134
C	6.0	-1.2461507875	0.7024137910	0.3233975060
C	6.0	-2.5490572873	0.0384008096	0.4378080320
C	6.0	-2.8184569612	-1.2854668672	0.9297828802
C	6.0	-4.1178624756	-1.8086058548	1.0554549890
C	6.0	-5.2288739384	-0.9946122375	0.6768509216
C	6.0	-5.0168389166	0.3197144573	0.1737208907
C	6.0	-3.6986620391	0.8237705308	0.0590535393
O	8.0	-1.6959655585	-2.1436005721	1.3206120291
N	7.0	1.6281753822	-1.9532996955	-0.4261493933
H	1.0	5.8427364935	1.2817629778	0.7693339012
H	1.0	6.1988789465	-1.1382859477	0.1211806838
H	1.0	4.2064491744	-2.5760474050	-0.4328520294
H	1.0	4.4218538459	3.1579678797	1.2313440660
H	1.0	2.1360921805	4.1996121211	1.5131603336
H	1.0	0.0905240935	2.7820865748	1.2700700449
H	1.0	-1.2911125056	1.7529791288	-0.0271416297
H	1.0	-4.2889258623	-2.8330705081	1.4380585273
H	1.0	-6.2527258708	-1.3982953004	0.7766210077
H	1.0	-5.8752551668	0.9483793431	-0.1216333719
H	1.0	-3.5366983314	1.8487058096	-0.3237365209
H	1.0	-2.0137195644	-2.9595396161	1.7866866509

H 1.0 1.2652152091 -1.6754636656 -1.3647053402
H 1.0 2.0213183810 -2.9090195181 -0.5376144598

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3720253	5.1675025	4.0091225
2 C	5.3720253	0.0000000	1.4014718 *	2.4411597 *
3 C	5.1675025	1.4014718 *	0.0000000	1.4319271 *
4 C	4.0091225	2.4411597 *	1.4319271 *	0.0000000
5 C	2.8128208 *	2.8380326 *	2.4725197 *	1.4076071 *
6 C	3.1330017	2.5314832 *	2.9234337 *	2.5083671 *
7 C	4.5444261	1.4440441 *	2.4798915 *	2.8450280 *
8 C	5.4440294	2.4847576 *	3.7792371	4.2884206
9 C	5.3055283	3.7778636	4.9555371	5.1792290
10 C	4.1665162	4.2918293	5.1853665	5.0074826
11 C	2.8962280 *	3.8348442	4.3843202	3.8937792
12 N	1.9398131 *	5.0499850	5.3225061	4.4910811
13 C	2.8608129 *	6.2315174	6.5837700	5.7586196
14 C	3.2626313	7.5529061	7.7711330	6.7987818
15 C	3.0106006	8.0368845	8.0532653	6.9427283
16 C	4.2814804	9.4299743	9.4022260	8.2468467
17 C	5.4413173	10.3369077	10.4251040	9.3204221
18 C	5.6103688	10.0092320	10.2511419	9.2524151
19 C	4.6968063	8.6958900	9.0141618	8.0951948
20 O	1.9520932 *	7.2658407	7.1125477	5.9428159
21 N	1.9777886 *	4.3417806	3.8148199	2.4744435 *
22 H	6.4316504	1.1049240 *	2.1797674 *	3.4509089
23 H	6.1153888	2.1866373 *	1.1040978 *	2.2013847 *
24 H	4.3383807	3.4384256	2.1938008 *	1.1078342 *
25 H	6.4927384	2.6806847 *	4.0801627	4.8901165
26 H	6.2795754	4.6675501	5.9297818	6.2527343
27 H	4.5263584	5.3917767	6.2690063	6.0098662
28 H	3.8771809	6.3998293	6.9317945	6.2668562
29 H	4.6176292	9.9306869	9.7825565	8.5714116
30 H	6.4211267	11.4151554	11.4691251	10.3342899
31 H	6.6761849	10.8819929	11.1863655	10.2252581
32 H	5.2810355	8.6504658	9.1032704	8.3044862
33 H	2.6581524 *	7.9521936	7.7015335	6.5008450
34 H	2.5016816 *	4.7752253	4.3261871	3.0592203
35 H	2.6212428 *	4.7370570	3.9170332	2.4857695 *

C C C C

1 CO	2.8128208 *	3.1330017	4.5444261	5.4440294
2 C	2.8380326 *	2.5314832 *	1.4440441 *	2.4847576 *
3 C	2.4725197 *	2.9234337 *	2.4798915 *	3.7792371
4 C	1.4076071 *	2.5083671 *	2.8450280 *	4.2884206
5 C	0.0000000	1.4578865 *	2.4749498 *	3.8149020
6 C	1.4578865 *	0.0000000	1.4672965 *	2.5277356 *
7 C	2.4749498 *	1.4672965 *	0.0000000	1.4442183 *
8 C	3.8149020	2.5277356 *	1.4442183 *	0.0000000
9 C	4.3648194	2.9131627 *	2.4779674 *	1.4016501 *
10 C	3.8870149	2.5043154 *	2.8490928 *	2.4446952 *
11 C	2.6254323 *	1.4660061 *	2.4963678 *	2.8590840 *
12 N	3.0916793	2.5279976 *	3.8339864	4.3070555
13 C	4.3516848	3.7324123	4.9331891	5.1570869
14 C	5.4084645	5.0257956	6.3083031	6.5906021
15 C	5.6383857	5.5536520	6.9260851	7.4052886
16 C	6.9796527	6.9561439	8.3305640	8.7891871
17 C	7.9940902	7.8156839	9.1412456	9.4403722
18 C	7.8703482	7.4888021	8.7249810	8.8586466
19 C	6.6946871	6.1960120	7.3846271	7.4799231
20 O	4.7591871	4.9305793	6.3254373	7.0205872
21 N	1.5094658 *	2.5927917 *	3.8867129	5.1109505
22 H	3.9427180	3.5191335	2.1958392 *	2.6785864 *
23 H	3.4665023	4.0273570	3.4865109	4.6703102
24 H	2.1829650 *	3.5076473	3.9523125	5.3953055
25 H	4.6715411	3.5174952	2.1973263 *	1.1050714 *
26 H	5.4688560	4.0172635	3.4835913	2.1841287 *
27 H	4.8041751	3.5059897	3.9506163	3.4307584
28 H	4.8907069	4.0401671	5.0263930	4.9859128
29 H	7.3963801	7.5334783	8.9263420	9.4887862
30 H	9.0305480	8.8991806	10.2331679	10.5369358
31 H	8.8349531	8.3829098	9.5630384	9.5933836
32 H	6.9061301	6.2358537	7.2892354	7.2138573
33 H	5.4325890	5.7295178	7.0995263	7.8424113
34 H	2.1106798 *	2.9594848 *	4.2435586	5.3714467
35 H	2.0889769 *	3.4244049	4.5631639	5.8894699

C C C N

1 CO	5.3055283	4.1665162	2.8962280 *	1.9398131 *
2 C	3.7778636	4.2918293	3.8348442	5.0499850
3 C	4.9555371	5.1853665	4.3843202	5.3225061
4 C	5.1792290	5.0074826	3.8937792	4.4910811
5 C	4.3648194	3.8870149	2.6254323 *	3.0916793
6 C	2.9131627 *	2.5043154 *	1.4660061 *	2.5279976 *
7 C	2.4779674 *	2.8490928 *	2.4963678 *	3.8339864
8 C	1.4016501 *	2.4446952 *	2.8590840 *	4.3070555

9 C	0.0000000	1.4300445 *	2.4829058 *	3.7962523
10 C	1.4300445 *	0.0000000	1.4149028 *	2.4713544 *
11 C	2.4829058 *	1.4149028 *	0.0000000	1.4538953 *
12 N	3.7962523	2.4713544 *	1.4538953 *	0.0000000
13 C	4.3481189	2.9253851 *	2.4457440 *	1.3320093 *
14 C	5.7602227	4.3311270	3.8348160	2.5073929 *
15 C	6.7290201	5.3167150	4.5895667	3.1504350
16 C	8.0601975	6.6423400	5.9858894	4.5514350
17 C	8.5556528	7.1370775	6.6897497	5.3107906
18 C	7.8566010	6.4732000	6.2324327	4.9859258
19 C	6.4800038	5.1007234	4.8988156	3.7426228
20 O	6.5912711	5.2733049	4.2880903	2.9394395 *
21 N	5.3877005	4.5653629	3.1560056	2.8987047 *
22 H	4.0778514	4.8915069	4.6913801	5.9978353
23 H	5.9310474	6.2589319	5.4880951	6.4039946
24 H	6.2665245	6.0082019	4.8023640	5.1733835
25 H	2.1808036 *	3.4533314	3.9640010	5.4110043
26 H	1.1042259 *	2.1979476 *	3.4747285	4.6677996
27 H	2.1811687 *	1.1044632 *	2.1892147 *	2.6929588 *
28 H	3.9935760	2.6582246 *	2.6585392 *	2.0964916 *
29 H	8.8536875	7.4582086	6.7001425	5.2690267
30 H	9.6409948	8.2268237	7.7886529	6.4027632
31 H	8.5131411	7.1801691	7.0794736	5.9183882
32 H	6.1174877	4.8318560	4.8758342	3.9718007
33 H	7.4601482	6.1743991	5.1882183	3.8913261
34 H	5.5508684	4.6793468	3.3298770	2.9995068 *
35 H	6.3031822	5.5571914	4.1534384	3.8867879

C C C C

1 CO	2.8608129 *	3.2626313	3.0106006	4.2814804
2 C	6.2315174	7.5529061	8.0368845	9.4299743
3 C	6.5837700	7.7711330	8.0532653	9.4022260
4 C	5.7586196	6.7987818	6.9427283	8.2468467
5 C	4.3516848	5.4084645	5.6383857	6.9796527
6 C	3.7324123	5.0257956	5.5536520	6.9561439
7 C	4.9331891	6.3083031	6.9260851	8.3305640
8 C	5.1570869	6.5906021	7.4052886	8.7891871
9 C	4.3481189	5.7602227	6.7290201	8.0601975
10 C	2.9253851 *	4.3311270	5.3167150	6.6423400
11 C	2.4457440 *	3.8348160	4.5895667	5.9858894
12 N	1.3320093 *	2.5073929 *	3.1504350	4.5514350
13 C	0.0000000	1.4668225 *	2.6060544 *	3.8843089
14 C	1.4668225 *	0.0000000	1.4377903 *	2.5008141 *
15 C	2.6060544 *	1.4377903 *	0.0000000	1.4063864 *
16 C	3.8843089	2.5008141 *	1.4063864 *	0.0000000

17 C	4.3436057	2.8819568 *	2.4410410 *	1.4283813 *
18 C	3.7930134	2.4977641 *	2.8250876 *	2.4729256 *
19 C	2.4696997 *	1.4428623 *	2.4457745 *	2.8456898 *
20 O	3.0490274	2.5036450 *	1.4659904 *	2.4592914 *
21 N	3.9845182	4.7077135	4.6964979	5.9357425
22 H	7.1264877	8.4898800	9.0350808	10.4329179
23 H	7.6718665	8.8323968	9.0547141	10.3806238
24 H	6.4071107	7.2959068	7.2712914	8.4910652
25 H	6.2434277	7.6782159	8.5004207	9.8805135
26 H	5.0085426	6.3578839	7.4144439	8.6844762
27 H	2.6472490 *	3.8971607	5.0122806	6.2314552
28 H	1.1084163 *	2.1767825 *	3.5327949	4.6741222
29 H	4.7958939	3.5032829	2.1944703 *	1.1068767 *
30 H	5.4483194	3.9869852	3.4395337	2.1917447 *
31 H	4.6569474	3.4935123	3.9293206	3.4749005
32 H	2.6418508 *	2.1983151 *	3.4511186	3.9516895
33 H	4.0174967	3.3307217	2.0455820 *	2.5073423 *
34 H	3.8484999	4.5535767	4.7003353	5.9035945
35 H	4.9457201	5.5251307	5.3115538	6.4372604

C C C O

1 CO	5.4413173	5.6103688	4.6968063	1.9520932 *
2 C	10.3369077	10.0092320	8.6958900	7.2658407
3 C	10.4251040	10.2511419	9.0141618	7.1125477
4 C	9.3204221	9.2524151	8.0951948	5.9428159
5 C	7.9940902	7.8703482	6.6946871	4.7591871
6 C	7.8156839	7.4888021	6.1960120	4.9305793
7 C	9.1412456	8.7249810	7.3846271	6.3254373
8 C	9.4403722	8.8586466	7.4799231	7.0205872
9 C	8.5556528	7.8566010	6.4800038	6.5912711
10 C	7.1370775	6.4732000	5.1007234	5.2733049
11 C	6.6897497	6.2324327	4.8988156	4.2880903
12 N	5.3107906	4.9859258	3.7426228	2.9394395 *
13 C	4.3436057	3.7930134	2.4696997 *	3.0490274
14 C	2.8819568 *	2.4977641 *	1.4428623 *	2.5036450 *
15 C	2.4410410 *	2.8250876 *	2.4457745 *	1.4659904 *
16 C	1.4283813 *	2.4729256 *	2.8456898 *	2.4592914 *
17 C	0.0000000	1.4232194 *	2.4555525 *	3.7704170
18 C	1.4232194 *	0.0000000	1.4159136 *	4.2908601
19 C	2.4555525 *	1.4159136 *	0.0000000	3.7957363
20 O	3.7704170	4.2908601	3.7957363	0.0000000
21 N	7.0110496	7.0485923	6.0268348	3.7599605
22 H	11.3035833	10.9183639	9.5787547	8.2987380
23 H	11.4421566	11.3102101	10.0903341	8.0484696
24 H	9.6310799	9.6861969	8.6192527	6.1725316

25 H	10.5208332	9.9127781	8.5302708	8.0958206
26 H	9.0510831	8.2469465	6.8960199	7.4133723
27 H	6.5506762	5.7749818	4.4339028	5.2398944
28 H	4.8529196	3.9969527	2.5820831 *	4.1429071
29 H	2.2006518 *	3.4739689	3.9525375	2.6856295 *
30 H	1.1050732 *	2.2005596 *	3.4605956	4.6492441
31 H	2.1978631 *	1.1042337 *	2.1876318 *	5.3950786
32 H	3.4567457	2.1854278 *	1.1060076 *	4.6936861
33 H	3.9280902	4.7301048	4.4874473	0.9919424 *
34 H	6.8413964	6.7684337	5.7370148	4.0247575
35 H	7.5963919	7.7760131	6.8562315	4.2257629

N H H H

1 CO	1.9777886 *	6.4316504	6.1153888	4.3383807
2 C	4.3417806	1.1049240 *	2.1866373 *	3.4384256
3 C	3.8148199	2.1797674 *	1.1040978 *	2.1938008 *
4 C	2.4744435 *	3.4509089	2.2013847 *	1.1078342 *
5 C	1.5094658 *	3.9427180	3.4665023	2.1829650 *
6 C	2.5927917 *	3.5191335	4.0273570	3.5076473
7 C	3.8867129	2.1958392 *	3.4865109	3.9523125
8 C	5.1109505	2.6785864 *	4.6703102	5.3953055
9 C	5.3877005	4.0778514	5.9310474	6.2665245
10 C	4.5653629	4.8915069	6.2589319	6.0082019
11 C	3.1560056	4.6913801	5.4880951	4.8023640
12 N	2.8987047 *	5.9978353	6.4039946	5.1733835
13 C	3.9845182	7.1264877	7.6718665	6.4071107
14 C	4.7077135	8.4898800	8.8323968	7.2959068
15 C	4.6964979	9.0350808	9.0547141	7.2712914
16 C	5.9357425	10.4329179	10.3806238	8.4910652
17 C	7.0110496	11.3035833	11.4421566	9.6310799
18 C	7.0485923	10.9183639	11.3102101	9.6861969
19 C	6.0268348	9.5787547	10.0903341	8.6192527
20 O	3.7599605	8.2987380	8.0484696	6.1725316
21 N	0.0000000	5.4458550	4.6749491	2.6524244 *
22 H	5.4458550	0.0000000	2.5305290 *	4.3595170
23 H	4.6749491	2.5305290 *	0.0000000	2.5187073 *
24 H	2.6524244 *	4.3595170	2.5187073 *	0.0000000
25 H	6.0561523	2.3984382 *	4.7799663	5.9745192
26 H	6.4712615	4.7755977	6.8510583	7.3473059
27 H	5.2597923	5.9657066	7.3485554	6.9678105
28 H	4.7347599	7.1936235	8.0300302	7.0091552
29 H	6.2658882	10.9558035	10.7051629	8.7027446
30 H	7.9914511	12.3888246	12.4715544	10.5945395
31 H	8.0507106	11.7565427	12.2555231	10.6845310
32 H	6.4141761	9.4599167	10.1932103	8.9188946

33 H	4.3786483	8.9859644	8.5754096	6.6154302
34 H	1.0439445 *	5.8526075	5.1804879	3.2140720
35 H	1.0394163 *	5.8201382	4.5849232	2.2128358 *

H H H H

1 CO	6.4927384	6.2795754	4.5263584	3.8771809
2 C	2.6806847 *	4.6675501	5.3917767	6.3998293
3 C	4.0801627	5.9297818	6.2690063	6.9317945
4 C	4.8901165	6.2527343	6.0098662	6.2668562
5 C	4.6715411	5.4688560	4.8041751	4.8907069
6 C	3.5174952	4.0172635	3.5059897	4.0401671
7 C	2.1973263 *	3.4835913	3.9506163	5.0263930
8 C	1.1050714 *	2.1841287 *	3.4307584	4.9859128
9 C	2.1808036 *	1.1042259 *	2.1811687 *	3.9935760
10 C	3.4533314	2.1979476 *	1.1044632 *	2.6582246 *
11 C	3.9640010	3.4747285	2.1892147 *	2.6585392 *
12 N	5.4110043	4.6677996	2.6929588 *	2.0964916 *
13 C	6.2434277	5.0085426	2.6472490 *	1.1084163 *
14 C	7.6782159	6.3578839	3.8971607	2.1767825 *
15 C	8.5004207	7.4144439	5.0122806	3.5327949
16 C	9.8805135	8.6844762	6.2314552	4.6741222
17 C	10.5208332	9.0510831	6.5506762	4.8529196
18 C	9.9127781	8.2469465	5.7749818	3.9969527
19 C	8.5302708	6.8960199	4.4339028	2.5820831 *
20 O	8.0958206	7.4133723	5.2398944	4.1429071
21 N	6.0561523	6.4712615	5.2597923	4.7347599
22 H	2.3984382 *	4.7755977	5.9657066	7.1936235
23 H	4.7799663	6.8510583	7.3485554	8.0300302
24 H	5.9745192	7.3473059	6.9678105	7.0091552
25 H	0.0000000	2.5276767 *	4.3477815	6.0162916
26 H	2.5276767 *	0.0000000	2.5005640 *	4.4837791
27 H	4.3477815	2.5005640 *	0.0000000	2.1565574 *
28 H	6.0162916	4.4837791	2.1565574 *	0.0000000
29 H	10.5741645	9.5260234	7.1230465	5.6714679
30 H	11.6152038	10.1119398	7.6128776	5.9324676
31 H	10.6180640	8.7991336	6.3945166	4.6551771
32 H	8.2140730	6.4094854	4.0704007	2.2671100 *
33 H	8.8965672	8.2794449	6.1368563	5.1009771
34 H	6.3297631	6.5997767	5.3095852	4.4808602
35 H	6.7601865	7.3994253	6.2756974	5.7416907

H H H H

1 CO	4.6176292	6.4211267	6.6761849	5.2810355
2 C	9.9306869	11.4151554	10.8819929	8.6504658

3 C	9.7825565	11.4691251	11.1863655	9.1032704
4 C	8.5714116	10.3342899	10.2252581	8.3044862
5 C	7.3963801	9.0305480	8.8349531	6.9061301
6 C	7.5334783	8.8991806	8.3829098	6.2358537
7 C	8.9263420	10.2331679	9.5630384	7.2892354
8 C	9.4887862	10.5369358	9.5933836	7.2138573
9 C	8.8536875	9.6409948	8.5131411	6.1174877
10 C	7.4582086	8.2268237	7.1801691	4.8318560
11 C	6.7001425	7.7886529	7.0794736	4.8758342
12 N	5.2690267	6.4027632	5.9183882	3.9718007
13 C	4.7958939	5.4483194	4.6569474	2.6418508 *
14 C	3.5032829	3.9869852	3.4935123	2.1983151 *
15 C	2.1944703 *	3.4395337	3.9293206	3.4511186
16 C	1.1068767 *	2.1917447 *	3.4749005	3.9516895
17 C	2.2006518 *	1.1050732 *	2.1978631 *	3.4567457
18 C	3.4739689	2.2005596 *	1.1042337 *	2.1854278 *
19 C	3.9525375	3.4605956	2.1876318 *	1.1060076 *
20 O	2.6856295 *	4.6492441	5.3950786	4.6936861
21 N	6.2658882	7.9914511	8.0507106	6.4141761
22 H	10.9558035	12.3888246	11.7565427	9.4599167
23 H	10.7051629	12.4715544	12.2555231	10.1932103
24 H	8.7027446	10.5945395	10.6845310	8.9188946
25 H	10.5741645	11.6152038	10.6180640	8.2140730
26 H	9.5260234	10.1119398	8.7991336	6.4094854
27 H	7.1230465	7.6128776	6.3945166	4.0704007
28 H	5.6714679	5.9324676	4.6551771	2.2671100 *
29 H	0.0000000	2.5204345 *	4.3873047	5.0585371
30 H	2.5204345 *	0.0000000	2.5409107 *	4.3738551
31 H	4.3873047	2.5409107 *	0.0000000	2.5140170 *
32 H	5.0585371	4.3738551	2.5140170 *	0.0000000
33 H	2.3052331 *	4.6289190	5.8159241	5.4674102
34 H	6.3280346	7.8218629	7.7081838	6.0466321
35 H	6.6127327	8.5128909	8.7982066	7.3193746

H H H

1 CO	2.6581524 *	2.5016816 *	2.6212428 *
2 C	7.9521936	4.7752253	4.7370570
3 C	7.7015335	4.3261871	3.9170332
4 C	6.5008450	3.0592203	2.4857695 *
5 C	5.4325890	2.1106798 *	2.0889769 *
6 C	5.7295178	2.9594848 *	3.4244049
7 C	7.0995263	4.2435586	4.5631639
8 C	7.8424113	5.3714467	5.8894699
9 C	7.4601482	5.5508684	6.3031822
10 C	6.1743991	4.6793468	5.5571914

11	C	5.1882183	3.3298770	4.1534384
12	N	3.8913261	2.9995068 *	3.8867879
13	C	4.0174967	3.8484999	4.9457201
14	C	3.3307217	4.5535767	5.5251307
15	C	2.0455820 *	4.7003353	5.3115538
16	C	2.5073423 *	5.9035945	6.4372604
17	C	3.9280902	6.8413964	7.5963919
18	C	4.7301048	6.7684337	7.7760131
19	C	4.4874473	5.7370148	6.8562315
20	O	0.9919424 *	4.0247575	4.2257629
21	N	4.3786483	1.0439445 *	1.0394163 *
22	H	8.9859644	5.8526075	5.8201382
23	H	8.5754096	5.1804879	4.5849232
24	H	6.6154302	3.2140720	2.2128358 *
25	H	8.8965672	6.3297631	6.7601865
26	H	8.2794449	6.5997767	7.3994253
27	H	6.1368563	5.3095852	6.2756974
28	H	5.1009771	4.4808602	5.7416907
29	H	2.3052331 *	6.3280346	6.6127327
30	H	4.6289190	7.8218629	8.5128909
31	H	5.8159241	7.7081838	8.7982066
32	H	5.4674102	6.0466321	7.3193746
33	H	0.0000000	4.7256254	4.6568723
34	H	4.7256254	0.0000000	1.6665627 *
35	H	4.6568723	1.6665627 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.71 , TOTAL = 8180.6 SECONDS (136.3 MIN)

WALL CLOCK TIME: STEP = 0.72 , TOTAL = 7564.7 SECONDS (126.1 MIN)

CPU UTILIZATION: STEP = 98.44%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.95 , TOTAL = 8181.5 SECONDS (136.4 MIN)

WALL CLOCK TIME: STEP = 0.95 , TOTAL = 7565.6 SECONDS (126.1 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636937812	-284.636937812	0.003379576	0.000189335	198258724
11324457						
2	1	-284.636942779	-0.000004968	0.000877368	0.000025221	144599091
15824225						
3	2	-284.636942684	0.000000096	0.000593843	0.000063117	130205287
16934559						
4	3	-284.636942872	-0.000000189	0.000209211	0.000009783	124612054
17354624						
5	4	-284.636942846	0.000000026	0.000118441	0.000017355	115272601
18020678						
6	5	-284.636942872	-0.000000026	0.000041105	0.000006203	108787465
18490272						
7	6	-284.636942868	0.000000004	0.000034469	0.000010002	103121266
18949151						
8	7	-284.636942873	-0.000000006	0.000039629	0.000003855	122540219
17574234						
9	8	-284.636942873	0.000000000	0.000043844	0.000002479	147895771
15602169						

-----DISABLING FDIFF OPTION-----

10	9	-284.636942882	-0.000000008	0.000067083	0.000001476	198259409
11324440						
11	10	-284.636942882	0.000000000	0.000027582	0.000001012	198259405
11324443						
12	11	-284.636942882	0.000000000	0.000031928	0.000001046	198259426
11324441						

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 38.4 SECONDS (3.2 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 13.1 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.1
TIME TO SOLVE SCF EQUATIONS= 1.8 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6369428818 AFTER 12 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6014608093
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998512122

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 41.45 , TOTAL = 8223.0 SECONDS (137.0 MIN)
WALL CLOCK TIME: STEP = 38.05 , TOTAL = 7603.7 SECONDS (126.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.72 , TOTAL = 8226.7 SECONDS (137.1 MIN)
WALL CLOCK TIME: STEP = 3.71 , TOTAL = 7607.4 SECONDS (126.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.89 , TOTAL = 8229.6 SECONDS (137.2 MIN)
WALL CLOCK TIME: STEP = 2.71 , TOTAL = 7610.1 SECONDS (126.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 91 ENERGY= -284.6369429

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000678	-0.0000323	-0.0000484
2 C	6.0	-0.0000525	0.0000483	-0.0001042
3 C	6.0	0.0000722	-0.0000936	-0.0000225
4 C	6.0	0.0000140	-0.0000155	0.0000050
5 C	6.0	0.0000048	-0.0000205	0.0000366
6 C	6.0	-0.0000774	0.0000096	0.0000417
7 C	6.0	-0.0000418	-0.0000666	-0.0000506
8 C	6.0	0.0000323	0.0000575	0.0000931
9 C	6.0	0.0000059	-0.0000245	-0.0000062

10	C	6.0	-0.0000359	0.0000631	-0.0000059
11	C	6.0	-0.0000067	-0.0000308	0.0000718
12	N	7.0	-0.0000248	-0.0000116	-0.0000438
13	C	6.0	0.0000868	0.0000034	-0.0000881
14	C	6.0	-0.0000010	-0.0000566	-0.0000292
15	C	6.0	-0.0000465	0.0000449	0.0000192
16	C	6.0	0.0000619	0.0000111	0.0000995
17	C	6.0	-0.0000094	-0.0000367	-0.0000198
18	C	6.0	-0.0000587	0.0001144	0.0000355
19	C	6.0	0.0000276	0.0000174	0.0000921
20	O	8.0	0.0000556	-0.0000360	-0.0000533
21	N	7.0	0.0000514	-0.0000586	0.0001032
22	H	1.0	-0.0001319	-0.0000280	0.0000907
23	H	1.0	-0.0000147	0.0000412	0.0000492
24	H	1.0	0.0000878	0.0000482	-0.0001469
25	H	1.0	0.0000247	-0.0000032	0.0000962
26	H	1.0	0.0000448	0.0000118	-0.0001776
27	H	1.0	-0.0001046	0.0001180	0.0001042
28	H	1.0	-0.0000146	0.0000224	-0.0000677
29	H	1.0	-0.0000219	-0.0000307	-0.0000290
30	H	1.0	0.0000668	0.0000688	0.0001029
31	H	1.0	-0.0000310	0.0000454	0.0000196
32	H	1.0	-0.0001089	0.0000321	-0.0001327
33	H	1.0	-0.0000933	-0.0001226	-0.0000252
34	H	1.0	0.0001626	-0.0000514	0.0000464
35	H	1.0	0.0000086	-0.0000383	-0.0000560

MAXIMUM GRADIENT = 0.0001776 RMS GRADIENT = 0.0000647
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000020374
 PREDICTED ENERGY CHANGE WAS -0.0000013864 RATIO= 1.470
 GDIIS STEP HAS LENGTH = 0.023979
 RADIUS OF STEP TAKEN= 0.02398 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8229.6 SECONDS (137.2 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7610.1 SECONDS (126.8
 MIN)
 CPU UTILIZATION: STEP = 80.41% , TOTAL = 100.00%

INSERCH= 92

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z

CO	27.0	0.1597587750	-1.7251200488	0.8816747293
C	6.0	4.9801890471	0.6216216741	0.5643757060
C	6.0	5.1808090059	-0.7173184420	0.2022898972
C	6.0	4.0426388878	-1.5346366826	-0.0933799502
C	6.0	2.7352910704	-1.0212704339	0.0001608124
C	6.0	2.4673308293	0.3445948418	0.4339562895
C	6.0	3.6515003322	1.1744604969	0.6828917533
C	6.0	3.5084426142	2.5616550558	1.0579369614
C	6.0	2.2424638339	3.1421468828	1.2156692120
C	6.0	1.0745432217	2.3359461517	1.0391346755
C	6.0	1.1631005075	0.9806840427	0.6428294953
N	7.0	-0.0501692146	0.1814759952	0.5924301857
C	6.0	-1.2460427435	0.7033469353	0.3244333495
C	6.0	-2.5487990702	0.0390315594	0.4381802987
C	6.0	-2.8177470472	-1.2850300347	0.9301125907
C	6.0	-4.1167864793	-1.8092519470	1.0551189331
C	6.0	-5.2281373340	-0.9964751532	0.6753076848
C	6.0	-5.0165103271	0.3178313436	0.1719950944
C	6.0	-3.6987690647	0.8236090683	0.0586970719
O	8.0	-1.6952622600	-2.1424524715	1.3218520146
N	7.0	1.6262253863	-1.9525808597	-0.4255164192
H	1.0	5.8429241260	1.2814370162	0.7677400869
H	1.0	6.1977458376	-1.1395639917	0.1205787093
H	1.0	4.2044677677	-2.5766186841	-0.4333558327
H	1.0	4.4230167021	3.1572867125	1.2306803821
H	1.0	2.1377697140	4.2004021094	1.5130991831
H	1.0	0.0916768628	2.7832160849	1.2703375440
H	1.0	-1.2908208607	1.7533855984	-0.0275491622
H	1.0	-4.2872696022	-2.8337849332	1.4378872894
H	1.0	-6.2516093114	-1.4017839749	0.7731989593
H	1.0	-5.8750865004	0.9458159901	-0.1240706821
H	1.0	-3.5374346867	1.8495560345	-0.3217572246
H	1.0	-2.0129035633	-2.9586982548	1.7871741083
H	1.0	1.2605169389	-1.6735601853	-1.3626716464
H	1.0	2.0189336048	-2.9082524963	-0.5385551004

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3707005	5.1660597	4.0079638
2 C	5.3707005	0.0000000	1.4014689 *	2.4415349 *
3 C	5.1660597	1.4014689 *	0.0000000	1.4320827 *
4 C	4.0079638	2.4415349 *	1.4320827 *	0.0000000
5 C	2.8117321 *	2.8384855 *	2.4726101 *	1.4076410 *

6 C	3.1319419	2.5314442 *	2.9230623 *	2.5082245 *
7 C	4.5430542	1.4439843 *	2.4796352 *	2.8451353 *
8 C	5.4425355	2.4846267 *	3.7789692	4.2884149
9 C	5.3046678	3.7778790	4.9554296	5.1794348
10 C	4.1657992	4.2916633	5.1849930	5.0073539
11 C	2.8957067 *	3.8347419	4.3839787	3.8936595
12 N	1.9398043 *	5.0496554	5.3219521	4.4907078
13 C	2.8608124 *	6.2313894	6.5831324	5.7578895
14 C	3.2626989	7.5525491	7.7701062	6.7975027
15 C	3.0102436	8.0359748	8.0516409	6.9408022
16 C	4.2808878	9.4289416	9.4002616	8.2444336
17 C	5.4408579	10.3363664	10.4234274	9.3181431
18 C	5.6099071	10.0090084	10.2497695	9.2504187
19 C	4.6969724	8.6960234	9.0134335	8.0940625
20 O	1.9516725 *	7.2646766	7.1108918	5.9410295
21 N	1.9776277 *	4.3422894	3.8151119	2.4746810 *
22 H	6.4304537	1.1050001 *	2.1801729 *	3.4514962
23 H	6.1138720	2.1865899 *	1.1041415 *	2.2014420 *
24 H	4.3375138	3.4388884	2.1941479 *	1.1079254 *
25 H	6.4911531	2.6802985 *	4.0797551	4.8899865
26 H	6.2787767	4.6676647	5.9297795	6.2529970
27 H	4.5255705	5.3915141	6.2684714	6.0094658
28 H	3.8769667	6.3997523	6.9310315	6.2658772
29 H	4.6167707	9.9291816	9.7801147	8.5685437
30 H	6.4204325	11.4145115	11.4671103	10.3315127
31 H	6.6756858	10.8819147	11.1850504	10.2232512
32 H	5.2816472	8.6511831	9.1033644	8.3043622
33 H	2.6574623 *	7.9509289	7.6996845	6.4987714
34 H	2.5002835 *	4.7767491	4.3280703	3.0611442
35 H	2.6217144 *	4.7376684	3.9174608	2.4860379 *

C C C C

1 CO	2.8117321 *	3.1319419	4.5430542	5.4425355
2 C	2.8384855 *	2.5314442 *	1.4439843 *	2.4846267 *
3 C	2.4726101 *	2.9230623 *	2.4796352 *	3.7789692
4 C	1.4076410 *	2.5082245 *	2.8451353 *	4.2884149
5 C	0.0000000	1.4579332 *	2.4752364 *	3.8149717
6 C	1.4579332 *	0.0000000	1.4672775 *	2.5275723 *
7 C	2.4752364 *	1.4672775 *	0.0000000	1.4441029 *
8 C	3.8149717	2.5275723 *	1.4441029 *	0.0000000
9 C	4.3651327	2.9134065 *	2.4781092 *	1.4016249 *
10 C	3.8869594	2.5043119 *	2.8489763 *	2.4444149 *
11 C	2.6253815 *	1.4660335 *	2.4962548 *	2.8587433 *
12 N	3.0913057	2.5277516 *	3.8336091	4.3064681
13 C	4.3509168	3.7322703	4.9331905	5.1571763

14 C	5.4071906	5.0254299	6.3081531	6.5907438
15 C	5.6365425	5.5528278	6.9254150	7.4049984
16 C	6.9774507	6.9552498	8.3299083	8.7891385
17 C	7.9920354	7.8151743	9.1411697	9.4411082
18 C	7.8684907	7.4884724	8.7252070	8.8597100
19 C	6.6935892	6.1960521	7.3850644	7.4808545
20 O	4.7574909	4.9295988	6.3244013	7.0197452
21 N	1.5094923 *	2.5929072 *	3.8869905	5.1109394
22 H	3.9432249	3.5190503	2.1956733 *	2.6782413 *
23 H	3.4665670	4.0270248	3.4862977	4.6701194
24 H	2.1830083 *	3.5076151	3.9525152	5.3953927
25 H	4.6715025	3.5172023	2.1970229 *	1.1050172 *
26 H	5.4691753	4.0175129	3.4838122	2.1843555 *
27 H	4.8037655	3.5057294	3.9503836	3.4305235
28 H	4.8896893	4.0399731	5.0265713	4.9864325
29 H	7.3938234	7.5322375	8.9252517	9.4883225
30 H	9.0281093	8.8985865	10.2331213	10.5379570
31 H	8.8330892	8.3826480	9.5634368	9.5947223
32 H	6.9059658	6.2364429	7.2901207	7.2149170
33 H	5.4306901	5.7284766	7.0984444	7.8416421
34 H	2.1113391 *	2.9592603 *	4.2440963	5.3711790
35 H	2.0890391 *	3.4245955	4.5635241	5.8895936

C C C N

1 CO	5.3046678	4.1657992	2.8957067 *	1.9398043 *
2 C	3.7778790	4.2916633	3.8347419	5.0496554
3 C	4.9554296	5.1849930	4.3839787	5.3219521
4 C	5.1794348	5.0073539	3.8936595	4.4907078
5 C	4.3651327	3.8869594	2.6253815 *	3.0913057
6 C	2.9134065 *	2.5043119 *	1.4660335 *	2.5277516 *
7 C	2.4781092 *	2.8489763 *	2.4962548 *	3.8336091
8 C	1.4016249 *	2.4444149 *	2.8587433 *	4.3064681
9 C	0.0000000	1.4300918 *	2.4829604 *	3.7960723
10 C	1.4300918 *	0.0000000	1.4147917 *	2.4710857 *
11 C	2.4829604 *	1.4147917 *	0.0000000	1.4537183 *
12 N	3.7960723	2.4710857 *	1.4537183 *	0.0000000
13 C	4.3487613	2.9259695 *	2.4458666 *	1.3320229 *
14 C	5.7610775	4.3319248	3.8349432	2.5074359 *
15 C	6.7295744	5.3172623	4.5894596	3.1502629
16 C	8.0611532	6.6432542	5.9858944	4.5513135
17 C	8.5574567	7.1387102	6.6901521	5.3109125
18 C	7.8586716	6.4750021	6.2328684	4.9859706
19 C	6.4817012	5.1022477	4.8993529	3.7429249
20 O	6.5912026	5.2733107	4.2878072	2.9392228 *
21 N	5.3879023	4.5651966	3.1559294	2.8983983 *

22 H	4.0775233	4.8911247	4.6911410	5.9974325
23 H	5.9309803	6.2586037	5.4877911	6.4034548
24 H	6.2668192	6.0081569	4.8023424	5.1731286
25 H	2.1806571 *	3.4530515	3.9636122	5.4103794
26 H	1.1042326 *	2.1980193 *	3.4747567	4.6675984
27 H	2.1812163 *	1.1043240 *	2.1887980 *	2.6923466 *
28 H	3.9947904	2.6593493 *	2.6586097 *	2.0963041 *
29 H	8.8542962	7.4588310	6.6999123	5.2687395
30 H	9.6432550	8.2288431	7.7891637	6.4029094
31 H	8.5154798	7.1821210	7.0799314	5.9183824
32 H	6.1189622	4.8331090	4.8765149	3.9723104
33 H	7.4602333	6.1745567	5.1879918	3.8910710
34 H	5.5500537	4.6775422	3.3281432	2.9969118 *
35 H	6.3035388	5.5572113	4.1535463	3.8867385

C C C C

1 CO	2.8608124 *	3.2626989	3.0102436	4.2808878
2 C	6.2313894	7.5525491	8.0359748	9.4289416
3 C	6.5831324	7.7701062	8.0516409	9.4002616
4 C	5.7578895	6.7975027	6.9408022	8.2444336
5 C	4.3509168	5.4071906	5.6365425	6.9774507
6 C	3.7322703	5.0254299	5.5528278	6.9552498
7 C	4.9331905	6.3081531	6.9254150	8.3299083
8 C	5.1571763	6.5907438	7.4049984	8.7891385
9 C	4.3487613	5.7610775	6.7295744	8.0611532
10 C	2.9259695 *	4.3319248	5.3172623	6.6432542
11 C	2.4458666 *	3.8349432	4.5894596	5.9858944
12 N	1.3320229 *	2.5074359 *	3.1502629	4.5513135
13 C	0.0000000	1.4667745 *	2.6059057 *	3.8843563
14 C	1.4667745 *	0.0000000	1.4378698 *	2.5010697 *
15 C	2.6059057 *	1.4378698 *	0.0000000	1.4063921 *
16 C	3.8843563	2.5010697 *	1.4063921 *	0.0000000
17 C	4.3439136	2.8822486 *	2.4409365 *	1.4282729 *
18 C	3.7931894	2.4976354 *	2.8246180 *	2.4726290 *
19 C	2.4700091 *	1.4429138 *	2.4457971 *	2.8459712 *
20 O	3.0488057	2.5036520 *	1.4658121 *	2.4588511 *
21 N	3.9832526	4.7056691	4.6938518	5.9325382
22 H	7.1263006	8.4895936	9.0343978	10.4321992
23 H	7.6712363	8.8313083	9.0529342	10.3784115
24 H	6.4062847	7.2943687	7.2690266	8.4880905
25 H	6.2435038	7.6783974	8.5001870	9.8805651
26 H	5.0092423	6.3589608	7.4153210	8.6859174
27 H	2.6476564 *	3.8980954	5.0130956	6.2328361
28 H	1.1083673 *	2.1767919 *	3.5327877	4.6744666
29 H	4.7958464	3.5035366	2.1945326 *	1.1069074 *

30 H	5.4487304	3.9873538	3.4394278	2.1915697 *
31 H	4.6570370	3.4932180	3.9287785	3.4745513
32 H	2.6423161 *	2.1983867 *	3.4511966	3.9520010
33 H	4.0172455	3.3306685	2.0453588 *	2.5066821 *
34 H	3.8443273	4.5482883	4.6946834	5.8974160
35 H	4.9445394	5.5231039	5.3089844	6.4338682

C C C O

1 CO	5.4408579	5.6099071	4.6969724	1.9516725 *
2 C	10.3363664	10.0090084	8.6960234	7.2646766
3 C	10.4234274	10.2497695	9.0134335	7.1108918
4 C	9.3181431	9.2504187	8.0940625	5.9410295
5 C	7.9920354	7.8684907	6.6935892	4.7574909
6 C	7.8151743	7.4884724	6.1960521	4.9295988
7 C	9.1411697	8.7252070	7.3850644	6.3244013
8 C	9.4411082	8.8597100	7.4808545	7.0197452
9 C	8.5574567	7.8586716	6.4817012	6.5912026
10 C	7.1387102	6.4750021	5.1022477	5.2733107
11 C	6.6901521	6.2328684	4.8993529	4.2878072
12 N	5.3109125	4.9859706	3.7429249	2.9392228 *
13 C	4.3439136	3.7931894	2.4700091 *	3.0488057
14 C	2.8822486 *	2.4976354 *	1.4429138 *	2.5036520 *
15 C	2.4409365 *	2.8246180 *	2.4457971 *	1.4658121 *
16 C	1.4282729 *	2.4726290 *	2.8459712 *	2.4588511 *
17 C	0.0000000	1.4232045 *	2.4559891 *	3.7699456
18 C	1.4232045 *	0.0000000	1.4160119 *	4.2902047
19 C	2.4559891 *	1.4160119 *	0.0000000	3.7956713
20 O	3.7699456	4.2902047	3.7956713	0.0000000
21 N	7.0077272	7.0454048	6.0247207	3.7578754
22 H	11.3033548	10.9183682	9.5789487	8.2978499
23 H	11.4402362	11.3086775	10.0895434	8.0466403
24 H	9.6280853	9.6835287	8.6177037	6.1705810
25 H	10.5217371	9.9140301	8.5312953	8.0949914
26 H	9.0535084	8.2496448	6.8980578	7.4135359
27 H	6.5529039	5.7773744	4.4357201	5.2400397
28 H	4.8536793	3.9976738	2.5826609 *	4.1427057
29 H	2.2005606 *	3.4737530	3.9528508	2.6851270 *
30 H	1.1051483 *	2.2009072 *	3.4611964	4.6486459
31 H	2.1977361 *	1.1041615 *	2.1873948 *	5.3943512
32 H	3.4572399	2.1857806 *	1.1060477 *	4.6937386
33 H	3.9273776	4.7292815	4.4872736	0.9918053 *
34 H	6.8347961	6.7617981	5.7315496	4.0203430
35 H	7.5926539	7.7723851	6.8538766	4.2240757

N H H H

1	CO	1.9776277 *	6.4304537	6.1138720	4.3375138
2	C	4.3422894	1.1050001 *	2.1865899 *	3.4388884
3	C	3.8151119	2.1801729 *	1.1041415 *	2.1941479 *
4	C	2.4746810 *	3.4514962	2.2014420 *	1.1079254 *
5	C	1.5094923 *	3.9432249	3.4665670	2.1830083 *
6	C	2.5929072 *	3.5190503	4.0270248	3.5076151
7	C	3.8869905	2.1956733 *	3.4862977	3.9525152
8	C	5.1109394	2.6782413 *	4.6701194	5.3953927
9	C	5.3879023	4.0775233	5.9309803	6.2668192
10	C	4.5651966	4.8911247	6.2586037	6.0081569
11	C	3.1559294	4.6911410	5.4877911	4.8023424
12	N	2.8983983 *	5.9974325	6.4034548	5.1731286
13	C	3.9832526	7.1263006	7.6712363	6.4062847
14	C	4.7056691	8.4895936	8.8313083	7.2943687
15	C	4.6938518	9.0343978	9.0529342	7.2690266
16	C	5.9325382	10.4321992	10.3784115	8.4880905
17	C	7.0077272	11.3033548	11.4402362	9.6280853
18	C	7.0454048	10.9183682	11.3086775	9.6835287
19	C	6.0247207	9.5789487	10.0895434	8.6177037
20	O	3.7578754	8.2978499	8.0466403	6.1705810
21	N	0.0000000	5.4464007	4.6752557	2.6527002 *
22	H	5.4464007	0.0000000	2.5310002 *	4.3602482
23	H	4.6752557	2.5310002 *	0.0000000	2.5189536 *
24	H	2.6527002 *	4.3602482	2.5189536 *	0.0000000
25	H	6.0560528	2.3977621 *	4.7796355	5.9744833
26	H	6.4714069	4.7753625	6.8511136	7.3476485
27	H	5.2591380	5.9652988	7.3480764	6.9674564
28	H	4.7330460	7.1934371	8.0293045	7.0079821
29	H	6.2624450	10.9546782	10.7023939	8.6992694
30	H	7.9875262	12.3886014	12.4692067	10.5908243
31	H	8.0474377	11.7566892	12.2540583	10.6817891
32	H	6.4132984	9.4604913	10.1933429	8.9185498
33	H	4.3762462	8.9851000	8.5733047	6.6130511
34	H	1.0439613 *	5.8539831	5.1827997	3.2165182
35	H	1.0393776 *	5.8208942	4.5853231	2.2130539 *

H H H H

1	CO	6.4911531	6.2787767	4.5255705	3.8769667
2	C	2.6802985 *	4.6676647	5.3915141	6.3997523
3	C	4.0797551	5.9297795	6.2684714	6.9310315
4	C	4.8899865	6.2529970	6.0094658	6.2658772
5	C	4.6715025	5.4691753	4.8037655	4.8896893
6	C	3.5172023	4.0175129	3.5057294	4.0399731
7	C	2.1970229 *	3.4838122	3.9503836	5.0265713

8 C	1.1050172 *	2.1843555 *	3.4305235	4.9864325
9 C	2.1806571 *	1.1042326 *	2.1812163 *	3.9947904
10 C	3.4530515	2.1980193 *	1.1043240 *	2.6593493 *
11 C	3.9636122	3.4747567	2.1887980 *	2.6586097 *
12 N	5.4103794	4.6675984	2.6923466 *	2.0963041 *
13 C	6.2435038	5.0092423	2.6476564 *	1.1083673 *
14 C	7.6783974	6.3589608	3.8980954	2.1767919 *
15 C	8.5001870	7.4153210	5.0130956	3.5327877
16 C	9.8805651	8.6859174	6.2328361	4.6744666
17 C	10.5217371	9.0535084	6.5529039	4.8536793
18 C	9.9140301	8.2496448	5.7773744	3.9976738
19 C	8.5312953	6.8980578	4.4357201	2.5826609 *
20 O	8.0949914	7.4135359	5.2400397	4.1427057
21 N	6.0560528	6.4714069	5.2591380	4.7330460
22 H	2.3977621 *	4.7753625	5.9652988	7.1934371
23 H	4.7796355	6.8511136	7.3480764	8.0293045
24 H	5.9744833	7.3476485	6.9674564	7.0079821
25 H	0.0000000	2.5278853 *	4.3476438	6.0168114
26 H	2.5278853 *	0.0000000	2.5007690 *	4.4851667
27 H	4.3476438	2.5007690 *	0.0000000	2.1578602 *
28 H	6.0168114	4.4851667	2.1578602 *	0.0000000
29 H	10.5737865	9.5271493	7.1241803	5.6717143
30 H	11.6164562	10.1150196	7.6156846	5.9334404
31 H	10.6196461	8.8021884	6.3970836	4.6558540
32 H	8.2151694	6.4110155	4.0714785	2.2678362 *
33 H	8.8958432	8.2798505	6.1372599	5.1008194
34 H	6.3296099	6.5987168	5.3067673	4.4761405
35 H	6.7602201	7.3997552	6.2752869	5.7399017

H H H H

1 CO	4.6167707	6.4204325	6.6756858	5.2816472
2 C	9.9291816	11.4145115	10.8819147	8.6511831
3 C	9.7801147	11.4671103	11.1850504	9.1033644
4 C	8.5685437	10.3315127	10.2232512	8.3043622
5 C	7.3938234	9.0281093	8.8330892	6.9059658
6 C	7.5322375	8.8985865	8.3826480	6.2364429
7 C	8.9252517	10.2331213	9.5634368	7.2901207
8 C	9.4883225	10.5379570	9.5947223	7.2149170
9 C	8.8542962	9.6432550	8.5154798	6.1189622
10 C	7.4588310	8.2288431	7.1821210	4.8331090
11 C	6.6999123	7.7891637	7.0799314	4.8765149
12 N	5.2687395	6.4029094	5.9183824	3.9723104
13 C	4.7958464	5.4487304	4.6570370	2.6423161 *
14 C	3.5035366	3.9873538	3.4932180	2.1983867 *
15 C	2.1945326 *	3.4394278	3.9287785	3.4511966

16 C	1.1069074 *	2.1915697 *	3.4745513	3.9520010
17 C	2.2005606 *	1.1051483 *	2.1977361 *	3.4572399
18 C	3.4737530	2.2009072 *	1.1041615 *	2.1857806 *
19 C	3.9528508	3.4611964	2.1873948 *	1.1060477 *
20 O	2.6851270 *	4.6486459	5.3943512	4.6937386
21 N	6.2624450	7.9875262	8.0474377	6.4132984
22 H	10.9546782	12.3886014	11.7566892	9.4604913
23 H	10.7023939	12.4692067	12.2540583	10.1933429
24 H	8.6992694	10.5908243	10.6817891	8.9185498
25 H	10.5737865	11.6164562	10.6196461	8.2151694
26 H	9.5271493	10.1150196	8.8021884	6.4110155
27 H	7.1241803	7.6156846	6.3970836	4.0714785
28 H	5.6717143	5.9334404	4.6558540	2.2678362 *
29 H	0.0000000	2.5201325 *	4.3870558	5.0588817
30 H	2.5201325 *	0.0000000	2.5412768 *	4.3745725
31 H	4.3870558	2.5412768 *	0.0000000	2.5140489 *
32 H	5.0588817	4.3745725	2.5140489 *	0.0000000
33 H	2.3044187 *	4.6280400	5.8150275	5.4672750
34 H	6.3219607	7.8145919	7.7014350	6.0428628
35 H	6.6090899	8.5083504	8.7943843	7.3182629

H H H

1 CO	2.6574623 *	2.5002835 *	2.6217144 *
2 C	7.9509289	4.7767491	4.7376684
3 C	7.6996845	4.3280703	3.9174608
4 C	6.4987714	3.0611442	2.4860379 *
5 C	5.4306901	2.1113391 *	2.0890391 *
6 C	5.7284766	2.9592603 *	3.4245955
7 C	7.0984444	4.2440963	4.5635241
8 C	7.8416421	5.3711790	5.8895936
9 C	7.4602333	5.5500537	6.3035388
10 C	6.1745567	4.6775422	5.5572113
11 C	5.1879918	3.3281432	4.1535463
12 N	3.8910710	2.9969118 *	3.8867385
13 C	4.0172455	3.8443273	4.9445394
14 C	3.3306685	4.5482883	5.5231039
15 C	2.0453588 *	4.6946834	5.3089844
16 C	2.5066821 *	5.8974160	6.4338682
17 C	3.9273776	6.8347961	7.5926539
18 C	4.7292815	6.7617981	7.7723851
19 C	4.4872736	5.7315496	6.8538766
20 O	0.9918053 *	4.0203430	4.2240757
21 N	4.3762462	1.0439613 *	1.0393776 *
22 H	8.9851000	5.8539831	5.8208942
23 H	8.5733047	5.1827997	4.5853231

24 H	6.6130511	3.2165182	2.2130539 *
25 H	8.8958432	6.3296099	6.7602201
26 H	8.2798505	6.5987168	7.3997552
27 H	6.1372599	5.3067673	6.2752869
28 H	5.1008194	4.4761405	5.7399017
29 H	2.3044187 *	6.3219607	6.6090899
30 H	4.6280400	7.8145919	8.5083504
31 H	5.8150275	7.7014350	8.7943843
32 H	5.4672750	6.0428628	7.3182629
33 H	0.0000000	4.7210581	4.6548117
34 H	4.7210581	0.0000000	1.6669820 *
35 H	4.6548117	1.6669820 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80 , TOTAL = 8230.4 SECONDS (137.2 MIN)
WALL CLOCK TIME: STEP = 0.81 , TOTAL = 7610.9 SECONDS (126.8 MIN)

CPU UTILIZATION: STEP = 98.38%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.85 , TOTAL = 8231.3 SECONDS (137.2 MIN)
WALL CLOCK TIME: STEP = 0.85 , TOTAL = 7611.8 SECONDS (126.9 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636936306	-284.636936306	0.002953643	0.000306817	198289447
11322297						
2	1	-284.636946325	-0.000010019	0.001492198	0.000039758	148086022
15530033						
3	2	-284.636946153	0.000000172	0.000614355	0.000082939	133114782
16695530						
4	3	-284.636946521	-0.000000368	0.000366401	0.000016188	127316089
17136056						
5	4	-284.636946491	0.000000031	0.000186474	0.000039141	118747564
17802273						

6 5	-284.636946531	-0.000000041	0.000073704	0.000011082	112586467
18263619					
7 6	-284.636946538	-0.000000006	0.000082703	0.000011612	108802733
18524812					
8 7	-284.636946546	-0.000000008	0.000070505	0.000008602	128432993
17126761					
9 8	-284.636946546	0.000000000	0.000111019	0.000007023	129707004
17032610					
10 9	-284.636946550	-0.000000004	0.000077835	0.000005670	152344441
15356642					
11 10	-284.636946553	-0.000000002	0.000105882	0.000006379	149566826
15523862					
-----DISABLING FDIFF OPTION-----					
12 11	-284.636946524	0.000000029	0.000043772	0.000007700	198290603
11322121					
13 12	-284.636946525	-0.000000002	0.000065800	0.000006108	198290898
11322113					
14 13	-284.636946527	-0.000000002	0.000054956	0.000003912	198290856
11322117					
15 14	-284.636946528	-0.000000001	0.000046044	0.000004300	198290855
11322117					
16 15	-284.636946529	-0.000000001	0.000037785	0.000003799	198290685
11322119					
17 16	-284.636946529	0.000000000	0.000033130	0.000002150	198290610
11322119					

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 54.4 SECONDS (3.2 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 18.5 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 3.3 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6369465291 AFTER 17 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6016946659
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998521972

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 58.49 , TOTAL = 8289.8 SECONDS (138.2 MIN)
WALL CLOCK TIME: STEP = 54.03 , TOTAL = 7665.8 SECONDS (127.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.67 , TOTAL = 8293.4 SECONDS (138.2 MIN)
WALL CLOCK TIME: STEP = 3.62 , TOTAL = 7669.4 SECONDS (127.8 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.86 , TOTAL = 8296.3 SECONDS (138.3 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 7672.1 SECONDS (127.9 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 92 ENERGY= -284.6369465

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000277	-0.0000185	-0.0000563
2 C	6.0	-0.0000281	0.0000185	-0.0000077
3 C	6.0	0.0000434	0.0000340	-0.0000592
4 C	6.0	-0.0000196	-0.0000414	-0.0000189
5 C	6.0	-0.0000310	-0.0000499	0.0000829
6 C	6.0	-0.0000083	-0.0000034	0.0000226
7 C	6.0	0.0000273	-0.0000142	0.0000294
8 C	6.0	-0.0000106	-0.0000763	0.0000767
9 C	6.0	0.0000697	0.0000665	0.0000551
10 C	6.0	-0.0000761	-0.0000128	0.0000112
11 C	6.0	-0.0000843	-0.0000012	0.0000027
12 N	7.0	0.0000668	0.0001038	0.0000073

13 C	6.0	0.0000201	-0.0000221	-0.0000200
14 C	6.0	0.0000441	0.0000264	-0.0000859
15 C	6.0	0.0000040	0.0000153	0.0000136
16 C	6.0	0.0000258	0.0000340	0.0000998
17 C	6.0	-0.0000057	0.0000137	0.0001176
18 C	6.0	-0.0000562	-0.0000290	0.0000195
19 C	6.0	0.0000263	0.0000903	-0.0000806
20 O	8.0	-0.0000020	-0.0000552	-0.0000550
21 N	7.0	0.0000525	-0.0001474	0.0000287
22 H	1.0	-0.0001210	0.0000693	0.0000437
23 H	1.0	0.0000078	0.0000253	0.0000874
24 H	1.0	0.0000684	-0.0000181	-0.0001638
25 H	1.0	-0.0000076	-0.0000229	0.0000602
26 H	1.0	0.0000210	0.0000255	-0.0001885
27 H	1.0	-0.0000219	0.0000645	0.0000655
28 H	1.0	0.0000114	-0.0000372	-0.0000979
29 H	1.0	-0.0000372	-0.0000451	-0.0000192
30 H	1.0	0.0000382	-0.0000237	0.0000628
31 H	1.0	0.0000233	0.0000247	0.0000356
32 H	1.0	-0.0000829	0.0001038	-0.0000274
33 H	1.0	-0.0000428	-0.0000332	-0.0000842
34 H	1.0	0.0000334	-0.0000353	0.0000683
35 H	1.0	0.0000237	-0.0000289	-0.0000260

MAXIMUM GRADIENT = 0.0001885 RMS GRADIENT = 0.0000570
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000036473
 PREDICTED ENERGY CHANGE WAS -0.0000021784 RATIO= 1.674
 GDIIS STEP HAS LENGTH = 0.018987
 RADIUS OF STEP TAKEN= 0.01899 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8296.3 SECONDS (138.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7672.2 SECONDS (127.9 MIN)
 CPU UTILIZATION: STEP = 80.73% , TOTAL = 100.00%

INSERCH= 93

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z

CO	27.0	0.1601050373	-1.7240803872	0.8829259457
C	6.0	4.9801611111	0.6210227210	0.5646242394
C	6.0	5.1800086591	-0.7178981344	0.2019982036

C	6.0	4.0415862053	-1.5347647777	-0.0939633292
C	6.0	2.7344395438	-1.0210103329	-0.0005868735
C	6.0	2.4672156652	0.3447711036	0.4338515499
C	6.0	3.6515953482	1.1742166760	0.6833595201
C	6.0	3.5088549312	2.5613282001	1.0586370745
C	6.0	2.2431089422	3.1422111763	1.2165994308
C	6.0	1.0751891366	2.3363278752	1.0394739559
C	6.0	1.1633398588	0.9812414562	0.6427295747
N	7.0	-0.0501203434	0.1822660948	0.5928002208
C	6.0	-1.2459951584	0.7039841208	0.3244150310
C	6.0	-2.5486472148	0.0393808970	0.4381487283
C	6.0	-2.8171104792	-1.2845105354	0.9306695445
C	6.0	-4.1158613798	-1.8094370795	1.0555558325
C	6.0	-5.2275124611	-0.9977274604	0.6744356637
C	6.0	-5.0162224656	0.3163239567	0.1703361123
C	6.0	-3.6988808354	0.8231042598	0.0577475059
O	8.0	-1.6945314845	-2.1409806827	1.3236785718
N	7.0	1.6248571308	-1.9516787582	-0.4261125836
H	1.0	5.8433085133	1.2807777905	0.7672949788
H	1.0	6.1967617768	-1.1405824812	0.1199104832
H	1.0	4.2028184956	-2.5768822474	-0.4336496799
H	1.0	4.4235868619	3.1566240859	1.2313596861
H	1.0	2.1386359242	4.2003329534	1.5148489785
H	1.0	0.0923156886	2.7836210084	1.2701367685
H	1.0	-1.2905748231	1.7537086791	-0.0285426183
H	1.0	-4.2857541428	-2.8335911961	1.4394806272
H	1.0	-6.2507670364	-1.4040721206	0.7715443539
H	1.0	-5.8750723174	0.9435534723	-0.1264877018
H	1.0	-3.5379024557	1.8495361545	-0.3217421755
H	1.0	-2.0118442492	-2.9567830712	1.7900470088
H	1.0	1.2573632237	-1.6719083323	-1.3624282699
H	1.0	2.0175417929	-2.9073200843	-0.5402093587

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3697081	5.1648328	4.0070000
2 C	5.3697081	0.0000000	1.4014798 *	2.4417371 *
3 C	5.1648328	1.4014798 *	0.0000000	1.4320859 *
4 C	4.0070000	2.4417371 *	1.4320859 *	0.0000000
5 C	2.8110675 *	2.8388381 *	2.4725950 *	1.4075849 *
6 C	3.1312256	2.5314643 *	2.9227158 *	2.5079646 *
7 C	4.5420763	1.4440251 *	2.4794867 *	2.8451545 *
8 C	5.4414821	2.4846682 *	3.7788769	4.2883876

9 C	5.3038700	3.7779515	4.9553244	5.1794014
10 C	4.1651892	4.2914520	5.1845159	5.0069502
11 C	2.8953308 *	3.8345772	4.3834858	3.8932385
12 N	1.9397228 *	5.0494587	5.3213975	4.4902006
13 C	2.8608652 *	6.2313405	6.5825725	5.7572175
14 C	3.2626617	7.5523015	7.7692574	6.7964884
15 C	3.0098693	8.0350787	8.0502128	6.9393242
16 C	4.2803009	9.4279252	9.3985753	8.2426204
17 C	5.4403565	10.3358120	10.4219958	9.3163854
18 C	5.6094029	10.0087956	10.2485973	9.2487989
19 C	4.6968970	8.6961791	9.0127784	8.0930459
20 O	1.9513445 *	7.2633565	7.1093342	5.9397182
21 N	1.9775949 *	4.3426279	3.8152117	2.4748171 *
22 H	6.4297236	1.1051586 *	2.1804203 *	3.4518472
23 H	6.1126007	2.1865819 *	1.1041682 *	2.2013413 *
24 H	4.3363780	3.4391000	2.1942586 *	1.1078770 *
25 H	6.4899892	2.6802211 *	4.0796668	4.8899422
26 H	6.2779443	4.6678319	5.9297995	6.2530667
27 H	4.5248093	5.3912533	6.2678685	6.0088237
28 H	3.8768884	6.3997620	6.9303997	6.2650043
29 H	4.6158890	9.9275836	9.7779438	8.5663877
30 H	6.4198202	11.4139201	11.4655070	10.3295072
31 H	6.6752192	10.8819922	11.1840574	10.2217041
32 H	5.2817819	8.6517222	9.1031861	8.3038560
33 H	2.6570262 *	7.9492449	7.6978733	6.4973573
34 H	2.4996626 *	4.7781051	4.3295165	3.0626311
35 H	2.6221063 *	4.7378237	3.9173508	2.4859202 *

C C C C

1 CO	2.8110675 *	3.1312256	4.5420763	5.4414821
2 C	2.8388381 *	2.5314643 *	1.4440251 *	2.4846682 *
3 C	2.4725950 *	2.9227158 *	2.4794867 *	3.7788769
4 C	1.4075849 *	2.5079646 *	2.8451545 *	4.2883876
5 C	0.0000000	1.4579109 *	2.4754755 *	3.8150785
6 C	1.4579109 *	0.0000000	1.4673069 *	2.5275472 *
7 C	2.4754755 *	1.4673069 *	0.0000000	1.4440521 *
8 C	3.8150785	2.5275472 *	1.4440521 *	0.0000000
9 C	4.3652447	2.9135183 *	2.4781407 *	1.4016027 *
10 C	3.8867156	2.5041595 *	2.8487171 *	2.4441198 *
11 C	2.6251138 *	1.4658843 *	2.4960580 *	2.8585126 *
12 N	3.0909151	2.5275785 *	3.8333883	4.3061869
13 C	4.3502980	3.7321502	4.9331889	5.1572675
14 C	5.4062856	5.0251529	6.3080099	6.5907933
15 C	5.6352798	5.5520707	6.9246413	7.4043696
16 C	6.9759356	6.9544254	8.3291118	8.7886232

17 C	7.9905492	7.8146672	9.1408958	9.4413242
18 C	7.8670477	7.4881303	8.7252644	8.8603650
19 C	6.6926656	6.1960474	7.3854025	7.4816213
20 O	4.7564479	4.9285792	6.3231016	7.0183464
21 N	1.5094333 *	2.5928340 *	3.8871350	5.1108865
22 H	3.9437213	3.5192749	2.1959069 *	2.6785002 *
23 H	3.4664813	4.0267044	3.4862074	4.6701385
24 H	2.1827546 *	3.5072687	3.9525055	5.3953417
25 H	4.6715672	3.5170904	2.1968646 *	1.1049637 *
26 H	5.4693650	4.0176955	3.4839347	2.1844830 *
27 H	4.8032048	3.5053547	3.9500584	3.4302896
28 H	4.8888227	4.0397899	5.0266949	4.9868562
29 H	7.3920473	7.5309945	8.9238870	9.4871559
30 H	9.0264534	8.8980735	10.2328945	10.5383605
31 H	8.8317074	8.3824990	9.5638096	9.5958223
32 H	6.9054654	6.2367206	7.2907588	7.2158772
33 H	5.4296221	5.7272597	7.0967925	7.8398107
34 H	2.1118794 *	2.9592837 *	4.2447642	5.3713186
35 H	2.0888512 *	3.4244851	4.5635725	5.8895194

C C C N

1 CO	5.3038700	4.1651892	2.8953308 *	1.9397228 *
2 C	3.7779515	4.2914520	3.8345772	5.0494587
3 C	4.9553244	5.1845159	4.3834858	5.3213975
4 C	5.1794014	5.0069502	3.8932385	4.4902006
5 C	4.3652447	3.8867156	2.6251138 *	3.0909151
6 C	2.9135183 *	2.5041595 *	1.4658843 *	2.5275785 *
7 C	2.4781407 *	2.8487171 *	2.4960580 *	3.8333883
8 C	1.4016027 *	2.4441198 *	2.8585126 *	4.3061869
9 C	0.0000000	1.4299853 *	2.4829454 *	3.7959585
10 C	1.4299853 *	0.0000000	1.4147211 *	2.4709960 *
11 C	2.4829454 *	1.4147211 *	0.0000000	1.4537332 *
12 N	3.7959585	2.4709960 *	1.4537332 *	0.0000000
13 C	4.3491139	2.9263889 *	2.4460358 *	1.3320424 *
14 C	5.7614641	4.3324066	3.8350753	2.5073831 *
15 C	6.7292973	5.3171708	4.5891749	3.1498927
16 C	8.0610954	6.6433900	5.9856727	4.5509641
17 C	8.5582251	7.1395536	6.6903151	5.3107851
18 C	7.8599108	6.4761958	6.2331582	4.9858417
19 C	6.4829343	5.1034671	4.8998369	3.7430480
20 O	6.5900375	5.2724204	4.2871192	2.9386641 *
21 N	5.3878059	4.5647650	3.1555416	2.8978360 *
22 H	4.0777746	4.8911379	4.6911987	5.9974728
23 H	5.9309712	6.2581953	5.4873320	6.4028969
24 H	6.2667227	6.0076445	4.8017983	5.1724257

25 H	2.1805755 *	3.4527487	3.9633301	5.4100480
26 H	1.1043048 *	2.1980481 *	3.4748158	4.6675142
27 H	2.1811384 *	1.1042267 *	2.1884480 *	2.6918618 *
28 H	3.9956525	2.6602526 *	2.6587608 *	2.0962409 *
29 H	8.8535836	7.4584034	6.6992825	5.2680980
30 H	9.6443089	8.2299461	7.7894348	6.4028461
31 H	8.5172088	7.1836913	7.0804210	5.9183612
32 H	6.1202611	4.8343034	4.8770709	3.9725057
33 H	7.4586326	6.1733426	5.1871156	3.8904229
34 H	5.5496689	4.6763532	3.3269659	2.9950617 *
35 H	6.3034979	5.5569121	4.1533019	3.8864483

C C C C

1 CO	2.8608652 *	3.2626617	3.0098693	4.2803009
2 C	6.2313405	7.5523015	8.0350787	9.4279252
3 C	6.5825725	7.7692574	8.0502128	9.3985753
4 C	5.7572175	6.7964884	6.9393242	8.2426204
5 C	4.3502980	5.4062856	5.6352798	6.9759356
6 C	3.7321502	5.0251529	5.5520707	6.9544254
7 C	4.9331889	6.3080099	6.9246413	8.3291118
8 C	5.1572675	6.5907933	7.4043696	8.7886232
9 C	4.3491139	5.7614641	6.7292973	8.0610954
10 C	2.9263889 *	4.3324066	5.3171708	6.6433900
11 C	2.4460358 *	3.8350753	4.5891749	5.9856727
12 N	1.3320424 *	2.5073831 *	3.1498927	4.5509641
13 C	0.0000000	1.4668112 *	2.6057741 *	3.8843256
14 C	1.4668112 *	0.0000000	1.4378240 *	2.5010957 *
15 C	2.6057741 *	1.4378240 *	0.0000000	1.4063777 *
16 C	3.8843256	2.5010957 *	1.4063777 *	0.0000000
17 C	4.3440553	2.8823158 *	2.4408888 *	1.4282483 *
18 C	3.7932354	2.4974685 *	2.8243356 *	2.4724733 *
19 C	2.4702124 *	1.4429015 *	2.4457212 *	2.8460092 *
20 O	3.0485303	2.5035282 *	1.4656674 *	2.4585869 *
21 N	3.9821640	4.7041901	4.6922327	5.9305500
22 H	7.1265041	8.4896599	9.0338393	10.4315669
23 H	7.6706505	8.8303889	9.0514053	10.3765599
24 H	6.4053350	7.2929524	7.2671173	8.4857021
25 H	6.2435688	7.6784397	8.4995170	9.8800226
26 H	5.0097221	6.3595148	7.4151329	8.6860246
27 H	2.6477075 *	3.8984283	5.0129525	6.2330556
28 H	1.1083718 *	2.1770316 *	3.5328707	4.6747750
29 H	4.7956173	3.5034518	2.1944142 *	1.1068665 *
30 H	5.4489969	3.9875306	3.4394205	2.1915304 *
31 H	4.6571517	3.4930569	3.9284833	3.4743355
32 H	2.6424700 *	2.1983453 *	3.4511338	3.9520971

33 H	4.0169414	3.3305833	2.0453554 *	2.5065451 *
34 H	3.8414982	4.5449207	4.6914508	5.8938191
35 H	4.9436593	5.5218034	5.3076226	6.4319863

C C C O

1 CO	5.4403565	5.6094029	4.6968970	1.9513445 *
2 C	10.3358120	10.0087956	8.6961791	7.2633565
3 C	10.4219958	10.2485973	9.0127784	7.1093342
4 C	9.3163854	9.2487989	8.0930459	5.9397182
5 C	7.9905492	7.8670477	6.6926656	4.7564479
6 C	7.8146672	7.4881303	6.1960474	4.9285792
7 C	9.1408958	8.7252644	7.3854025	6.3231016
8 C	9.4413242	8.8603650	7.4816213	7.0183464
9 C	8.5582251	7.8599108	6.4829343	6.5900375
10 C	7.1395536	6.4761958	5.1034671	5.2724204
11 C	6.6903151	6.2331582	4.8998369	4.2871192
12 N	5.3107851	4.9858417	3.7430480	2.9386641 *
13 C	4.3440553	3.7932354	2.4702124 *	3.0485303
14 C	2.8823158 *	2.4974685 *	1.4429015 *	2.5035282 *
15 C	2.4408888 *	2.8243356 *	2.4457212 *	1.4656674 *
16 C	1.4282483 *	2.4724733 *	2.8460092 *	2.4585869 *
17 C	0.0000000	1.4231974 *	2.4561040 *	3.7696815
18 C	1.4231974 *	0.0000000	1.4159419 *	4.2897757
19 C	2.4561040 *	1.4159419 *	0.0000000	3.7954970
20 O	3.7696815	4.2897757	3.7954970	0.0000000
21 N	7.0054406	7.0429770	6.0229334	3.7571193
22 H	11.3032423	10.9186054	9.5794729	8.2968082
23 H	11.4386165	11.3073487	10.0887894	8.0450210
24 H	9.6256285	9.6812271	8.6161611	6.1690315
25 H	10.5220017	9.9147908	8.5321253	8.0934857
26 H	9.0546269	8.2513780	6.8996681	7.4122856
27 H	6.5539322	5.7787783	4.4369680	5.2390258
28 H	4.8542824	3.9982594	2.5832941 *	4.1424978
29 H	2.2005904 *	3.4736547	3.9528507	2.6846889 *
30 H	1.1052583 *	2.2012075 *	3.4614944	4.6483512
31 H	2.1975859 *	1.1041487 *	2.1872951 *	5.3939090
32 H	3.4574647	2.1859348 *	1.1061143 *	4.6935755
33 H	3.9272140	4.7289514	4.4871486	0.9918268 *
34 H	6.8305891	6.7572414	5.7276821	4.0185671
35 H	7.5903042	7.7698517	6.8520877	4.2238421

N H H H

1 CO	1.9775949 *	6.4297236	6.1126007	4.3363780
2 C	4.3426279	1.1051586 *	2.1865819 *	3.4391000

3 C	3.8152117	2.1804203 *	1.1041682 *	2.1942586 *
4 C	2.4748171 *	3.4518472	2.2013413 *	1.1078770 *
5 C	1.5094333 *	3.9437213	3.4664813	2.1827546 *
6 C	2.5928340 *	3.5192749	4.0267044	3.5072687
7 C	3.8871350	2.1959069 *	3.4862074	3.9525055
8 C	5.1108865	2.6785002 *	4.6701385	5.3953417
9 C	5.3878059	4.0777746	5.9309712	6.2667227
10 C	4.5647650	4.8911379	6.2581953	6.0076445
11 C	3.1555416	4.6911987	5.4873320	4.8017983
12 N	2.8978360 *	5.9974728	6.4028969	5.1724257
13 C	3.9821640	7.1265041	7.6706505	6.4053350
14 C	4.7041901	8.4896599	8.8303889	7.2929524
15 C	4.6922327	9.0338393	9.0514053	7.2671173
16 C	5.9305500	10.4315669	10.3765599	8.4857021
17 C	7.0054406	11.3032423	11.4386165	9.6256285
18 C	7.0429770	10.9186054	11.3073487	9.6812271
19 C	6.0229334	9.5794729	10.0887894	8.6161611
20 O	3.7571193	8.2968082	8.0450210	6.1690315
21 N	0.0000000	5.4468641	4.6752893	2.6527007 *
22 H	5.4468641	0.0000000	2.5312095 *	4.3606211
23 H	4.6752893	2.5312095 *	0.0000000	2.5189672 *
24 H	2.6527007 *	4.3606211	2.5189672 *	0.0000000
25 H	6.0559772	2.3978667 *	4.7796917	5.9744531
26 H	6.4713637	4.7756924	6.8512493	7.3476624
27 H	5.2582325	5.9653421	7.3475612	6.9666431
28 H	4.7315644	7.1936995	8.0286468	7.0068181
29 H	6.2604739	10.9534367	10.7000320	8.6965730
30 H	7.9849678	12.3885068	12.4673585	10.5879850
31 H	8.0449417	11.7572538	12.2528982	10.6794990
32 H	6.4120367	9.4613216	10.1931131	8.9176490
33 H	4.3757508	8.9836723	8.5714149	6.6114435
34 H	1.0440356 *	5.8553369	5.1843315	3.2182781
35 H	1.0394564 *	5.8211874	4.5850845	2.2126858 *

H H H H

1 CO	6.4899892	6.2779443	4.5248093	3.8768884
2 C	2.6802211 *	4.6678319	5.3912533	6.3997620
3 C	4.0796668	5.9297995	6.2678685	6.9303997
4 C	4.8899422	6.2530667	6.0088237	6.2650043
5 C	4.6715672	5.4693650	4.8032048	4.8888227
6 C	3.5170904	4.0176955	3.5053547	4.0397899
7 C	2.1968646 *	3.4839347	3.9500584	5.0266949
8 C	1.1049637 *	2.1844830 *	3.4302896	4.9868562
9 C	2.1805755 *	1.1043048 *	2.1811384 *	3.9956525
10 C	3.4527487	2.1980481 *	1.1042267 *	2.6602526 *

11 C	3.9633301	3.4748158	2.1884480 *	2.6587608 *
12 N	5.4100480	4.6675142	2.6918618 *	2.0962409 *
13 C	6.2435688	5.0097221	2.6477075 *	1.1083718 *
14 C	7.6784397	6.3595148	3.8984283	2.1770316 *
15 C	8.4995170	7.4151329	5.0129525	3.5328707
16 C	9.8800226	8.6860246	6.2330556	4.6747750
17 C	10.5220017	9.0546269	6.5539322	4.8542824
18 C	9.9147908	8.2513780	5.7787783	3.9982594
19 C	8.5321253	6.8996681	4.4369680	2.5832941 *
20 O	8.0934857	7.4122856	5.2390258	4.1424978
21 N	6.0559772	6.4713637	5.2582325	4.7315644
22 H	2.3978667 *	4.7756924	5.9653421	7.1936995
23 H	4.7796917	6.8512493	7.3475612	8.0286468
24 H	5.9744531	7.3476624	6.9666431	7.0068181
25 H	0.0000000	2.5279824 *	4.3474757	6.0172393
26 H	2.5279824 *	0.0000000	2.5008765 *	4.4863698
27 H	4.3474757	2.5008765 *	0.0000000	2.1586277 *
28 H	6.0172393	4.4863698	2.1586277 *	0.0000000
29 H	10.5725406	9.5265186	7.1238505	5.6718173
30 H	11.6169364	10.1165182	7.6170904	5.9342418
31 H	10.6209139	8.8045510	6.3989162	4.6565612
32 H	8.2161984	6.4126750	4.0724780	2.2683982 *
33 H	8.8938547	8.2780752	6.1359624	5.1006108
34 H	6.3298842	6.5983774	5.3046655	4.4728169
35 H	6.7600983	7.3997743	6.2746043	5.7385214

H H H H

1 CO	4.6158890	6.4198202	6.6752192	5.2817819
2 C	9.9275836	11.4139201	10.8819922	8.6517222
3 C	9.7779438	11.4655070	11.1840574	9.1031861
4 C	8.5663877	10.3295072	10.2217041	8.3038560
5 C	7.3920473	9.0264534	8.8317074	6.9054654
6 C	7.5309945	8.8980735	8.3824990	6.2367206
7 C	8.9238870	10.2328945	9.5638096	7.2907588
8 C	9.4871559	10.5383605	9.5958223	7.2158772
9 C	8.8535836	9.6443089	8.5172088	6.1202611
10 C	7.4584034	8.2299461	7.1836913	4.8343034
11 C	6.6992825	7.7894348	7.0804210	4.8770709
12 N	5.2680980	6.4028461	5.9183612	3.9725057
13 C	4.7956173	5.4489969	4.6571517	2.6424700 *
14 C	3.5034518	3.9875306	3.4930569	2.1983453 *
15 C	2.1944142 *	3.4394205	3.9284833	3.4511338
16 C	1.1068665 *	2.1915304 *	3.4743355	3.9520971
17 C	2.2005904 *	1.1052583 *	2.1975859 *	3.4574647
18 C	3.4736547	2.2012075 *	1.1041487 *	2.1859348 *

19 C	3.9528507	3.4614944	2.1872951 *	1.1061143 *
20 O	2.6846889 *	4.6483512	5.3939090	4.6935755
21 N	6.2604739	7.9849678	8.0449417	6.4120367
22 H	10.9534367	12.3885068	11.7572538	9.4613216
23 H	10.7000320	12.4673585	12.2528982	10.1931131
24 H	8.6965730	10.5879850	10.6794990	8.9176490
25 H	10.5725406	11.6169364	10.6209139	8.2161984
26 H	9.5265186	10.1165182	8.8045510	6.4126750
27 H	7.1238505	7.6170904	6.3989162	4.0724780
28 H	5.6718173	5.9342418	4.6565612	2.2683982 *
29 H	0.0000000	2.5201070 *	4.3869136	5.0589396
30 H	2.5201070 *	0.0000000	2.5414472 *	4.3750287
31 H	4.3869136	2.5414472 *	0.0000000	2.5142179 *
32 H	5.0589396	4.3750287	2.5142179 *	0.0000000
33 H	2.3040701 *	4.6278208	5.8146592	5.4671027
34 H	6.3187301	7.8100957	7.6967413	6.0397162
35 H	6.6072799	8.5056089	8.7916864	7.3169919

H H H

1 CO	2.6570262 *	2.4996626 *	2.6221063 *
2 C	7.9492449	4.7781051	4.7378237
3 C	7.6978733	4.3295165	3.9173508
4 C	6.4973573	3.0626311	2.4859202 *
5 C	5.4296221	2.1118794 *	2.0888512 *
6 C	5.7272597	2.9592837 *	3.4244851
7 C	7.0967925	4.2447642	4.5635725
8 C	7.8398107	5.3713186	5.8895194
9 C	7.4586326	5.5496689	6.3034979
10 C	6.1733426	4.6763532	5.5569121
11 C	5.1871156	3.3269659	4.1533019
12 N	3.8904229	2.9950617 *	3.8864483
13 C	4.0169414	3.8414982	4.9436593
14 C	3.3305833	4.5449207	5.5218034
15 C	2.0453554 *	4.6914508	5.3076226
16 C	2.5065451 *	5.8938191	6.4319863
17 C	3.9272140	6.8305891	7.5903042
18 C	4.7289514	6.7572414	7.7698517
19 C	4.4871486	5.7276821	6.8520877
20 O	0.9918268 *	4.0185671	4.2238421
21 N	4.3757508	1.0440356 *	1.0394564 *
22 H	8.9836723	5.8553369	5.8211874
23 H	8.5714149	5.1843315	4.5850845
24 H	6.6114435	3.2182781	2.2126858 *
25 H	8.8938547	6.3298842	6.7600983
26 H	8.2780752	6.5983774	7.3997743

27 H	6.1359624	5.3046655	6.2746043
28 H	5.1006108	4.4728169	5.7385214
29 H	2.3040701 *	6.3187301	6.6072799
30 H	4.6278208	7.8100957	8.5056089
31 H	5.8146592	7.6967413	8.7916864
32 H	5.4671027	6.0397162	7.3169919
33 H	0.0000000	4.7198221	4.6549429
34 H	4.7198221	0.0000000	1.6673805 *
35 H	4.6549429	1.6673805 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.73 , TOTAL = 8297.0 SECONDS (138.3 MIN)
WALL CLOCK TIME: STEP = 0.74 , TOTAL = 7672.9 SECONDS (127.9 MIN)
CPU UTILIZATION: STEP = 98.58% , TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.13 , TOTAL = 8298.2 SECONDS (138.3 MIN)
WALL CLOCK TIME: STEP = 1.13 , TOTAL = 7674.0 SECONDS (127.9 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
INTEGRALS	SKIPPED				

-----START SECOND ORDER SCF-----

1	0	-284.636942602	-284.636942602	0.004435974	0.000294423	198313743
11320228						
2	1	-284.636948551	-0.000005948	0.000507297	0.000019872	145576504
15713320						
3	2	-284.636948533	0.000000018	0.000286932	0.000043662	129372071
16982635						
4	3	-284.636948650	-0.000000116	0.000084142	0.000019415	122764479
17493407						
5	4	-284.636948608	0.000000042	0.000060000	0.000040517	115627659
18052569						
6	5	-284.636948656	-0.000000049	0.000041403	0.000009169	109699835
18485061						

7 6	-284.636948624	0.000000033	0.000041187	0.000008059	104852921
18808414					
8 7	-284.636948629	-0.000000005	0.000104466	0.000006679	126796192
17283787					
9 8	-284.636948632	-0.000000003	0.000139808	0.000004833	155017252
15078008					
-----DISABLING FDIFF OPTION-----					
10 9	-284.636948653	-0.000000021	0.000113299	0.000006239	198315906
11320047					
11 10	-284.636948656	-0.000000003	0.000119035	0.000007473	198315994
11320037					
12 11	-284.636948658	-0.000000003	0.000079038	0.000006275	198316241
11320029					
13 12	-284.636948660	-0.000000001	0.000052544	0.000003351	198316208
11320033					
14 13	-284.636948660	-0.000000001	0.000037854	0.000002607	198316068
11320038					
15 14	-284.636948661	0.000000000	0.000014369	0.000002486	198316080
11320038					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 49.0 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 16.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.1
TIME TO SOLVE SCF EQUATIONS= 2.0 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369486607 AFTER 15 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6019180298
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998521546

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 51.98 , TOTAL = 8350.1 SECONDS (139.2 MIN)

WALL CLOCK TIME: STEP = 47.73 , TOTAL = 7721.8 SECONDS (128.7 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.69 , TOTAL = 8353.8 SECONDS (139.2 MIN)

WALL CLOCK TIME: STEP = 3.67 , TOTAL = 7725.4 SECONDS (128.8 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.86 , TOTAL = 8356.7 SECONDS (139.3 MIN)

WALL CLOCK TIME: STEP = 2.68 , TOTAL = 7728.1 SECONDS (128.8 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 93 ENERGY= -284.6369487

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000166	-0.0000008	-0.0000478
2 C	6.0	-0.0000324	-0.0000431	0.0000662
3 C	6.0	-0.0000334	0.0000703	-0.0000558
4 C	6.0	0.0000054	-0.0000222	-0.0000429
5 C	6.0	-0.0000190	-0.0001203	0.0000478
6 C	6.0	-0.0000386	-0.0000176	0.0000234
7 C	6.0	0.0000147	0.0000312	0.0000966
8 C	6.0	-0.0000539	-0.0001055	0.0000498
9 C	6.0	0.0000481	0.0000172	0.0000385
10 C	6.0	0.0000140	-0.0000243	0.0000372
11 C	6.0	-0.0000269	0.0000196	-0.0000338
12 N	7.0	0.0000823	0.0000735	0.0000387
13 C	6.0	-0.0000086	-0.0000029	0.0000022
14 C	6.0	0.0000085	0.0000157	-0.0000673
15 C	6.0	0.0000462	0.0000102	-0.0000214
16 C	6.0	0.0000246	0.0000032	0.0000926
17 C	6.0	0.0000095	0.0001003	0.0001648

18 C	6.0	0.0000655	-0.0000709	0.0000072
19 C	6.0	-0.0000595	0.0000242	-0.0001553
20 O	8.0	-0.0000227	0.0000364	-0.0001024
21 N	7.0	0.0000222	-0.0000868	0.0000192
22 H	1.0	-0.0000375	0.0001548	0.0000156
23 H	1.0	0.0000185	0.0000180	0.0000790
24 H	1.0	0.0000245	-0.0000028	-0.0001247
25 H	1.0	-0.0000397	-0.0000407	0.0000361
26 H	1.0	0.0000114	0.0000680	-0.0001456
27 H	1.0	0.0000323	0.0000261	0.0000204
28 H	1.0	0.0000387	-0.0000492	-0.0001233
29 H	1.0	-0.0000231	-0.0000121	-0.0000038
30 H	1.0	-0.0000184	-0.0000963	0.0000494
31 H	1.0	0.0000280	0.0000111	0.0000445
32 H	1.0	-0.0000553	0.0001733	0.0000311
33 H	1.0	-0.0000300	-0.0000530	-0.0000690
34 H	1.0	-0.0000682	-0.0000207	0.0000319
35 H	1.0	0.0000893	-0.0000840	0.0000009

MAXIMUM GRADIENT = 0.0001733 RMS GRADIENT = 0.0000603
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000021316
 PREDICTED ENERGY CHANGE WAS -0.0000015520 RATIO= 1.373
 GDIIS STEP HAS LENGTH = 0.023361
 RADIUS OF STEP TAKEN= 0.02336 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8356.7 SECONDS (139.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7728.1 SECONDS (128.8
 MIN)
 CPU UTILIZATION: STEP = 81.69%, TOTAL = 100.00%

INSERCH= 94

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1606218409	-1.7230128652	0.8845306424
C	6.0	4.9801086237	0.6203165409	0.5647384061
C	6.0	5.1790393479	-0.7186824540	0.2018383187
C	6.0	4.0402311181	-1.5348259817	-0.0946435709
C	6.0	2.7334210129	-1.0203739642	-0.0017678127
C	6.0	2.4671209874	0.3451777481	0.4335349928
C	6.0	3.6517268476	1.1740641378	0.6835583760
C	6.0	3.5093825728	2.5611399893	1.0592911358

C	6.0	2.2437726397	3.1423090031	1.2176336229
C	6.0	1.0758090827	2.3367548121	1.0399211358
C	6.0	1.1635799417	0.9818662729	0.6427469769
N	7.0	-0.0500805348	0.1830644375	0.5932649627
C	6.0	-1.2458736678	0.7046371532	0.3244141096
C	6.0	-2.5483241332	0.0397202924	0.4382322779
C	6.0	-2.8163631248	-1.2839424682	0.9315802444
C	6.0	-4.1148010425	-1.8096443952	1.0559501356
C	6.0	-5.2267352729	-0.9991866963	0.6732139221
C	6.0	-5.0158891906	0.3146371205	0.1684123408
C	6.0	-3.6987781027	0.8223093506	0.0566181070
O	8.0	-1.6935801474	-2.1392986756	1.3264345983
N	7.0	1.6231771533	-1.9503156785	-0.4271330740
H	1.0	5.8437917568	1.2795426745	0.7669546779
H	1.0	6.1954984605	-1.1419261596	0.1192544345
H	1.0	4.2006805801	-2.5771704251	-0.4338578262
H	1.0	4.4243451724	3.1559968232	1.2321951060
H	1.0	2.1395420720	4.2001276184	1.5172824938
H	1.0	0.0929526954	2.7839201799	1.2703267591
H	1.0	-1.2903444608	1.7540852133	-0.0293432436
H	1.0	-4.2839642602	-2.8333831552	1.4412463427
H	1.0	-6.2497258235	-1.4063210154	0.7699100195
H	1.0	-5.8750263708	0.9409343553	-0.1293995224
H	1.0	-3.5380461854	1.8487568001	-0.3229856373
H	1.0	-2.0106644886	-2.9545506982	1.7939276386
H	1.0	1.2537363902	-1.6697104066	-1.3624435135
H	1.0	2.0156555098	-2.9059104842	-0.5425505772

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3685112	5.1632609	4.0056915
2 C	5.3685112	0.0000000	1.4014950 *	2.4418832 *
3 C	5.1632609	1.4014950 *	0.0000000	1.4320880 *
4 C	4.0056915	2.4418832 *	1.4320880 *	0.0000000
5 C	2.8104309 *	2.8390843 *	2.4725538 *	1.4074940 *
6 C	3.1306146	2.5314072 *	2.9223249 *	2.5076009 *
7 C	4.5410637	1.4440750 *	2.4793603 *	2.8451045 *
8 C	5.4404692	2.4848366 *	3.7789171	4.2883916
9 C	5.3030021	3.7781282	4.9552887	5.1792785
10 C	4.1645441	4.2913301	5.1840697	5.0064132
11 C	2.8949534 *	3.8344093	4.3829420	3.8926349
12 N	1.9396809 *	5.0492382	5.3207196	4.4894337
13 C	2.8610216 *	6.2311894	6.5818212	5.7561887

14 C	3.2626368	7.5518472	7.7680888	6.7950138
15 C	3.0095574	8.0340368	8.0485094	6.9375041
16 C	4.2797349	9.4267376	9.3965512	8.2403847
17 C	5.4398709	10.3350965	10.4202218	9.3141388
18 C	5.6090204	10.0085207	10.2472159	9.2467847
19 C	4.6967087	8.6960946	9.0117361	8.0914295
20 O	1.9510607 *	7.2618027	7.1074444	5.9381346
21 N	1.9776745 *	4.3429193	3.8153219	2.4749406 *
22 H	6.4286534	1.1051783 *	2.1804027 *	3.4519347
23 H	6.1108956	2.1865790 *	1.1041487 *	2.2012042 *
24 H	4.3347212	3.4392769	2.1943730 *	1.1078322 *
25 H	6.4888322	2.6803071 *	4.0797473	4.8899758
26 H	6.2769494	4.6681052	5.9298929	6.2530486
27 H	4.5239212	5.3910415	6.2672299	6.0079713
28 H	3.8769421	6.3997614	6.9297151	6.2638835
29 H	4.6148890	9.9256916	9.7753020	8.5637280
30 H	6.4191891	11.4130862	11.4635172	10.3270122
31 H	6.6748572	10.8820301	11.1828626	10.2197323
32 H	5.2816455	8.6519409	9.1024593	8.3024731
33 H	2.6567222 *	7.9474204	7.6958233	6.4958184
34 H	2.4993266 *	4.7795506	4.3312164	3.0643210
35 H	2.6223954 *	4.7379688	3.9172795	2.4858399 *

C C C C

1 CO	2.8104309 *	3.1306146	4.5410637	5.4404692
2 C	2.8390843 *	2.5314072 *	1.4440750 *	2.4848366 *
3 C	2.4725538 *	2.9223249 *	2.4793603 *	3.7789171
4 C	1.4074940 *	2.5076009 *	2.8451045 *	4.2883916
5 C	0.0000000	1.4577845 *	2.4755840 *	3.8151284
6 C	1.4577845 *	0.0000000	1.4672612 *	2.5275222 *
7 C	2.4755840 *	1.4672612 *	0.0000000	1.4440971 *
8 C	3.8151284	2.5275222 *	1.4440971 *	0.0000000
9 C	4.3651603	2.9135268 *	2.4782170 *	1.4016413 *
10 C	3.8862716	2.5039633 *	2.8485428 *	2.4439730 *
11 C	2.6246459 *	1.4657289 *	2.4958927 *	2.8583919 *
12 N	3.0903412	2.5274687 *	3.8332246	4.3060656
13 C	4.3493499	3.7319496	4.9331366	5.1574324
14 C	5.4050191	5.0247404	6.3077376	6.5908332
15 C	5.6338895	5.5513319	6.9238356	7.4037847
16 C	6.9742283	6.9535859	8.3282740	8.7881706
17 C	7.9887507	7.8141017	9.1405807	9.4416490
18 C	7.8653051	7.4877676	8.7253400	8.8611906
19 C	6.6911939	6.1958077	7.3855744	7.4824104
20 O	4.7554656	4.9276086	6.3217062	7.0168590
21 N	1.5094266 *	2.5927362 *	3.8872096	5.1108179

22 H	3.9439773	3.5193909	2.1961852 *	2.6790705 *
23 H	3.4663239	4.0262947	3.4861188	4.6702876
24 H	2.1824682 *	3.5068102	3.9524334	5.3953332
25 H	4.6716124	3.5169999	2.1968155 *	1.1049466 *
26 H	5.4693549	4.0177674	3.4840865	2.1846051 *
27 H	4.8023902	3.5049052	3.9497857	3.4301837
28 H	4.8876449	4.0395325	5.0268004	4.9873682
29 H	7.3900601	7.5296669	8.9223830	9.4859383
30 H	9.0244872	8.8974330	10.2325270	10.5387231
31 H	8.8299709	8.3823173	9.5642186	9.5971445
32 H	6.9040852	6.2365941	7.2911712	7.2169544
33 H	5.4288036	5.7262063	7.0951431	7.8379496
34 H	2.1124731 *	2.9593268 *	4.2454135	5.3714834
35 H	2.0887511 *	3.4243450	4.5635803	5.8894616

C C C N

1 CO	5.3030021	4.1645441	2.8949534 *	1.9396809 *
2 C	3.7781282	4.2913301	3.8344093	5.0492382
3 C	4.9552887	5.1840697	4.3829420	5.3207196
4 C	5.1792785	5.0064132	3.8926349	4.4894337
5 C	4.3651603	3.8862716	2.6246459 *	3.0903412
6 C	2.9135268 *	2.5039633 *	1.4657289 *	2.5274687 *
7 C	2.4782170 *	2.8485428 *	2.4958927 *	3.8332246
8 C	1.4016413 *	2.4439730 *	2.8583919 *	4.3060656
9 C	0.0000000	1.4299084 *	2.4829063 *	3.7958829
10 C	1.4299084 *	0.0000000	1.4146286 *	2.4709333 *
11 C	2.4829063 *	1.4146286 *	0.0000000	1.4537897 *
12 N	3.7958829	2.4709333 *	1.4537897 *	0.0000000
13 C	4.3494501	2.9267677 *	2.4461518 *	1.3320060 *
14 C	5.7617458	4.3327519	3.8350616	2.5071505 *
15 C	6.7289303	5.3169720	4.5888191	3.1494263
16 C	8.0609828	6.6434416	5.9853634	4.5504856
17 C	8.5590226	7.1403813	6.6904131	5.3105427
18 C	7.8612520	6.4774436	6.2334603	4.9856862
19 C	6.4841549	5.1046168	4.9001562	3.7429424
20 O	6.5886239	5.2713055	4.2863111	2.9380264 *
21 N	5.3875061	4.5640808	3.1549269	2.8969491 *
22 H	4.0783756	4.8914075	4.6913134	5.9975131
23 H	5.9310408	6.2578006	5.4867789	6.4021514
24 H	6.2665268	6.0069549	4.8010208	5.1713487
25 H	2.1806641 *	3.4526542	3.9631910	5.4099024
26 H	1.1043703 *	2.1980810 *	3.4748411	4.6674460
27 H	2.1811111 *	1.1041061 *	2.1880350 *	2.6913420 *
28 H	3.9965110	2.6611112 *	2.6589043 *	2.0961875 *
29 H	8.8526972	7.4577851	6.6984675	5.2672384

30 H	9.6452065	8.2308556	7.7895257	6.4025738
31 H	8.5191224	7.1853837	7.0809508	5.9183279
32 H	6.1217819	4.8356300	4.8774406	3.9723986
33 H	7.4568122	6.1719332	5.1861762	3.8897441
34 H	5.5490991	4.6749094	3.3256241	2.9929098 *
35 H	6.3032725	5.5563538	4.1528028	3.8857571

C C C C

1 CO	2.8610216 *	3.2626368	3.0095574	4.2797349
2 C	6.2311894	7.5518472	8.0340368	9.4267376
3 C	6.5818212	7.7680888	8.0485094	9.3965512
4 C	5.7561887	6.7950138	6.9375041	8.2403847
5 C	4.3493499	5.4050191	5.6338895	6.9742283
6 C	3.7319496	5.0247404	5.5513319	6.9535859
7 C	4.9331366	6.3077376	6.9238356	8.3282740
8 C	5.1574324	6.5908332	7.4037847	8.7881706
9 C	4.3494501	5.7617458	6.7289303	8.0609828
10 C	2.9267677 *	4.3327519	5.3169720	6.6434416
11 C	2.4461518 *	3.8350616	4.5888191	5.9853634
12 N	1.3320060 *	2.5071505 *	3.1494263	4.5504856
13 C	0.0000000	1.4667809 *	2.6056740 *	3.8842632
14 C	1.4667809 *	0.0000000	1.4378179 *	2.5011148 *
15 C	2.6056740 *	1.4378179 *	0.0000000	1.4063326 *
16 C	3.8842632	2.5011148 *	1.4063326 *	0.0000000
17 C	4.3441842	2.8824348 *	2.4408468 *	1.4281899 *
18 C	3.7933433	2.4974506 *	2.8241453 *	2.4722975 *
19 C	2.4702837 *	1.4427818 *	2.4455085 *	2.8458602 *
20 O	3.0483532	2.5035204 *	1.4656691 *	2.4584842 *
21 N	3.9805842	4.7021828	4.6903809	5.9282137
22 H	7.1266903	8.4895717	9.0330969	10.4307318
23 H	7.6698048	8.8290695	9.0495133	10.3742721
24 H	6.4039199	7.2909343	7.2646928	8.4826799
25 H	6.2437659	7.6785203	8.4988992	9.8795583
26 H	5.0102324	6.3599865	7.4147871	8.6860230
27 H	2.6477584 *	3.8986353	5.0126215	6.2331360
28 H	1.1083606 *	2.1771970 *	3.5329477	4.6749958
29 H	4.7952994	3.5033138	2.1941693 *	1.1068471 *
30 H	5.4491419	3.9876585	3.4393449	2.1914362 *
31 H	4.6573424	3.4930417	3.9282535	3.4740654
32 H	2.6423836 *	2.1980936 *	3.4508791	3.9519627
33 H	4.0167189	3.3305625	2.0454156 *	2.5065538 *
34 H	3.8381070	4.5409526	4.6879710	5.8897711
35 H	4.9421913	5.5198357	5.3058690	6.4295802

C C C O

1 CO	5.4398709	5.6090204	4.6967087	1.9510607 *
2 C	10.3350965	10.0085207	8.6960946	7.2618027
3 C	10.4202218	10.2472159	9.0117361	7.1074444
4 C	9.3141388	9.2467847	8.0914295	5.9381346
5 C	7.9887507	7.8653051	6.6911939	4.7554656
6 C	7.8141017	7.4877676	6.1958077	4.9276086
7 C	9.1405807	8.7253400	7.3855744	6.3217062
8 C	9.4416490	8.8611906	7.4824104	7.0168590
9 C	8.5590226	7.8612520	6.4841549	6.5886239
10 C	7.1403813	6.4774436	5.1046168	5.2713055
11 C	6.6904131	6.2334603	4.9001562	4.2863111
12 N	5.3105427	4.9856862	3.7429424	2.9380264 *
13 C	4.3441842	3.7933433	2.4702837 *	3.0483532
14 C	2.8824348 *	2.4974506 *	1.4427818 *	2.5035204 *
15 C	2.4408468 *	2.8241453 *	2.4455085 *	1.4656691 *
16 C	1.4281899 *	2.4722975 *	2.8458602 *	2.4584842 *
17 C	0.0000000	1.4231703 *	2.4561538 *	3.7695806
18 C	1.4231703 *	0.0000000	1.4159840 *	4.2895867
19 C	2.4561538 *	1.4159840 *	0.0000000	3.7953096
20 O	3.7695806	4.2895867	3.7953096	0.0000000
21 N	7.0026217	7.0400204	6.0203548	3.7565400
22 H	11.3030068	10.9188812	9.5798893	8.2953884
23 H	11.4365497	11.3057156	10.0875593	8.0429843
24 H	9.6224638	9.6783490	8.6138538	6.1670634
25 H	10.5224220	9.9157947	8.5330657	8.0918506
26 H	9.0557917	8.2532832	6.9013897	7.4106393
27 H	6.5549616	5.7802975	4.4382686	5.2376456
28 H	4.8548188	3.9988500	2.5838243 *	4.1423629
29 H	2.2006744 *	3.4735936	3.9526859	2.6842177 *
30 H	1.1052684 *	2.2013290 *	3.4616344	4.6481652
31 H	2.1973938 *	1.1041091 *	2.1874028 *	5.3936797
32 H	3.4575810	2.1860959 *	1.1061321 *	4.6933174
33 H	3.9271566	4.7287699	4.4869415	0.9918307 *
34 H	6.8256880	6.7519893	5.7228750	4.0171200
35 H	7.5872197	7.7665962	6.8493341	4.2236511

N H H H

1 CO	1.9776745 *	6.4286534	6.1108956	4.3347212
2 C	4.3429193	1.1051783 *	2.1865790 *	3.4392769
3 C	3.8153219	2.1804027 *	1.1041487 *	2.1943730 *
4 C	2.4749406 *	3.4519347	2.2012042 *	1.1078322 *
5 C	1.5094266 *	3.9439773	3.4663239	2.1824682 *
6 C	2.5927362 *	3.5193909	4.0262947	3.5068102
7 C	3.8872096	2.1961852 *	3.4861188	3.9524334

8 C	5.1108179	2.6790705 *	4.6702876	5.3953332
9 C	5.3875061	4.0783756	5.9310408	6.2665268
10 C	4.5640808	4.8914075	6.2578006	6.0069549
11 C	3.1549269	4.6913134	5.4867789	4.8010208
12 N	2.8969491 *	5.9975131	6.4021514	5.1713487
13 C	3.9805842	7.1266903	7.6698048	6.4039199
14 C	4.7021828	8.4895717	8.8290695	7.2909343
15 C	4.6903809	9.0330969	9.0495133	7.2646928
16 C	5.9282137	10.4307318	10.3742721	8.4826799
17 C	7.0026217	11.3030068	11.4365497	9.6224638
18 C	7.0400204	10.9188812	11.3057156	9.6783490
19 C	6.0203548	9.5798893	10.0875593	8.6138538
20 O	3.7565400	8.2953884	8.0429843	6.1670634
21 N	0.0000000	5.4471477	4.6752706	2.6526432 *
22 H	5.4471477	0.0000000	2.5311508 *	4.3607340
23 H	4.6752706	2.5311508 *	0.0000000	2.5189596 *
24 H	2.6526432 *	4.3607340	2.5189596 *	0.0000000
25 H	6.0559343	2.3984073 *	4.7799334	5.9745263
26 H	6.4711156	4.7764290	6.8514818	7.3475853
27 H	5.2569902	5.9656253	7.3469927	6.9655557
28 H	4.7296333	7.1941074	8.0278769	7.0053382
29 H	6.2581922	10.9518158	10.6970944	8.6931501
30 H	7.9819449	12.3881815	12.4650257	10.5844669
31 H	8.0418299	11.7579252	12.2514369	10.6765925
32 H	6.4095261	9.4620747	10.1922349	8.9156613
33 H	4.3756604	8.9819098	8.5692035	6.6095576
34 H	1.0440457 *	5.8567089	5.1860387	3.2202849
35 H	1.0394816 *	5.8212928	4.5848352	2.2122881 *

H H H H

1 CO	6.4888322	6.2769494	4.5239212	3.8769421
2 C	2.6803071 *	4.6681052	5.3910415	6.3997614
3 C	4.0797473	5.9298929	6.2672299	6.9297151
4 C	4.8899758	6.2530486	6.0079713	6.2638835
5 C	4.6716124	5.4693549	4.8023902	4.8876449
6 C	3.5169999	4.0177674	3.5049052	4.0395325
7 C	2.1968155 *	3.4840865	3.9497857	5.0268004
8 C	1.1049466 *	2.1846051 *	3.4301837	4.9873682
9 C	2.1806641 *	1.1043703 *	2.1811111 *	3.9965110
10 C	3.4526542	2.1980810 *	1.1041061 *	2.6611112 *
11 C	3.9631910	3.4748411	2.1880350 *	2.6589043 *
12 N	5.4099024	4.6674460	2.6913420 *	2.0961875 *
13 C	6.2437659	5.0102324	2.6477584 *	1.1083606 *
14 C	7.6785203	6.3599865	3.8986353	2.1771970 *
15 C	8.4988992	7.4147871	5.0126215	3.5329477

16 C	9.8795583	8.6860230	6.2331360	4.6749958
17 C	10.5224220	9.0557917	6.5549616	4.8548188
18 C	9.9157947	8.2532832	5.7802975	3.9988500
19 C	8.5330657	6.9013897	4.4382686	2.5838243 *
20 O	8.0918506	7.4106393	5.2376456	4.1423629
21 N	6.0559343	6.4711156	5.2569902	4.7296333
22 H	2.3984073 *	4.7764290	5.9656253	7.1941074
23 H	4.7799334	6.8514818	7.3469927	8.0278769
24 H	5.9745263	7.3475853	6.9655557	7.0053382
25 H	0.0000000	2.5282027 *	4.3475115	6.0178495
26 H	2.5282027 *	0.0000000	2.5010315 *	4.4876827
27 H	4.3475115	2.5010315 *	0.0000000	2.1594474 *
28 H	6.0178495	4.4876827	2.1594474 *	0.0000000
29 H	10.5712359	9.5256228	7.1232515	5.6717951
30 H	11.6174112	10.1178381	7.6182747	5.9348494
31 H	10.6224995	8.8072249	6.4009847	4.6573097
32 H	8.2174899	6.4148687	4.0739818	2.2687776 *
33 H	8.8917762	8.2758787	6.1342816	5.1004343
34 H	6.3302733	6.5979142	5.3022376	4.4689910
35 H	6.7600465	7.3995971	6.2735543	5.7365998

H H H H

1 CO	4.6148890	6.4191891	6.6748572	5.2816455
2 C	9.9256916	11.4130862	10.8820301	8.6519409
3 C	9.7753020	11.4635172	11.1828626	9.1024593
4 C	8.5637280	10.3270122	10.2197323	8.3024731
5 C	7.3900601	9.0244872	8.8299709	6.9040852
6 C	7.5296669	8.8974330	8.3823173	6.2365941
7 C	8.9223830	10.2325270	9.5642186	7.2911712
8 C	9.4859383	10.5387231	9.5971445	7.2169544
9 C	8.8526972	9.6452065	8.5191224	6.1217819
10 C	7.4577851	8.2308556	7.1853837	4.8356300
11 C	6.6984675	7.7895257	7.0809508	4.8774406
12 N	5.2672384	6.4025738	5.9183279	3.9723986
13 C	4.7952994	5.4491419	4.6573424	2.6423836 *
14 C	3.5033138	3.9876585	3.4930417	2.1980936 *
15 C	2.1941693 *	3.4393449	3.9282535	3.4508791
16 C	1.1068471 *	2.1914362 *	3.4740654	3.9519627
17 C	2.2006744 *	1.1052684 *	2.1973938 *	3.4575810
18 C	3.4735936	2.2013290 *	1.1041091 *	2.1860959 *
19 C	3.9526859	3.4616344	2.1874028 *	1.1061321 *
20 O	2.6842177 *	4.6481652	5.3936797	4.6933174
21 N	6.2581922	7.9819449	8.0418299	6.4095261
22 H	10.9518158	12.3881815	11.7579252	9.4620747
23 H	10.6970944	12.4650257	12.2514369	10.1922349

24 H	8.6931501	10.5844669	10.6765925	8.9156613
25 H	10.5712359	11.6174112	10.6224995	8.2174899
26 H	9.5256228	10.1178381	8.8072249	6.4148687
27 H	7.1232515	7.6182747	6.4009847	4.0739818
28 H	5.6717951	5.9348494	4.6573097	2.2687776 *
29 H	0.0000000	2.5202018 *	4.3867847	5.0587887
30 H	2.5202018 *	0.0000000	2.5414101 *	4.3752896
31 H	4.3867847	2.5414101 *	0.0000000	2.5145762 *
32 H	5.0587887	4.3752896	2.5145762 *	0.0000000
33 H	2.3036835 *	4.6276634	5.8144031	5.4668071
34 H	6.3151358	7.8050145	7.6912367	6.0350033
35 H	6.6049920	8.5022262	8.7881608	7.3142787

H H H

1 CO	2.6567222 *	2.4993266 *	2.6223954 *
2 C	7.9474204	4.7795506	4.7379688
3 C	7.6958233	4.3312164	3.9172795
4 C	6.4958184	3.0643210	2.4858399 *
5 C	5.4288036	2.1124731 *	2.0887511 *
6 C	5.7262063	2.9593268 *	3.4243450
7 C	7.0951431	4.2454135	4.5635803
8 C	7.8379496	5.3714834	5.8894616
9 C	7.4568122	5.5490991	6.3032725
10 C	6.1719332	4.6749094	5.5563538
11 C	5.1861762	3.3256241	4.1528028
12 N	3.8897441	2.9929098 *	3.8857571
13 C	4.0167189	3.8381070	4.9421913
14 C	3.3305625	4.5409526	5.5198357
15 C	2.0454156 *	4.6879710	5.3058690
16 C	2.5065538 *	5.8897711	6.4295802
17 C	3.9271566	6.8256880	7.5872197
18 C	4.7287699	6.7519893	7.7665962
19 C	4.4869415	5.7228750	6.8493341
20 O	0.9918307 *	4.0171200	4.2236511
21 N	4.3756604	1.0440457 *	1.0394816 *
22 H	8.9819098	5.8567089	5.8212928
23 H	8.5692035	5.1860387	4.5848352
24 H	6.6095576	3.2202849	2.2122881 *
25 H	8.8917762	6.3302733	6.7600465
26 H	8.2758787	6.5979142	7.3995971
27 H	6.1342816	5.3022376	6.2735543
28 H	5.1004343	4.4689910	5.7365998
29 H	2.3036835 *	6.3151358	6.6049920
30 H	4.6276634	7.8050145	8.5022262
31 H	5.8144031	7.6912367	8.7881608

-----DISABLING FDIFF OPTION-----

10	9	-284.636951106	-0.000000015	0.000147503	0.000009892	198347051
11317424						
11	10	-284.636951111	-0.000000005	0.000150774	0.000010055	198346902
11317430						
12	11	-284.636951116	-0.000000005	0.000106216	0.000007276	198347075
11317429						
13	12	-284.636951119	-0.000000002	0.000050709	0.000004016	198347055
11317423						
14	13	-284.636951120	-0.000000001	0.000021490	0.000002319	198347096
11317426						
15	14	-284.636951120	0.000000000	0.000013958	0.000001541	198347080
11317425						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 50.3 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 16.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 1.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369511200 AFTER 15 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6022643637
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998525024

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 52.77 , TOTAL = 8411.1 SECONDS (140.2 MIN)
WALL CLOCK TIME: STEP = 48.44 , TOTAL = 7778.2 SECONDS (129.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.78 , TOTAL = 8414.9 SECONDS (140.2 MIN)

WALL CLOCK TIME: STEP = 3.75 , TOTAL = 7781.9 SECONDS (129.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.85 , TOTAL = 8417.7 SECONDS (140.3 MIN)

WALL CLOCK TIME: STEP = 2.69 , TOTAL = 7784.6 SECONDS (129.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 94 ENERGY= -284.6369511

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000546	0.0000027	-0.0000090
2 C	6.0	0.0000220	-0.0000315	0.0001263
3 C	6.0	-0.0000532	0.0000772	-0.0000008
4 C	6.0	-0.0000125	0.0000243	-0.0000574
5 C	6.0	0.0000292	-0.0000820	-0.0000024
6 C	6.0	-0.0000080	-0.0000521	0.0000296
7 C	6.0	-0.0000496	-0.0000188	0.0001166
8 C	6.0	-0.0000484	-0.0000724	0.0000355
9 C	6.0	-0.0000261	-0.0000078	-0.0000003
10 C	6.0	0.0000616	-0.0000279	0.0000406
11 C	6.0	0.0000439	0.0000221	-0.0000237
12 N	7.0	0.0000221	0.0000254	0.0000583
13 C	6.0	-0.0000431	0.0000053	-0.0000062
14 C	6.0	0.0000079	0.0000860	-0.0000732
15 C	6.0	0.0000053	0.0000084	-0.0000490
16 C	6.0	-0.0000054	0.0000355	0.0000446
17 C	6.0	0.0000168	0.0001057	0.0001544
18 C	6.0	0.0000624	-0.0000775	0.0000056
19 C	6.0	-0.0000089	-0.0000564	-0.0001388
20 O	8.0	0.0000084	0.0000874	-0.0001116
21 N	7.0	-0.0000111	-0.0000454	-0.0000539
22 H	1.0	-0.0000084	0.0001559	-0.0000175
23 H	1.0	0.0000014	0.0000247	0.0000487
24 H	1.0	-0.0000206	0.0000078	-0.0000765

25 H	1.0	-0.0000433	-0.0000519	0.0000202
26 H	1.0	0.0000060	0.0000990	-0.0000821
27 H	1.0	0.0000963	-0.0000279	-0.0000258
28 H	1.0	0.0000577	-0.0000694	-0.0001295
29 H	1.0	0.0000055	0.0000082	0.0000206
30 H	1.0	-0.0000195	-0.0001179	0.0000580
31 H	1.0	0.0000328	-0.0000243	0.0000593
32 H	1.0	-0.0000240	0.0001879	0.0000538
33 H	1.0	-0.0000180	-0.0000587	-0.0000676
34 H	1.0	-0.0001433	-0.0000363	0.0000261
35 H	1.0	0.0001186	-0.0001056	0.0000269

MAXIMUM GRADIENT = 0.0001879 RMS GRADIENT = 0.0000623
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000024593
 PREDICTED ENERGY CHANGE WAS -0.0000017785 RATIO= 1.383
 GDIIS STEP HAS LENGTH = 0.039364
 RADIUS OF STEP TAKEN= 0.03936 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 8417.8 SECONDS (140.3 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7784.6 SECONDS (129.7
 MIN)
 CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 95

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1617523234	-1.7216529554	0.8881031676
C	6.0	4.9800729959	0.6193132007	0.5638689034
C	6.0	5.1775731254	-0.7201152396	0.2018179735
C	6.0	4.0380323355	-1.5349141830	-0.0953476226
C	6.0	2.7317951611	-1.0189499301	-0.0037222074
C	6.0	2.4670765064	0.3463206121	0.4327321100
C	6.0	3.6522383051	1.1744128438	0.6826832943
C	6.0	3.5106256581	2.5613331424	1.0592166769
C	6.0	2.2450955102	3.1425129094	1.2188926323
C	6.0	1.0766948971	2.3375216467	1.0409555305
C	6.0	1.1639430149	0.9828374515	0.6433605724
N	7.0	-0.0498077809	0.1839892541	0.5947394368
C	6.0	-1.2454424335	0.7054065120	0.3251415788
C	6.0	-2.5477568335	0.0398083312	0.4391604889
C	6.0	-2.8152764272	-1.2834675470	0.9336552798

C	6.0	-4.1133736493	-1.8103085352	1.0562275341
C	6.0	-5.2255678274	-1.0015284906	0.6705803725
C	6.0	-5.0153145585	0.3123064974	0.1655122046
C	6.0	-3.6984077145	0.8208674480	0.0551891858
O	8.0	-1.6923484613	-2.1373240352	1.3313422547
N	7.0	1.6202716451	-1.9473710944	-0.4285024070
H	1.0	5.8447529485	1.2770258526	0.7662206425
H	1.0	6.1936049497	-1.1442788046	0.1191493763
H	1.0	4.1973000382	-2.5776144139	-0.4337401308
H	1.0	4.4259809680	3.1556093589	1.2322845417
H	1.0	2.1411005961	4.1995656645	1.5211507444
H	1.0	0.0938772256	2.7841843887	1.2722428314
H	1.0	-1.2900811245	1.7546485267	-0.0294623403
H	1.0	-4.2816732071	-2.8336277850	1.4428883618
H	1.0	-6.2483597201	-1.4090534489	0.7669865981
H	1.0	-5.8748317422	0.9372049700	-0.1342737810
H	1.0	-3.5375183031	1.8461531587	-0.3269232808
H	1.0	-2.0094702433	-2.9519160605	1.8000432276
H	1.0	1.2477365379	-1.6648986738	-1.3620816695
H	1.0	2.0117022845	-2.9028955722	-0.5472050812

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3666996	5.1606708	4.0034477
2 C	5.3666996	0.0000000	1.4014834 *	2.4418646 *
3 C	5.1606708	1.4014834 *	0.0000000	1.4320468 *
4 C	4.0034477	2.4418646 *	1.4320468 *	0.0000000
5 C	2.8096733 *	2.8391581 *	2.4725248 *	1.4074338 *
6 C	3.1302391	2.5311802 *	2.9218827 *	2.5071527 *
7 C	4.5401417	1.4440905 *	2.4793375 *	2.8451049 *
8 C	5.4395039	2.4851733 *	3.7791203	4.2884051
9 C	5.3018723	3.7783190	4.9551753	5.1788198
10 C	4.1638182	4.2914115	5.1836761	5.0056432
11 C	2.8945731 *	3.8342296	4.3822636	3.8916773
12 N	1.9396629 *	5.0487781	5.3195210	4.4879044
13 C	2.8614228 *	6.2306858	6.5804597	5.7542118
14 C	3.2627803	7.5511324	7.7662435	6.7925009
15 C	3.0094487	8.0327324	8.0460298	6.9346891
16 C	4.2793490	9.4252984	9.3936270	8.2369525
17 C	5.4395877	10.3340999	10.4174984	9.3105013
18 C	5.6090240	10.0080325	10.2451048	9.2435579
19 C	4.6967000	8.6957120	9.0099480	8.0885643
20 O	1.9511363 *	7.2601152	7.1049369	5.9359587

21 N	1.9777961 *	4.3429177	3.8154757	2.4752130 *
22 H	6.4267742	1.1050808 *	2.1799660 *	3.4516005
23 H	6.1080191	2.1864794 *	1.1041148 *	2.2011584 *
24 H	4.3319263	3.4392301	2.1943502 *	1.1077452 *
25 H	6.4876648	2.6807827 *	4.0801953	4.8902068
26 H	6.2753007	4.6684431	5.9299296	6.2526535
27 H	4.5226917	5.3910454	6.2665692	6.0067692
28 H	3.8774243	6.3996766	6.9288165	6.2621368
29 H	4.6139251	9.9234782	9.7716187	8.5598088
30 H	6.4188725	11.4119775	11.4606279	10.3232419
31 H	6.6749627	10.8819766	11.1810251	10.2165436
32 H	5.2811110	8.6514744	9.1004461	8.2990488
33 H	2.6569512 *	7.9457863	7.6934291	6.4940502
34 H	2.4991828 *	4.7809251	4.3338220	3.0671260
35 H	2.6225481 *	4.7383188	3.9176911	2.4862747 *

C C C C

1 CO	2.8096733 *	3.1302391	4.5401417	5.4395039
2 C	2.8391581 *	2.5311802 *	1.4440905 *	2.4851733 *
3 C	2.4725248 *	2.9218827 *	2.4793375 *	3.7791203
4 C	1.4074338 *	2.5071527 *	2.8451049 *	4.2884051
5 C	0.0000000	1.4575774 *	2.4757238 *	3.8150810
6 C	1.4575774 *	0.0000000	1.4672494 *	2.5274015 *
7 C	2.4757238 *	1.4672494 *	0.0000000	1.4440843 *
8 C	3.8150810	2.5274015 *	1.4440843 *	0.0000000
9 C	4.3645660	2.9130766 *	2.4781019 *	1.4017250 *
10 C	3.8854356	2.5035931 *	2.8486146 *	2.4442676 *
11 C	2.6237434 *	1.4654948 *	2.4959689 *	2.8585843 *
12 N	3.0890992	2.5273117 *	3.8332517	4.3062965
13 C	4.3474102	3.7313959	4.9330599	5.1578594
14 C	5.4028496	5.0241959	6.3076597	6.5914001
15 C	5.6319312	5.5507104	6.9233597	7.4037352
16 C	6.9718059	6.9528498	8.3278344	8.7884370
17 C	7.9859009	7.8134529	9.1405858	9.4427802
18 C	7.8624801	7.4872384	8.7256613	8.8627583
19 C	6.6884907	6.1952344	7.3858473	7.4838128
20 O	4.7545983	4.9271500	6.3208360	7.0158657
21 N	1.5092676 *	2.5922625 *	3.8870499	5.1102994
22 H	3.9439603	3.5193927	2.1965037 *	2.6801944 *
23 H	3.4662562	4.0258210	3.4860358	4.6705101
24 H	2.1822133 *	3.5062578	3.9523666	5.3952964
25 H	4.6717153	3.5169154	2.1967883 *	1.1049851 *
26 H	5.4687350	4.0172643	3.4839797	2.1846711 *
27 H	4.8010966	3.5042878	3.9497947	3.4306286
28 H	4.8855910	4.0389658	5.0269619	4.9882610

29 H	7.3874540	7.5284866	8.9212809	9.4853956
30 H	9.0216049	8.8967350	10.2324604	10.5397895
31 H	8.8270954	8.3820089	9.5649752	9.5994282
32 H	6.9005482	6.2355219	7.2913058	7.2186702
33 H	5.4285841	5.7260262	7.0943659	7.8368488
34 H	2.1130121 *	2.9585722 *	4.2455132	5.3706972
35 H	2.0888175 *	3.4241858	4.5638172	5.8894106

C C C N

1 CO	5.3018723	4.1638182	2.8945731 *	1.9396629 *
2 C	3.7783190	4.2914115	3.8342296	5.0487781
3 C	4.9551753	5.1836761	4.3822636	5.3195210
4 C	5.1788198	5.0056432	3.8916773	4.4879044
5 C	4.3645660	3.8854356	2.6237434 *	3.0890992
6 C	2.9130766 *	2.5035931 *	1.4654948 *	2.5273117 *
7 C	2.4781019 *	2.8486146 *	2.4959689 *	3.8332517
8 C	1.4017250 *	2.4442676 *	2.8585843 *	4.3062965
9 C	0.0000000	1.4299764 *	2.4828061 *	3.7959203
10 C	1.4299764 *	0.0000000	1.4145187 *	2.4709955 *
11 C	2.4828061 *	1.4145187 *	0.0000000	1.4538616 *
12 N	3.7959203	2.4709955 *	1.4538616 *	0.0000000
13 C	4.3499579	2.9272019 *	2.4460927 *	1.3319539 *
14 C	5.7624814	4.3333929	3.8350642	2.5069389 *
15 C	6.7288950	5.3170026	4.5885288	3.1489856
16 C	8.0614534	6.6439100	5.9851646	4.5500288
17 C	8.5606388	7.1417749	6.6906127	5.3103386
18 C	7.8634110	6.4792343	6.2338732	4.9856754
19 C	6.4860985	5.1062295	4.9004729	3.7428612
20 O	6.5873203	5.2703102	4.2856887	2.9375192 *
21 N	5.3862078	4.5623555	3.1532916	2.8946306 *
22 H	4.0795205	4.8922907	4.6916546	5.9974979
23 H	5.9309987	6.2574299	5.4860660	6.4008347
24 H	6.2659520	6.0059526	4.7998144	5.1693471
25 H	2.1809659 *	3.4530554	3.9634153	5.4101455
26 H	1.1043258 *	2.1978978 *	3.4745781	4.6672445
27 H	2.1815100 *	1.1040525 *	2.1875522 *	2.6908495 *
28 H	3.9977533	2.6621728 *	2.6590633 *	2.0963960 *
29 H	8.8522958	7.4575093	6.6977151	5.2663131
30 H	9.6467485	8.2321509	7.7896507	6.4023043
31 H	8.5221864	7.1878907	7.0817475	5.9185892
32 H	6.1244361	4.8377163	4.8775510	3.9719486
33 H	7.4552753	6.1708007	5.1856293	3.8893362
34 H	5.5468333	4.6715320	3.3225482	2.9885041 *
35 H	6.3024231	5.5550397	4.1515134	3.8836476

	C	C	C	C
1 CO	2.8614228 *	3.2627803	3.0094487	4.2793490
2 C	6.2306858	7.5511324	8.0327324	9.4252984
3 C	6.5804597	7.7662435	8.0460298	9.3936270
4 C	5.7542118	6.7925009	6.9346891	8.2369525
5 C	4.3474102	5.4028496	5.6319312	6.9718059
6 C	3.7313959	5.0241959	5.5507104	6.9528498
7 C	4.9330599	6.3076597	6.9233597	8.3278344
8 C	5.1578594	6.5914001	7.4037352	8.7884370
9 C	4.3499579	5.7624814	6.7288950	8.0614534
10 C	2.9272019 *	4.3333929	5.3170026	6.6439100
11 C	2.4460927 *	3.8350642	4.5885288	5.9851646
12 N	1.3319539 *	2.5069389 *	3.1489856	4.5500288
13 C	0.0000000	1.4669847 *	2.6058181 *	3.8843710
14 C	1.4669847 *	0.0000000	1.4377590 *	2.5009718 *
15 C	2.6058181 *	1.4377590 *	0.0000000	1.4062865 *
16 C	3.8843710	2.5009718 *	1.4062865 *	0.0000000
17 C	4.3444624	2.8824658 *	2.4409430 *	1.4282243 *
18 C	3.7936717	2.4975948 *	2.8243064 *	2.4723199 *
19 C	2.4704745 *	1.4427352 *	2.4453730 *	2.8455863 *
20 O	3.0484884	2.5035209 *	1.4656715 *	2.4584528 *
21 N	3.9771253	4.6983170	4.6872517	5.9243479
22 H	7.1268626	8.4895168	9.0321797	10.4297662
23 H	7.6683241	8.8269970	9.0466976	10.3708977
24 H	6.4013728	7.2875681	7.2609101	8.4779749
25 H	6.2443131	7.6792109	8.4988465	9.8798742
26 H	5.0108143	6.3607915	7.4144775	8.6863795
27 H	2.6480361 *	3.8992123	5.0123456	6.2335373
28 H	1.1084428 *	2.1776208 *	3.5332656	4.6753205
29 H	4.7950828	3.5029374	2.1937718 *	1.1068033 *
30 H	5.4493439	3.9876224	3.4394202	2.1915363 *
31 H	4.6579006	3.4933616	3.9284523	3.4740263
32 H	2.6419885 *	2.1975882 *	3.4503938	3.9515095
33 H	4.0168497	3.3304908	2.0454027 *	2.5065792 *
34 H	3.8315807	4.5339022	4.6823042	5.8831000
35 H	4.9386055	5.5155318	5.3023785	6.4250524

	C	C	C	O
1 CO	5.4395877	5.6090240	4.6967000	1.9511363 *
2 C	10.3340999	10.0080325	8.6957120	7.2601152
3 C	10.4174984	10.2451048	9.0099480	7.1049369
4 C	9.3105013	9.2435579	8.0885643	5.9359587
5 C	7.9859009	7.8624801	6.6884907	4.7545983
6 C	7.8134529	7.4872384	6.1952344	4.9271500

7 C	9.1405858	8.7256613	7.3858473	6.3208360
8 C	9.4427802	8.8627583	7.4838128	7.0158657
9 C	8.5606388	7.8634110	6.4860985	6.5873203
10 C	7.1417749	6.4792343	5.1062295	5.2703102
11 C	6.6906127	6.2338732	4.9004729	4.2856887
12 N	5.3103386	4.9856754	3.7428612	2.9375192 *
13 C	4.3444624	3.7936717	2.4704745 *	3.0484884
14 C	2.8824658 *	2.4975948 *	1.4427352 *	2.5035209 *
15 C	2.4409430 *	2.8243064 *	2.4453730 *	1.4656715 *
16 C	1.4282243 *	2.4723199 *	2.8455863 *	2.4584528 *
17 C	0.0000000	1.4231875 *	2.4560235 *	3.7696521
18 C	1.4231875 *	0.0000000	1.4159975 *	4.2897498
19 C	2.4560235 *	1.4159975 *	0.0000000	3.7952256
20 O	3.7696521	4.2897498	3.7952256	0.0000000
21 N	6.9977224	7.0349130	6.0154345	3.7558737
22 H	11.3027855	10.9193681	9.5804782	8.2936750
23 H	11.4333705	11.3032591	10.0855245	8.0401375
24 H	9.6173806	9.6738314	8.6099322	6.1641975
25 H	10.5237684	9.9176830	8.5347680	8.0906682
26 H	9.0577400	8.2560776	6.9039483	7.4086119
27 H	6.5566848	5.7826355	4.4404119	5.2359660
28 H	4.8553710	3.9994662	2.5844051 *	4.1425908
29 H	2.2009054 *	3.4737331	3.9523718	2.6836326 *
30 H	1.1052032 *	2.2011933 *	3.4614243	4.6482377
31 H	2.1972759 *	1.1041465 *	2.1877505 *	5.3938785
32 H	3.4574290	2.1861061 *	1.1059413 *	4.6928229
33 H	3.9272104	4.7288414	4.4867495	0.9918705 *
34 H	6.8172901	6.7430477	5.7141957	4.0151984
35 H	7.5813110	7.7604417	6.8435843	4.2231542

N H H H

1 CO	1.9777961 *	6.4267742	6.1080191	4.3319263
2 C	4.3429177	1.1050808 *	2.1864794 *	3.4392301
3 C	3.8154757	2.1799660 *	1.1041148 *	2.1943502 *
4 C	2.4752130 *	3.4516005	2.2011584 *	1.1077452 *
5 C	1.5092676 *	3.9439603	3.4662562	2.1822133 *
6 C	2.5922625 *	3.5193927	4.0258210	3.5062578
7 C	3.8870499	2.1965037 *	3.4860358	3.9523666
8 C	5.1102994	2.6801944 *	4.6705101	5.3952964
9 C	5.3862078	4.0795205	5.9309987	6.2659520
10 C	4.5623555	4.8922907	6.2574299	6.0059526
11 C	3.1532916	4.6916546	5.4860660	4.7998144
12 N	2.8946306 *	5.9974979	6.4008347	5.1693471
13 C	3.9771253	7.1268626	7.6683241	6.4013728
14 C	4.6983170	8.4895168	8.8269970	7.2875681

15 C	4.6872517	9.0321797	9.0466976	7.2609101
16 C	5.9243479	10.4297662	10.3708977	8.4779749
17 C	6.9977224	11.3027855	11.4333705	9.6173806
18 C	7.0349130	10.9193681	11.3032591	9.6738314
19 C	6.0154345	9.5804782	10.0855245	8.6099322
20 O	3.7558737	8.2936750	8.0401375	6.1641975
21 N	0.0000000	5.4470488	4.6754954	2.6529812 *
22 H	5.4470488	0.0000000	2.5304377 *	4.3603049
23 H	4.6754954	2.5304377 *	0.0000000	2.5190020 *
24 H	2.6529812 *	4.3603049	2.5190020 *	0.0000000
25 H	6.0556278	2.3998345 *	4.7804396	5.9747626
26 H	6.4697173	4.7778865	6.8516475	7.3470895
27 H	5.2545249	5.9665867	7.3463682	6.9640034
28 H	4.7259217	7.1949352	8.0269186	7.0030918
29 H	6.2546389	10.9498794	10.6928779	8.6879379
30 H	7.9771135	12.3878326	12.4616325	10.5791818
31 H	8.0364124	11.7590405	12.2492433	10.6719948
32 H	6.4034320	9.4628687	10.1900159	8.9111472
33 H	4.3761344	8.9800646	8.5664111	6.6071088
34 H	1.0440993 *	5.8580842	5.1890948	3.2240957
35 H	1.0393918 *	5.8214352	4.5853104	2.2125821 *

H H H H

1 CO	6.4876648	6.2753007	4.5226917	3.8774243
2 C	2.6807827 *	4.6684431	5.3910454	6.3996766
3 C	4.0801953	5.9299296	6.2665692	6.9288165
4 C	4.8902068	6.2526535	6.0067692	6.2621368
5 C	4.6717153	5.4687350	4.8010966	4.8855910
6 C	3.5169154	4.0172643	3.5042878	4.0389658
7 C	2.1967883 *	3.4839797	3.9497947	5.0269619
8 C	1.1049851 *	2.1846711 *	3.4306286	4.9882610
9 C	2.1809659 *	1.1043258 *	2.1815100 *	3.9977533
10 C	3.4530554	2.1978978 *	1.1040525 *	2.6621728 *
11 C	3.9634153	3.4745781	2.1875522 *	2.6590633 *
12 N	5.4101455	4.6672445	2.6908495 *	2.0963960 *
13 C	6.2443131	5.0108143	2.6480361 *	1.1084428 *
14 C	7.6792109	6.3607915	3.8992123	2.1776208 *
15 C	8.4988465	7.4144775	5.0123456	3.5332656
16 C	9.8798742	8.6863795	6.2335373	4.6753205
17 C	10.5237684	9.0577400	6.5566848	4.8553710
18 C	9.9176830	8.2560776	5.7826355	3.9994662
19 C	8.5347680	6.9039483	4.4404119	2.5844051 *
20 O	8.0906682	7.4086119	5.2359660	4.1425908
21 N	6.0556278	6.4697173	5.2545249	4.7259217
22 H	2.3998345 *	4.7778865	5.9665867	7.1949352

23 H	4.7804396	6.8516475	7.3463682	8.0269186
24 H	5.9747626	7.3470895	6.9640034	7.0030918
25 H	0.0000000	2.5286294 *	4.3481808	6.0189752
26 H	2.5286294 *	0.0000000	2.5012762 *	4.4894352
27 H	4.3481808	2.5012762 *	0.0000000	2.1609538 *
28 H	6.0189752	4.4894352	2.1609538 *	0.0000000
29 H	10.5706460	9.5249125	7.1228067	5.6718356
30 H	11.6187004	10.1197044	7.6198751	5.9353069
31 H	10.6252314	8.8112768	6.4043039	4.6582333
32 H	8.2196791	6.4187725	4.0772869	2.2688830 *
33 H	8.8904021	8.2733736	6.1323317	5.1006236
34 H	6.3300293	6.5956857	5.2976785	4.4620282
35 H	6.7602372	7.3986347	6.2714689	5.7325865

H H H H

1 CO	4.6139251	6.4188725	6.6749627	5.2811110
2 C	9.9234782	11.4119775	10.8819766	8.6514744
3 C	9.7716187	11.4606279	11.1810251	9.1004461
4 C	8.5598088	10.3232419	10.2165436	8.2990488
5 C	7.3874540	9.0216049	8.8270954	6.9005482
6 C	7.5284866	8.8967350	8.3820089	6.2355219
7 C	8.9212809	10.2324604	9.5649752	7.2913058
8 C	9.4853956	10.5397895	9.5994282	7.2186702
9 C	8.8522958	9.6467485	8.5221864	6.1244361
10 C	7.4575093	8.2321509	7.1878907	4.8377163
11 C	6.6977151	7.7896507	7.0817475	4.8775510
12 N	5.2663131	6.4023043	5.9185892	3.9719486
13 C	4.7950828	5.4493439	4.6579006	2.6419885 *
14 C	3.5029374	3.9876224	3.4933616	2.1975882 *
15 C	2.1937718 *	3.4394202	3.9284523	3.4503938
16 C	1.1068033 *	2.1915363 *	3.4740263	3.9515095
17 C	2.2009054 *	1.1052032 *	2.1972759 *	3.4574290
18 C	3.4737331	2.2011933 *	1.1041465 *	2.1861061 *
19 C	3.9523718	3.4614243	2.1877505 *	1.1059413 *
20 O	2.6836326 *	4.6482377	5.3938785	4.6928229
21 N	6.2546389	7.9771135	8.0364124	6.4034320
22 H	10.9498794	12.3878326	11.7590405	9.4628687
23 H	10.6928779	12.4616325	12.2492433	10.1900159
24 H	8.6879379	10.5791818	10.6719948	8.9111472
25 H	10.5706460	11.6187004	10.6252314	8.2196791
26 H	9.5249125	10.1197044	8.8112768	6.4187725
27 H	7.1228067	7.6198751	6.4043039	4.0772869
28 H	5.6718356	5.9353069	4.6582333	2.2688830 *
29 H	0.0000000	2.5207362 *	4.3868866	5.0582951
30 H	2.5207362 *	0.0000000	2.5410081 *	4.3751194

31 H	4.3868866	2.5410081 *	0.0000000	2.5152206 *
32 H	5.0582951	4.3751194	2.5152206 *	0.0000000
33 H	2.3031409 *	4.6277224	5.8144530	5.4662954
34 H	6.3093706	7.7967844	7.6817599	6.0247574
35 H	6.6008973	8.4963103	8.7814750	7.3072455

H H H

1 CO	2.6569512 *	2.4991828 *	2.6225481 *
2 C	7.9457863	4.7809251	4.7383188
3 C	7.6934291	4.3338220	3.9176911
4 C	6.4940502	3.0671260	2.4862747 *
5 C	5.4285841	2.1130121 *	2.0888175 *
6 C	5.7260262	2.9585722 *	3.4241858
7 C	7.0943659	4.2455132	4.5638172
8 C	7.8368488	5.3706972	5.8894106
9 C	7.4552753	5.5468333	6.3024231
10 C	6.1708007	4.6715320	5.5550397
11 C	5.1856293	3.3225482	4.1515134
12 N	3.8893362	2.9885041 *	3.8836476
13 C	4.0168497	3.8315807	4.9386055
14 C	3.3304908	4.5339022	5.5155318
15 C	2.0454027 *	4.6823042	5.3023785
16 C	2.5065792 *	5.8831000	6.4250524
17 C	3.9272104	6.8172901	7.5813110
18 C	4.7288414	6.7430477	7.7604417
19 C	4.4867495	5.7141957	6.8435843
20 O	0.9918705 *	4.0151984	4.2231542
21 N	4.3761344	1.0440993 *	1.0393918 *
22 H	8.9800646	5.8580842	5.8214352
23 H	8.5664111	5.1890948	4.5853104
24 H	6.6071088	3.2240957	2.2125821 *
25 H	8.8904021	6.3300293	6.7602372
26 H	8.2733736	6.5956857	7.3986347
27 H	6.1323317	5.2976785	6.2714689
28 H	5.1006236	4.4620282	5.7325865
29 H	2.3031409 *	6.3093706	6.6008973
30 H	4.6277224	7.7967844	8.4963103
31 H	5.8144530	7.6817599	8.7814750
32 H	5.4662954	6.0247574	7.3072455
33 H	0.0000000	4.7185637	4.6563726
34 H	4.7185637	0.0000000	1.6674243 *
35 H	4.6563726	1.6674243 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.76 , TOTAL = 8418.5 SECONDS (140.3 MIN)

WALL CLOCK TIME: STEP = 0.77 , TOTAL = 7785.4 SECONDS (129.8 MIN)

CPU UTILIZATION: STEP = 98.65%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.32 , TOTAL = 8419.8 SECONDS (140.3 MIN)

WALL CLOCK TIME: STEP = 1.32 , TOTAL = 7786.7 SECONDS (129.8 MIN)

CPU UTILIZATION: STEP = 99.96%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.636928342 -284.636928342 0.005450627 0.000561280 198386279
11313978

2 1 -284.636954871 -0.000026529 0.001028092 0.000046867 152569943
15171832

3 2 -284.636954917 -0.000000046 0.000491427 0.000061801 135791203
16523404

4 3 -284.636955331 -0.000000413 0.000214471 0.000033087 129135859
17016151

5 4 -284.636955278 0.000000052 0.000089863 0.000060307 123587657
17466872

6 5 -284.636955368 -0.000000090 0.000119497 0.000016376 115871386
18061356

7 6 -284.636955367 0.000000001 0.000088141 0.000017229 140790967
16133578

8 7 -284.636955386 -0.000000019 0.000123603 0.000012621 134157781
16675864

9 8 -284.636955396 -0.000000010 0.000202775 0.000012158 156019325
15001580

-----DISABLING FDIFF OPTION-----

10 9 -284.636955412 -0.000000016 0.000233038 0.000011240 198387004
11313905

11 10 -284.636955423 -0.000000011 0.000225105 0.000015216 198387012
11313906

12 11 -284.636955434 -0.000000011 0.000148534 0.000014251 198386939
11313910

13 12 -284.636955442 -0.000000008 0.000108132 0.000006695 198386922
11313908
14 13 -284.636955444 -0.000000002 0.000049111 0.000004043 198386950
11313907
15 14 -284.636955445 -0.000000001 0.000019041 0.000002166 198386955
11313908
16 15 -284.636955445 0.000000000 0.000014093 0.000001375 198386978
11313905

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 53.6 SECONDS (3.4 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 17.5 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369554455 AFTER 16 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6026126473
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998541902

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 56.49 , TOTAL = 8476.3 SECONDS (141.3 MIN)
WALL CLOCK TIME: STEP = 51.82 , TOTAL = 7838.6 SECONDS (130.6
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.75 , TOTAL = 8480.1 SECONDS (141.3 MIN)
WALL CLOCK TIME: STEP = 3.74 , TOTAL = 7842.3 SECONDS (130.7
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.

USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.88 , TOTAL = 8483.0 SECONDS (141.4 MIN)

WALL CLOCK TIME: STEP = 2.70 , TOTAL = 7845.0 SECONDS (130.7 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 95 ENERGY= -284.6369554

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000166	-0.0000116	0.0000640
2 C	6.0	0.0000444	0.0000099	0.0000734
3 C	6.0	-0.0000297	0.0000518	0.0001410
4 C	6.0	0.0000071	0.0001038	-0.0000174
5 C	6.0	0.0000058	0.0000141	-0.0001550
6 C	6.0	0.0000193	-0.0000715	0.0000447
7 C	6.0	-0.0000515	0.0000130	0.0001225
8 C	6.0	-0.0000007	-0.0000565	0.0000031
9 C	6.0	-0.0000157	0.0000165	-0.0000558
10 C	6.0	0.0000333	-0.0000049	-0.0000322
11 C	6.0	0.0000819	-0.0000431	0.0000762
12 N	7.0	-0.0000473	-0.0001254	0.0000705
13 C	6.0	0.0001051	0.0000951	-0.0000667
14 C	6.0	-0.0000565	0.0000155	-0.0000337
15 C	6.0	-0.0000412	-0.0000081	-0.0000272
16 C	6.0	0.0000129	0.0000401	0.0000204
17 C	6.0	-0.0000300	0.0000158	-0.0000436
18 C	6.0	0.0000474	0.0000034	0.0000548
19 C	6.0	-0.0000229	0.0000249	-0.0000152
20 O	8.0	0.0000253	0.0001537	-0.0001315
21 N	7.0	0.0000025	0.0000161	-0.0000246
22 H	1.0	-0.0000204	0.0000529	-0.0000194
23 H	1.0	-0.0000136	0.0000538	0.0000018
24 H	1.0	-0.0000544	0.0000492	-0.0000166
25 H	1.0	-0.0000040	-0.0000583	0.0000139
26 H	1.0	-0.0000113	0.0000370	0.0000009
27 H	1.0	0.0001016	-0.0001052	-0.0000549
28 H	1.0	0.0000484	-0.0000234	-0.0001366
29 H	1.0	0.0000625	0.0000407	0.0000363

30 H	1.0	0.0000101	-0.0000538	0.0001148
31 H	1.0	-0.0000172	-0.0000447	0.0000548
32 H	1.0	0.0000085	0.0000221	0.0000085
33 H	1.0	-0.0000356	-0.0000848	-0.0000578
34 H	1.0	-0.0002017	-0.0000859	-0.0000308
35 H	1.0	0.0000542	-0.0000522	0.0000172

MAXIMUM GRADIENT = 0.0002017 RMS GRADIENT = 0.0000607
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000043255
 PREDICTED ENERGY CHANGE WAS -0.0000018273 RATIO= 2.367
 GDIIS STEP HAS LENGTH = 0.018199
 RADIUS OF STEP TAKEN= 0.01820 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8483.0 SECONDS (141.4 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7845.0 SECONDS (130.8
 MIN)
 CPU UTILIZATION: STEP = 81.97% , TOTAL = 100.00%

INSERCH= 96

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1623387328	-1.7211789200	0.8900260428
C	6.0	4.9800733528	0.6189757639	0.5628692274
C	6.0	5.1769507719	-0.7208328611	0.2016569574
C	6.0	4.0370600786	-1.5351944363	-0.0952292680
C	6.0	2.7311055445	-1.0183780224	-0.0040582622
C	6.0	2.4670768947	0.3470254223	0.4322125717
C	6.0	3.6525580701	1.1748261919	0.6815274596
C	6.0	3.5112088384	2.5617818075	1.0584234253
C	6.0	2.2456522838	3.1426403298	1.2193199376
C	6.0	1.0769624249	2.3378818713	1.0417355575
C	6.0	1.1640217608	0.9833819329	0.6436922931
N	7.0	-0.0495987363	0.1844441266	0.5956167305
C	6.0	-1.2453082718	0.7055652399	0.3260296110
C	6.0	-2.5473892268	0.0396556805	0.4399100243
C	6.0	-2.8148196169	-1.2835451914	0.9344774939
C	6.0	-4.1128587618	-1.8108698437	1.0558231966
C	6.0	-5.2250571750	-1.0024985732	0.6692354197
C	6.0	-5.0149981211	0.3114838458	0.1643015417
C	6.0	-3.6980248867	0.8202260006	0.0549666888
O	8.0	-1.6919028161	-2.1370130465	1.3334056611

N	7.0	1.6188890955	-1.9459761265	-0.4287485635
H	1.0	5.8452777229	1.2759627546	0.7653386455
H	1.0	6.1928570542	-1.1454692578	0.1196386343
H	1.0	4.1959526812	-2.5780940847	-0.4329801354
H	1.0	4.4267235220	3.1559568785	1.2311569851
H	1.0	2.1417106698	4.1992894105	1.5227166512
H	1.0	0.0941214818	2.7842857937	1.2738103153
H	1.0	-1.2899936869	1.7548206761	-0.0285126785
H	1.0	-4.2810671128	-2.8341232737	1.4426724139
H	1.0	-6.2478736063	-1.4098826190	0.7650663179
H	1.0	-5.8744995234	0.9360911988	-0.1363670628
H	1.0	-3.5368317200	1.8449237822	-0.3283593192
H	1.0	-2.0091996289	-2.9513162199	1.8023843689
H	1.0	1.2452856791	-1.6622813121	-1.3615047414
H	1.0	2.0095932310	-2.9014599191	-0.5493671410

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3659969	5.1595424	4.0023473
2 C	5.3659969	0.0000000	1.4015428 *	2.4418880 *
3 C	5.1595424	1.4015428 *	0.0000000	1.4320185 *
4 C	4.0023473	2.4418880 *	1.4320185 *	0.0000000
5 C	2.8092488 *	2.8390474 *	2.4724504 *	1.4074547 *
6 C	3.1303163	2.5310431 *	2.9217963 *	2.5071485 *
7 C	4.5400384	1.4440728 *	2.4794298 *	2.8452425 *
8 C	5.4393971	2.4854843 *	3.7794582	4.2886651
9 C	5.3014496	3.7784744	4.9552572	5.1787373
10 C	4.1635954	4.2916461	5.1837604	5.0055556
11 C	2.8945982 *	3.8342632	4.3821619	3.8914754
12 N	1.9398437 *	5.0485138	5.3189802	4.4872269
13 C	2.8615816 *	6.2304869	6.5799310	5.7534232
14 C	3.2627854	7.5507234	7.7653420	6.7912811
15 C	3.0094802	8.0323119	8.0450025	6.9333887
16 C	4.2793512	9.4248909	9.3924620	8.2354172
17 C	5.4396034	10.3336916	10.4163206	9.3088661
18 C	5.6092077	10.0077401	10.2441640	9.2421499
19 C	4.6966446	8.6952778	9.0089718	8.0871567
20 O	1.9513368 *	7.2597842	7.1040531	5.9349978
21 N	1.9776853 *	4.3427921	3.8155196	2.4753843 *
22 H	6.4260564	1.1050812 *	2.1798144 *	3.4514972
23 H	6.1067249	2.1864501 *	1.1041325 *	2.2012529 *
24 H	4.3306686	3.4391593	2.1942062 *	1.1076833 *
25 H	6.4875112	2.6812456 *	4.0807119	4.8906072

26 H	6.2745642	4.6686460	5.9300493	6.2525517
27 H	4.5222955	5.3913385	6.2666198	6.0065750
28 H	3.8775709	6.3995013	6.9284348	6.2614816
29 H	4.6138833	9.9230373	9.7703745	8.5582473
30 H	6.4189830	11.4115706	11.4594429	10.3216119
31 H	6.6751767	10.8816932	11.1800810	10.2150849
32 H	5.2806641	8.6507172	9.0991225	8.2971914
33 H	2.6572946 *	7.9456478	7.6927331	6.4933500
34 H	2.4991266 *	4.7807937	4.3344884	3.0681605
35 H	2.6224540 *	4.7385957	3.9180767	2.4866734 *

C C C C

1 CO	2.8092488 *	3.1303163	4.5400384	5.4393971
2 C	2.8390474 *	2.5310431 *	1.4440728 *	2.4854843 *
3 C	2.4724504 *	2.9217963 *	2.4794298 *	3.7794582
4 C	1.4074547 *	2.5071485 *	2.8452425 *	4.2886651
5 C	0.0000000	1.4575218 *	2.4757317 *	3.8150980
6 C	1.4575218 *	0.0000000	1.4672347 *	2.5273499 *
7 C	2.4757317 *	1.4672347 *	0.0000000	1.4441870 *
8 C	3.8150980	2.5273499 *	1.4441870 *	0.0000000
9 C	4.3642173	2.9127358 *	2.4780834 *	1.4017552 *
10 C	3.8851454	2.5034868 *	2.8488842 *	2.4445788 *
11 C	2.6234282 *	1.4654781 *	2.4961761 *	2.8587821 *
12 N	3.0884798	2.5272099 *	3.8333018	4.3064225
13 C	4.3465855	3.7311700	4.9331206	5.1581388
14 C	5.4017636	5.0238835	6.3076412	6.5916834
15 C	5.6310256	5.5506271	6.9234780	7.4040893
16 C	6.9707417	6.9527660	8.3280356	8.7889986
17 C	7.9846166	7.8132145	9.1407301	9.4434054
18 C	7.8612340	7.4869544	8.7257901	8.8633797
19 C	6.6871269	6.1947327	7.3857559	7.4841829
20 O	4.7542778	4.9274444	6.3211143	7.0161713
21 N	1.5092467 *	2.5920133 *	3.8868920	5.1100329
22 H	3.9438610	3.5193946	2.1966503 *	2.6808780 *
23 H	3.4662915	4.0257522	3.4860592	4.6707884
24 H	2.1823073 *	3.5062650	3.9524442	5.3955058
25 H	4.6718250	3.5169053	2.1968850 *	1.1050104 *
26 H	5.4683161	4.0168396	3.4839111	2.1846109 *
27 H	4.8007171	3.5042035	3.9501431	3.4310910
28 H	4.8847178	4.0385312	5.0268647	4.9884028
29 H	7.3865097	7.5284915	8.9215148	9.4859371
30 H	9.0203600	8.8965094	10.2326070	10.5403922
31 H	8.8257518	8.3816573	9.5650809	9.6000998
32 H	6.8986017	6.2345078	7.2908318	7.2188592
33 H	5.4286258	5.7265592	7.0948482	7.8372596

34 H	2.1130388 *	2.9576188 *	4.2447756	5.3696526
35 H	2.0890044 *	3.4242440	4.5640490	5.8895543

	C	C	C	N
--	---	---	---	---

1 CO	5.3014496	4.1635954	2.8945982 *	1.9398437 *
2 C	3.7784744	4.2916461	3.8342632	5.0485138
3 C	4.9552572	5.1837604	4.3821619	5.3189802
4 C	5.1787373	5.0055556	3.8914754	4.4872269
5 C	4.3642173	3.8851454	2.6234282 *	3.0884798
6 C	2.9127358 *	2.5034868 *	1.4654781 *	2.5272099 *
7 C	2.4780834 *	2.8488842 *	2.4961761 *	3.8333018
8 C	1.4017552 *	2.4445788 *	2.8587821 *	4.3064225
9 C	0.0000000	1.4300379 *	2.4826737 *	3.7958013
10 C	1.4300379 *	0.0000000	1.4144567 *	2.4709221 *
11 C	2.4826737 *	1.4144567 *	0.0000000	1.4537839 *
12 N	3.7958013	2.4709221 *	1.4537839 *	0.0000000
13 C	4.3501848	2.9273937 *	2.4460096 *	1.3319030 *
14 C	5.7627459	4.3335854	3.8349339	2.5068238 *
15 C	6.7290883	5.3171614	4.5885393	3.1490103
16 C	8.0619264	6.6442895	5.9852454	4.5500714
17 C	8.5613240	7.1422930	6.6906430	5.3103317
18 C	7.8641945	6.4798274	6.2339032	4.9857159
19 C	6.4866498	5.1066130	4.9002771	3.7426641
20 O	6.5872677	5.2703293	4.2858925	2.9377983 *
21 N	5.3854414	4.5615181	3.1524867	2.8934178 *
22 H	4.0801823	4.8929437	4.6919675	5.9974817
23 H	5.9310714	6.2575055	5.4859661	6.4002718
24 H	6.2658255	6.0058060	4.7995771	5.1685913
25 H	2.1811440 *	3.4534080	3.9636371	5.4102921
26 H	1.1042467 *	2.1976964 *	3.4742798	4.6669405
27 H	2.1818506 *	1.1041338 *	2.1874620 *	2.6906837 *
28 H	3.9979898	2.6623059 *	2.6587909 *	2.0962346 *
29 H	8.8526638	7.4578059	6.6978137	5.2663628
30 H	9.6473724	8.2325881	7.7896495	6.4022810
31 H	8.5231222	7.1885858	7.0817731	5.9186352
32 H	6.1250715	4.8381054	4.8770034	3.9713623
33 H	7.4552019	6.1707860	5.1859185	3.8896422
34 H	5.5451476	4.6696041	3.3206856	2.9862091 *
35 H	6.3019938	5.5544676	4.1509491	3.8825331

	C	C	C	C
--	---	---	---	---

1 CO	2.8615816 *	3.2627854	3.0094802	4.2793512
2 C	6.2304869	7.5507234	8.0323119	9.4248909
3 C	6.5799310	7.7653420	8.0450025	9.3924620

4 C	5.7534232	6.7912811	6.9333887	8.2354172
5 C	4.3465855	5.4017636	5.6310256	6.9707417
6 C	3.7311700	5.0238835	5.5506271	6.9527660
7 C	4.9331206	6.3076412	6.9234780	8.3280356
8 C	5.1581388	6.5916834	7.4040893	8.7889986
9 C	4.3501848	5.7627459	6.7290883	8.0619264
10 C	2.9273937 *	4.3335854	5.3171614	6.6442895
11 C	2.4460096 *	3.8349339	4.5885393	5.9852454
12 N	1.3319030 *	2.5068238 *	3.1490103	4.5500714
13 C	0.0000000	1.4669080 *	2.6057887 *	3.8843133
14 C	1.4669080 *	0.0000000	1.4376983 *	2.5008976 *
15 C	2.6057887 *	1.4376983 *	0.0000000	1.4063078 *
16 C	3.8843133	2.5008976 *	1.4063078 *	0.0000000
17 C	4.3443841	2.8824610 *	2.4410214 *	1.4282505 *
18 C	3.7936813	2.4977879 *	2.8245485 *	2.4724586 *
19 C	2.4703119 *	1.4427175 *	2.4452902 *	2.8454290 *
20 O	3.0486890	2.5036130 *	1.4657739 *	2.4585461 *
21 N	3.9754230	4.6962939	4.6856134	5.9224269
22 H	7.1270440	8.4894769	9.0319973	10.4296404
23 H	7.6678047	8.8260410	9.0455108	10.3695216
24 H	6.4004559	7.2860971	7.2592510	8.4759375
25 H	6.2446473	7.6795608	8.4992438	9.8805149
26 H	5.0109945	6.3610283	7.4144921	8.6867510
27 H	2.6482899 *	3.8994824	5.0124180	6.2339118
28 H	1.1084376 *	2.1776718 *	3.5332862	4.6753075
29 H	4.7950097	3.5028241	2.1937266 *	1.1067944 *
30 H	5.4491773	3.9875397	3.4395524	2.1917159 *
31 H	4.6579357	3.4936163	3.9287574	3.4742612
32 H	2.6414849 *	2.1973227 *	3.4501270	3.9512777
33 H	4.0169560	3.3304500	2.0454208 *	2.5066618 *
34 H	3.8285151	4.5305703	4.6796827	5.8800735
35 H	4.9367331	5.5131587	5.3004153	6.4226506

C C C O

1 CO	5.4396034	5.6092077	4.6966446	1.9513368 *
2 C	10.3336916	10.0077401	8.6952778	7.2597842
3 C	10.4163206	10.2441640	9.0089718	7.1040531
4 C	9.3088661	9.2421499	8.0871567	5.9349978
5 C	7.9846166	7.8612340	6.6871269	4.7542778
6 C	7.8132145	7.4869544	6.1947327	4.9274444
7 C	9.1407301	8.7257901	7.3857559	6.3211143
8 C	9.4434054	8.8633797	7.4841829	7.0161713
9 C	8.5613240	7.8641945	6.4866498	6.5872677
10 C	7.1422930	6.4798274	5.1066130	5.2703293
11 C	6.6906430	6.2339032	4.9002771	4.2858925

12 N	5.3103317	4.9857159	3.7426641	2.9377983 *
13 C	4.3443841	3.7936813	2.4703119 *	3.0486890
14 C	2.8824610 *	2.4977879 *	1.4427175 *	2.5036130 *
15 C	2.4410214 *	2.8245485 *	2.4452902 *	1.4657739 *
16 C	1.4282505 *	2.4724586 *	2.8454290 *	2.4585461 *
17 C	0.0000000	1.4232473 *	2.4559069 *	3.7698044
18 C	1.4232473 *	0.0000000	1.4160477 *	4.2900937
19 C	2.4559069 *	1.4160477 *	0.0000000	3.7952859
20 O	3.7698044	4.2900937	3.7952859	0.0000000
21 N	6.9953784	7.0325169	6.0129385	3.7553995
22 H	11.3027845	10.9195722	9.5805506	8.2933826
23 H	11.4320279	11.3022442	10.0845271	8.0390191
24 H	9.6152383	9.6720226	8.6082259	6.1629144
25 H	10.5245132	9.9184331	8.5352562	8.0909563
26 H	9.0584931	8.2570457	6.9046992	7.4081820
27 H	6.5573553	5.7834991	4.4411130	5.2357059
28 H	4.8553462	3.9995070	2.5843859 *	4.1427916
29 H	2.2009478 *	3.4738640	3.9522062	2.6835934 *
30 H	1.1051239 *	2.2009095 *	3.4611204	4.6485049
31 H	2.1974761 *	1.1042095 *	2.1879386 *	5.3942856
32 H	3.4573277	2.1861218 *	1.1058606 *	4.6926588
33 H	3.9272963	4.7290595	4.4866613	0.9918205 *
34 H	6.8135567	6.7390643	5.7101273	4.0143478
35 H	7.5783384	7.7573974	6.8405460	4.2225923

N H H H

1 CO	1.9776853 *	6.4260564	6.1067249	4.3306686
2 C	4.3427921	1.1050812 *	2.1864501 *	3.4391593
3 C	3.8155196	2.1798144 *	1.1041325 *	2.1942062 *
4 C	2.4753843 *	3.4514972	2.2012529 *	1.1076833 *
5 C	1.5092467 *	3.9438610	3.4662915	2.1823073 *
6 C	2.5920133 *	3.5193946	4.0257522	3.5062650
7 C	3.8868920	2.1966503 *	3.4860592	3.9524442
8 C	5.1100329	2.6808780 *	4.6707884	5.3955058
9 C	5.3854414	4.0801823	5.9310714	6.2658255
10 C	4.5615181	4.8929437	6.2575055	6.0058060
11 C	3.1524867	4.6919675	5.4859661	4.7995771
12 N	2.8934178 *	5.9974817	6.4002718	5.1685913
13 C	3.9754230	7.1270440	7.6678047	6.4004559
14 C	4.6962939	8.4894769	8.8260410	7.2860971
15 C	4.6856134	9.0319973	9.0455108	7.2592510
16 C	5.9224269	10.4296404	10.3695216	8.4759375
17 C	6.9953784	11.3027845	11.4320279	9.6152383
18 C	7.0325169	10.9195722	11.3022442	9.6720226
19 C	6.0129385	9.5805506	10.0845271	8.6082259

20	O	3.7553995	8.2933826	8.0390191	6.1629144
21	N	0.0000000	5.4469345	4.6757590	2.6534596 *
22	H	5.4469345	0.0000000	2.5300342 *	4.3600453
23	H	4.6757590	2.5300342 *	0.0000000	2.5190134 *
24	H	2.6534596 *	4.3600453	2.5190134 *	0.0000000
25	H	6.0554885	2.4007625 *	4.7808961	5.9751107
26	H	6.4688366	4.7786891	6.8517779	7.3469441
27	H	5.2534751	5.9673595	7.3464047	6.9637110
28	H	4.7241597	7.1952486	8.0266236	7.0023819
29	H	6.2530397	10.9496323	10.6913544	8.6858211
30	H	7.9748696	12.3878196	12.4602677	10.5770289
31	H	8.0338454	11.7593267	12.2482459	10.6701211
32	H	6.4001920	9.4627623	10.1887191	8.9089835
33	H	4.3762645	8.9798756	8.5654218	6.6060627
34	H	1.0440768 *	5.8580430	5.1903124	3.2260358
35	H	1.0393016 *	5.8216653	4.5859315	2.2132056 *

H H H H

1	CO	6.4875112	6.2745642	4.5222955	3.8775709
2	C	2.6812456 *	4.6686460	5.3913385	6.3995013
3	C	4.0807119	5.9300493	6.2666198	6.9284348
4	C	4.8906072	6.2525517	6.0065750	6.2614816
5	C	4.6718250	5.4683161	4.8007171	4.8847178
6	C	3.5169053	4.0168396	3.5042035	4.0385312
7	C	2.1968850 *	3.4839111	3.9501431	5.0268647
8	C	1.1050104 *	2.1846109 *	3.4310910	4.9884028
9	C	2.1811440 *	1.1042467 *	2.1818506 *	3.9979898
10	C	3.4534080	2.1976964 *	1.1041338 *	2.6623059 *
11	C	3.9636371	3.4742798	2.1874620 *	2.6587909 *
12	N	5.4102921	4.6669405	2.6906837 *	2.0962346 *
13	C	6.2446473	5.0109945	2.6482899 *	1.1084376 *
14	C	7.6795608	6.3610283	3.8994824	2.1776718 *
15	C	8.4992438	7.4144921	5.0124180	3.5332862
16	C	9.8805149	8.6867510	6.2339118	4.6753075
17	C	10.5245132	9.0584931	6.5573553	4.8553462
18	C	9.9184331	8.2570457	5.7834991	3.9995070
19	C	8.5352562	6.9046992	4.4411130	2.5843859 *
20	O	8.0909563	7.4081820	5.2357059	4.1427916
21	N	6.0554885	6.4688366	5.2534751	4.7241597
22	H	2.4007625 *	4.7786891	5.9673595	7.1952486
23	H	4.7808961	6.8517779	7.3464047	8.0266236
24	H	5.9751107	7.3469441	6.9637110	7.0023819
25	H	0.0000000	2.5288008 *	4.3487239	6.0192031
26	H	2.5288008 *	0.0000000	2.5013618 *	4.4898034
27	H	4.3487239	2.5013618 *	0.0000000	2.1613927 *

28 H	6.0192031	4.4898034	2.1613927 *	0.0000000
29 H	10.5712543	9.5250919	7.1230127	5.6717997
30 H	11.6194300	10.1203740	7.6204180	5.9351232
31 H	10.6260586	8.8125279	6.4053774	4.6582877
32 H	8.2200432	6.4199193	4.0783783	2.2685475 *
33 H	8.8907926	8.2728128	6.1319231	5.1007025
34 H	6.3292070	6.5939610	5.2954720	4.4588222
35 H	6.7605535	7.3980827	6.2706230	5.7305770

H H H H

1 CO	4.6138833	6.4189830	6.6751767	5.2806641
2 C	9.9230373	11.4115706	10.8816932	8.6507172
3 C	9.7703745	11.4594429	11.1800810	9.0991225
4 C	8.5582473	10.3216119	10.2150849	8.2971914
5 C	7.3865097	9.0203600	8.8257518	6.8986017
6 C	7.5284915	8.8965094	8.3816573	6.2345078
7 C	8.9215148	10.2326070	9.5650809	7.2908318
8 C	9.4859371	10.5403922	9.6000998	7.2188592
9 C	8.8526638	9.6473724	8.5231222	6.1250715
10 C	7.4578059	8.2325881	7.1885858	4.8381054
11 C	6.6978137	7.7896495	7.0817731	4.8770034
12 N	5.2663628	6.4022810	5.9186352	3.9713623
13 C	4.7950097	5.4491773	4.6579357	2.6414849 *
14 C	3.5028241	3.9875397	3.4936163	2.1973227 *
15 C	2.1937266 *	3.4395524	3.9287574	3.4501270
16 C	1.1067944 *	2.1917159 *	3.4742612	3.9512777
17 C	2.2009478 *	1.1051239 *	2.1974761 *	3.4573277
18 C	3.4738640	2.2009095 *	1.1042095 *	2.1861218 *
19 C	3.9522062	3.4611204	2.1879386 *	1.1058606 *
20 O	2.6835934 *	4.6485049	5.3942856	4.6926588
21 N	6.2530397	7.9748696	8.0338454	6.4001920
22 H	10.9496323	12.3878196	11.7593267	9.4627623
23 H	10.6913544	12.4602677	12.2482459	10.1887191
24 H	8.6858211	10.5770289	10.6701211	8.9089835
25 H	10.5712543	11.6194300	10.6260586	8.2200432
26 H	9.5250919	10.1203740	8.8125279	6.4199193
27 H	7.1230127	7.6204180	6.4053774	4.0783783
28 H	5.6717997	5.9351232	4.6582877	2.2685475 *
29 H	0.0000000	2.5210988 *	4.3871300	5.0580551
30 H	2.5210988 *	0.0000000	2.5407840 *	4.3748248
31 H	4.3871300	2.5407840 *	0.0000000	2.5154579 *
32 H	5.0580551	4.3748248	2.5154579 *	0.0000000
33 H	2.3031519 *	4.6280021	5.8147431	5.4660449
34 H	6.3069167	7.7931666	7.6774894	6.0196781
35 H	6.5988759	8.4934267	8.7781710	7.3034124

	H	H	H
1 CO	2.6572946 *	2.4991266 *	2.6224540 *
2 C	7.9456478	4.7807937	4.7385957
3 C	7.6927331	4.3344884	3.9180767
4 C	6.4933500	3.0681605	2.4866734 *
5 C	5.4286258	2.1130388 *	2.0890044 *
6 C	5.7265592	2.9576188 *	3.4242440
7 C	7.0948482	4.2447756	4.5640490
8 C	7.8372596	5.3696526	5.8895543
9 C	7.4552019	5.5451476	6.3019938
10 C	6.1707860	4.6696041	5.5544676
11 C	5.1859185	3.3206856	4.1509491
12 N	3.8896422	2.9862091 *	3.8825331
13 C	4.0169560	3.8285151	4.9367331
14 C	3.3304500	4.5305703	5.5131587
15 C	2.0454208 *	4.6796827	5.3004153
16 C	2.5066618 *	5.8800735	6.4226506
17 C	3.9272963	6.8135567	7.5783384
18 C	4.7290595	6.7390643	7.7573974
19 C	4.4866613	5.7101273	6.8405460
20 O	0.9918205 *	4.0143478	4.2225923
21 N	4.3762645	1.0440768 *	1.0393016 *
22 H	8.9798756	5.8580430	5.8216653
23 H	8.5654218	5.1903124	4.5859315
24 H	6.6060627	3.2260358	2.2132056 *
25 H	8.8907926	6.3292070	6.7605535
26 H	8.2728128	6.5939610	7.3980827
27 H	6.1319231	5.2954720	6.2706230
28 H	5.1007025	4.4588222	5.7305770
29 H	2.3031519 *	6.3069167	6.5988759
30 H	4.6280021	7.7931666	8.4934267
31 H	5.8147431	7.6774894	8.7781710
32 H	5.4660449	6.0196781	7.3034124
33 H	0.0000000	4.7184192	4.6565993
34 H	4.7184192	0.0000000	1.6671224 *
35 H	4.6565993	1.6671224 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.56 , TOTAL = 8483.5 SECONDS (141.4 MIN)

WALL CLOCK TIME: STEP = 0.56 , TOTAL = 7845.6 SECONDS (130.8 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.94 , TOTAL = 8484.5 SECONDS (141.4 MIN)

WALL CLOCK TIME: STEP = 0.94 , TOTAL = 7846.5 SECONDS (130.8 MIN)

CPU UTILIZATION: STEP = 99.93%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.636951183 -284.636951183 0.002680005 0.000247792 198391238
11313365

2 1 -284.636957405 -0.000006222 0.000257735 0.000019030 145736874
15720084

3 2 -284.636957423 -0.000000018 0.000128929 0.000052431 127389944
17173149

4 3 -284.636957501 -0.000000078 0.000119465 0.000034685 119874290
17759429

5 4 -284.636957473 0.000000028 0.000081582 0.000033404 118414811
17844075

6 5 -284.636957527 -0.000000054 0.000052628 0.000007122 112187783
18256151

7 6 -284.636957510 0.000000017 0.000033444 0.000007726 107553296
18603950

8 7 -284.636957516 -0.000000006 0.000059178 0.000005597 125486204
17310658

9 8 -284.636957518 -0.000000002 0.000086751 0.000005292 150347017
15420287

-----DISABLING FDIFF OPTION-----

10 9 -284.636957497 0.000000021 0.000090210 0.000004715 198390689
11313397

11 10 -284.636957499 -0.000000002 0.000124369 0.000006650 198390757
11313391

12 11 -284.636957502 -0.000000002 0.000071103 0.000006558 198390799
11313386

13 12 -284.636957503 -0.000000002 0.000080818 0.000003980 198390799
11313384

14 13 -284.636957504 -0.000000001 0.000018425 0.000001728 198390876
11313382

15 14 -284.636957504 0.000000000 0.000019450 0.000001009 198390788
11313384

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 49.1 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 16.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369575044 AFTER 15 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6026693324
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998561034

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 51.74 , TOTAL = 8536.2 SECONDS (142.3 MIN)
WALL CLOCK TIME: STEP = 47.93 , TOTAL = 7894.4 SECONDS (131.6
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.76 , TOTAL = 8540.0 SECONDS (142.3 MIN)
WALL CLOCK TIME: STEP = 3.82 , TOTAL = 7898.3 SECONDS (131.6
MIN)
CPU UTILIZATION: STEP = 98.48% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.83 , TOTAL = 8542.8 SECONDS (142.4 MIN)

WALL CLOCK TIME: STEP = 2.68 , TOTAL = 7900.9 SECONDS (131.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 96 ENERGY= -284.6369575

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000492	-0.0000500	0.0000867
2 C	6.0	0.0000079	0.0000368	0.0000585
3 C	6.0	-0.0000236	-0.0000060	0.0001231
4 C	6.0	0.0000103	0.0000816	-0.0000005
5 C	6.0	0.0000093	0.0000748	-0.0001454
6 C	6.0	0.0000324	-0.0000555	0.0000328
7 C	6.0	-0.0000144	-0.0000224	0.0000569
8 C	6.0	0.0000185	0.0000355	0.0000162
9 C	6.0	0.0000028	0.0000190	-0.0000629
10 C	6.0	0.0000219	-0.0000204	-0.0000514
11 C	6.0	0.0000387	-0.0000617	0.0001064
12 N	7.0	-0.0000431	-0.0000558	0.0000422
13 C	6.0	0.0000554	0.0000554	-0.0000796
14 C	6.0	-0.0000060	0.0000158	-0.0000246
15 C	6.0	-0.0000491	0.0000595	-0.0000427
16 C	6.0	0.0000255	0.0000139	-0.0000092
17 C	6.0	-0.0000478	-0.0000896	-0.0000630
18 C	6.0	-0.0000336	0.0000526	0.0000467
19 C	6.0	0.0000228	0.0000517	0.0000799
20 O	8.0	0.0000261	0.0000767	-0.0000886
21 N	7.0	-0.0000239	0.0000222	-0.0000049
22 H	1.0	-0.0000019	0.0000184	0.0000009
23 H	1.0	0.0000042	0.0000604	0.0000109
24 H	1.0	-0.0000393	0.0000873	0.0000072
25 H	1.0	0.0000221	-0.0000606	0.0000106
26 H	1.0	-0.0000219	-0.0000315	0.0000170
27 H	1.0	0.0000355	-0.0001128	-0.0000541
28 H	1.0	0.0000698	-0.0000266	-0.0001190
29 H	1.0	0.0000718	0.0000487	0.0000451
30 H	1.0	0.0000415	0.0000183	0.0001147
31 H	1.0	-0.0000543	-0.0000186	0.0000387
32 H	1.0	0.0000239	-0.0000584	-0.0000308
33 H	1.0	-0.0000327	-0.0000474	-0.0000786
34 H	1.0	-0.0001853	-0.0001186	-0.0000313
35 H	1.0	-0.0000128	0.0000071	-0.0000080

MAXIMUM GRADIENT = 0.0001853 RMS GRADIENT = 0.0000557
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0000020589
PREDICTED ENERGY CHANGE WAS -0.0000014529 RATIO= 1.417
GDIIS STEP HAS LENGTH = 0.024029
RADIUS OF STEP TAKEN= 0.02403 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.04 , TOTAL = 8542.9 SECONDS (142.4 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7901.0 SECONDS (131.7
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 97

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1627834349	-1.7201958787	0.8922261844
C	6.0	4.9801611773	0.6184612483	0.5613533856
C	6.0	5.1762205123	-0.7217835331	0.2010208589
C	6.0	4.0358272711	-1.5358886008	-0.0949102929
C	6.0	2.7302222995	-1.0179610201	-0.0036994297
C	6.0	2.4670256140	0.3480049611	0.4315484850
C	6.0	3.6530239131	1.1753334896	0.6798932529
C	6.0	3.5119909202	2.5623112610	1.0572309814
C	6.0	2.2464155884	3.1428263552	1.2200916029
C	6.0	1.0772386831	2.3385413890	1.0429333185
C	6.0	1.1640633822	0.9843674792	0.6437135572
N	7.0	-0.0493433817	0.1852188910	0.5965527024
C	6.0	-1.2453010868	0.7058310459	0.3274253061
C	6.0	-2.5470199697	0.0393250097	0.4408968699
C	6.0	-2.8141639767	-1.2839827621	0.9354360074
C	6.0	-4.1122271555	-1.8117717263	1.0551250146
C	6.0	-5.2243986902	-1.0037017594	0.6675255297
C	6.0	-5.0145557130	0.3102613537	0.1625513311
C	6.0	-3.6976107109	0.8193619644	0.0546071409
O	8.0	-1.6913494723	-2.1367283521	1.3360091680
N	7.0	1.6171573055	-1.9443096050	-0.4287764146
H	1.0	5.8460110895	1.2745540733	0.7639572358
H	1.0	6.1919122663	-1.1471839558	0.1200743770
H	1.0	4.1944697444	-2.5791812255	-0.4319846719
H	1.0	4.4276703250	3.1567029858	1.2292759369
H	1.0	2.1427303241	4.1990788953	1.5246246476

H	1.0	0.0944077874	2.7848950325	1.2759765524
H	1.0	-1.2903063356	1.7552526895	-0.0269282592
H	1.0	-4.2805270639	-2.8350703504	1.4420302839
H	1.0	-6.2473207360	-1.4111698526	0.7618748082
H	1.0	-5.8738756976	0.9347039608	-0.1390789591
H	1.0	-3.5361704999	1.8438096399	-0.3291365871
H	1.0	-2.0087342179	-2.9504893465	1.8056654556
H	1.0	1.2428262984	-1.6584980479	-1.3605047818
H	1.0	2.0067437710	-2.8998207090	-0.5517135982

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3652514	5.1584051	4.0011094
2 C	5.3652514	0.0000000	1.4016187 *	2.4420630 *
3 C	5.1584051	1.4016187 *	0.0000000	1.4320751 *
4 C	4.0011094	2.4420630 *	1.4320751 *	0.0000000
5 C	2.8084798 *	2.8389060 *	2.4723549 *	1.4075414 *
6 C	3.1303691	2.5309773 *	2.9218705 *	2.5074594 *
7 C	4.5399289	1.4441093 *	2.4796168 *	2.8456254 *
8 C	5.4391438	2.4859548 *	3.7799517	4.2891813
9 C	5.3007550	3.7788517	4.9555496	5.1789572
10 C	4.1632066	4.2922487	5.1842123	5.0059107
11 C	2.8946473 *	3.8344847	4.3822749	3.8915657
12 N	1.9398521 *	5.0482526	5.3184224	4.4865300
13 C	2.8613474 *	6.2304684	6.5795137	5.7527377
14 C	3.2623069	7.5503884	7.7643590	6.7898649
15 C	3.0090472	8.0318575	8.0437353	6.9316268
16 C	4.2790931	9.4245089	9.3911037	8.2334369
17 C	5.4392633	10.3332341	10.4148924	9.3067887
18 C	5.6089235	10.0074170	10.2429740	9.2403457
19 C	4.6961263	8.6948765	9.0078547	8.0855194
20 O	1.9514742 *	7.2594914	7.1030828	5.9337250
21 N	1.9774929 *	4.3425737	3.8155138	2.4755280 *
22 H	6.4252671	1.1050802 *	2.1796515 *	3.4515224
23 H	6.1053219	2.1864517 *	1.1041502 *	2.2013660 *
24 H	4.3296518	3.4393239	2.1941870 *	1.1078114 *
25 H	6.4874498	2.6821704 *	4.0817023	4.8915668
26 H	6.2735900	4.6690179	5.9303353	6.2527243
27 H	4.5219226	5.3920968	6.2671481	6.0069368
28 H	3.8775066	6.3997760	6.9284658	6.2613043
29 H	4.6139178	9.9228433	9.7691433	8.5563900
30 H	6.4188725	11.4112209	11.4580585	10.3195333
31 H	6.6748286	10.8812100	11.1787408	10.2131284

32 H	5.2797843	8.6499917	9.0977521	8.2953223
33 H	2.6577212 *	7.9454628	7.6919171	6.4923037
34 H	2.4990190 *	4.7797233	4.3344419	3.0688136
35 H	2.6223399 *	4.7390334	3.9186781	2.4871992 *

C C C C

1 CO	2.8084798 *	3.1303691	4.5399289	5.4391438
2 C	2.8389060 *	2.5309773 *	1.4441093 *	2.4859548 *
3 C	2.4723549 *	2.9218705 *	2.4796168 *	3.7799517
4 C	1.4075414 *	2.5074594 *	2.8456254 *	4.2891813
5 C	0.0000000	1.4575926 *	2.4757630 *	3.8151127
6 C	1.4575926 *	0.0000000	1.4672217 *	2.5271691 *
7 C	2.4757630 *	1.4672217 *	0.0000000	1.4442927 *
8 C	3.8151127	2.5271691 *	1.4442927 *	0.0000000
9 C	4.3639300	2.9123007 *	2.4781827 *	1.4018567 *
10 C	3.8850873	2.5035044 *	2.8494772 *	2.4450554 *
11 C	2.6232264 *	1.4654971 *	2.4965379 *	2.8589626 *
12 N	3.0877063	2.5270217 *	3.8333792	4.3064945
13 C	4.3457898	3.7309852	4.9333816	5.1585814
14 C	5.4004449	5.0235469	6.3077871	6.5921878
15 C	5.6296503	5.5505180	6.9237315	7.4046639
16 C	6.9692438	6.9527009	8.3284285	8.7898412
17 C	7.9829031	7.8128615	9.1409507	9.4441952
18 C	7.8596056	7.4865107	8.7259916	8.8642077
19 C	6.6855211	6.1941104	7.3857652	7.4847500
20 O	4.7536046	4.9278831	6.3215954	7.0166546
21 N	1.5092136 *	2.5917448 *	3.8866534	5.1096227
22 H	3.9437371	3.5194505	2.1968396 *	2.6817864 *
23 H	3.4663116	4.0258399	3.4861782	4.6712520
24 H	2.1828553 *	3.5068749	3.9529504	5.3961547
25 H	4.6721919	3.5169989	2.1972081 *	1.1051560 *
26 H	5.4679454	4.0163109	3.4839050	2.1845685 *
27 H	4.8007086	3.5043983	3.9509179	3.4318024
28 H	4.8842506	4.0383277	5.0271679	4.9888680
29 H	7.3852981	7.5287787	8.9221871	9.4869982
30 H	9.0187026	8.8962713	10.2329636	10.5413449
31 H	8.8239294	8.3809585	9.5650632	9.6007685
32 H	6.8966165	6.2333327	7.2903716	7.2190608
33 H	5.4282756	5.7271885	7.0954409	7.8376993
34 H	2.1127128 *	2.9557018 *	4.2429798	5.3674748
35 H	2.0892909 *	3.4244759	4.5644250	5.8897672

C C C N

1 CO	5.3007550	4.1632066	2.8946473 *	1.9398521 *
------	-----------	-----------	-------------	-------------

2 C	3.7788517	4.2922487	3.8344847	5.0482526
3 C	4.9555496	5.1842123	4.3822749	5.3184224
4 C	5.1789572	5.0059107	3.8915657	4.4865300
5 C	4.3639300	3.8850873	2.6232264 *	3.0877063
6 C	2.9123007 *	2.5035044 *	1.4654971 *	2.5270217 *
7 C	2.4781827 *	2.8494772 *	2.4965379 *	3.8333792
8 C	1.4018567 *	2.4450554 *	2.8589626 *	4.3064945
9 C	0.0000000	1.4301168 *	2.4824671 *	3.7956227
10 C	1.4301168 *	0.0000000	1.4144617 *	2.4708785 *
11 C	2.4824671 *	1.4144617 *	0.0000000	1.4536914 *
12 N	3.7956227	2.4708785 *	1.4536914 *	0.0000000
13 C	4.3506189	2.9277783 *	2.4459472 *	1.3318338 *
14 C	5.7633228	4.3340621	3.8348898	2.5067713 *
15 C	6.7295716	5.3176359	4.5887697	3.1492266
16 C	8.0627287	6.6449833	5.9855573	4.5503060
17 C	8.5622480	7.1429793	6.6906976	5.3103453
18 C	7.8653366	6.4806598	6.2338808	4.9857122
19 C	6.4875488	5.1072381	4.9000151	3.7424186
20 O	6.5873461	5.2705800	4.2864782	2.9384382 *
21 N	5.3845783	4.5607296	3.1516152	2.8919571 *
22 H	4.0811258	4.8939848	4.6924728	5.9974895
23 H	5.9313717	6.2579418	5.4860709	6.3996563
24 H	6.2662303	6.0063723	4.7999342	5.1681473
25 H	2.1813182 *	3.4539114	3.9639696	5.4105183
26 H	1.1041560 *	2.1974755 *	3.4739261	4.6666451
27 H	2.1822868 *	1.1043085 *	2.1876515 *	2.6908358 *
28 H	3.9986024	2.6627240 *	2.6585626 *	2.0961211 *
29 H	8.8535578	7.4586320	6.6984312	5.2668676
30 H	9.6484403	8.2333771	7.7898123	6.4023989
31 H	8.5242172	7.1892909	7.0815123	5.9184507
32 H	6.1258350	4.8384791	4.8761949	3.9706155
33 H	7.4550448	6.1708051	5.1865089	3.8902226
34 H	5.5425071	4.6669324	3.3178054	2.9831307 *
35 H	6.3016125	5.5540360	4.1504306	3.8811698

C C C C

1 CO	2.8613474 *	3.2623069	3.0090472	4.2790931
2 C	6.2304684	7.5503884	8.0318575	9.4245089
3 C	6.5795137	7.7643590	8.0437353	9.3911037
4 C	5.7527377	6.7898649	6.9316268	8.2334369
5 C	4.3457898	5.4004449	5.6296503	6.9692438
6 C	3.7309852	5.0235469	5.5505180	6.9527009
7 C	4.9333816	6.3077871	6.9237315	8.3284285
8 C	5.1585814	6.5921878	7.4046639	8.7898412
9 C	4.3506189	5.7633228	6.7295716	8.0627287

10 C	2.9277783 *	4.3340621	5.3176359	6.6449833
11 C	2.4459472 *	3.8348898	4.5887697	5.9855573
12 N	1.3318338 *	2.5067713 *	3.1492266	4.5503060
13 C	0.0000000	1.4668259 *	2.6058332 *	3.8842162
14 C	1.4668259 *	0.0000000	1.4377338 *	2.5007417 *
15 C	2.6058332 *	1.4377338 *	0.0000000	1.4063622 *
16 C	3.8842162	2.5007417 *	1.4063622 *	0.0000000
17 C	4.3441211	2.8822946 *	2.4412220 *	1.4283333 *
18 C	3.7935391	2.4979222 *	2.8250113 *	2.4726320 *
19 C	2.4700489 *	1.4427531 *	2.4454850 *	2.8453132 *
20 O	3.0489907	2.5037185 *	1.4657238 *	2.4586869 *
21 N	3.9735066	4.6937736	4.6833445	5.9199135
22 H	7.1274620	8.4895895	9.0318408	10.4296066
23 H	7.6673856	8.8249457	9.0439448	10.3678004
24 H	6.3999309	7.2846538	7.2572946	8.4735840
25 H	6.2452152	7.6802273	8.5000115	9.8815949
26 H	5.0114692	6.3617432	7.4149787	8.6876492
27 H	2.6489765 *	3.9003402	5.0131352	6.2348936
28 H	1.1085476 *	2.1777505 *	3.5334458	4.6752262
29 H	4.7950937	3.5027794	2.1937938 *	1.1068697 *
30 H	5.4489118	3.9873786	3.4398932	2.1920543 *
31 H	4.6576509	3.4937150	3.9292479	3.4745730
32 H	2.6408619 *	2.1971652 *	3.4501482	3.9511133
33 H	4.0170515	3.3303656	2.0453021 *	2.5069247 *
34 H	3.8249102	4.5266528	4.6766201	5.8766791
35 H	4.9345117	5.5100469	5.2975181	6.4193135

C C C O

1 CO	5.4392633	5.6089235	4.6961263	1.9514742 *
2 C	10.3332341	10.0074170	8.6948765	7.2594914
3 C	10.4148924	10.2429740	9.0078547	7.1030828
4 C	9.3067887	9.2403457	8.0855194	5.9337250
5 C	7.9829031	7.8596056	6.6855211	4.7536046
6 C	7.8128615	7.4865107	6.1941104	4.9278831
7 C	9.1409507	8.7259916	7.3857652	6.3215954
8 C	9.4441952	8.8642077	7.4847500	7.0166546
9 C	8.5622480	7.8653366	6.4875488	6.5873461
10 C	7.1429793	6.4806598	5.1072381	5.2705800
11 C	6.6906976	6.2338808	4.9000151	4.2864782
12 N	5.3103453	4.9857122	3.7424186	2.9384382 *
13 C	4.3441211	3.7935391	2.4700489 *	3.0489907
14 C	2.8822946 *	2.4979222 *	1.4427531 *	2.5037185 *
15 C	2.4412220 *	2.8250113 *	2.4454850 *	1.4657238 *
16 C	1.4283333 *	2.4726320 *	2.8453132 *	2.4586869 *
17 C	0.0000000	1.4232119 *	2.4556693 *	3.7700207

18 C	1.4232119 *	0.0000000	1.4160436 *	4.2905083
19 C	2.4556693 *	1.4160436 *	0.0000000	3.7954638
20 O	3.7700207	4.2905083	3.7954638	0.0000000
21 N	6.9923894	7.0293937	6.0098502	3.7546918
22 H	11.3028192	10.9198654	9.5807669	8.2931234
23 H	11.4303301	11.3009237	10.0833652	8.0376309
24 H	9.6128113	9.6699794	8.6064976	6.1615286
25 H	10.5255388	9.9194639	8.5359945	8.0916136
26 H	9.0596984	8.2586251	6.9060134	7.4079820
27 H	6.5584587	5.7848972	4.4423494	5.2359249
28 H	4.8550158	3.9992419	2.5841157 *	4.1431812
29 H	2.2010593 *	3.4740432	3.9521652	2.6837963 *
30 H	1.1051251 *	2.2005053 *	3.4607110	4.6489719
31 H	2.1976915 *	1.1042374 *	2.1879094 *	5.3947296
32 H	3.4571333	2.1861268 *	1.1058098 *	4.6926280
33 H	3.9275746	4.7294061	4.4866789	0.9917243 *
34 H	6.8093072	6.7342812	5.7052826	4.0136366
35 H	7.5743800	7.7532863	6.8366369	4.2215756

N H H H

1 CO	1.9774929 *	6.4252671	6.1053219	4.3296518
2 C	4.3425737	1.1050802 *	2.1864517 *	3.4393239
3 C	3.8155138	2.1796515 *	1.1041502 *	2.1941870 *
4 C	2.4755280 *	3.4515224	2.2013660 *	1.1078114 *
5 C	1.5092136 *	3.9437371	3.4663116	2.1828553 *
6 C	2.5917448 *	3.5194505	4.0258399	3.5068749
7 C	3.8866534	2.1968396 *	3.4861782	3.9529504
8 C	5.1096227	2.6817864 *	4.6712520	5.3961547
9 C	5.3845783	4.0811258	5.9313717	6.2662303
10 C	4.5607296	4.8939848	6.2579418	6.0063723
11 C	3.1516152	4.6924728	5.4860709	4.7999342
12 N	2.8919571 *	5.9974895	6.3996563	5.1681473
13 C	3.9735066	7.1274620	7.6673856	6.3999309
14 C	4.6937736	8.4895895	8.8249457	7.2846538
15 C	4.6833445	9.0318408	9.0439448	7.2572946
16 C	5.9199135	10.4296066	10.3678004	8.4735840
17 C	6.9923894	11.3028192	11.4303301	9.6128113
18 C	7.0293937	10.9198654	11.3009237	9.6699794
19 C	6.0098502	9.5807669	10.0833652	8.6064976
20 O	3.7546918	8.2931234	8.0376309	6.1615286
21 N	0.0000000	5.4467331	4.6760057	2.6543571 *
22 H	5.4467331	0.0000000	2.5296339 *	4.3599474
23 H	4.6760057	2.5296339 *	0.0000000	2.5189605 *
24 H	2.6543571 *	4.3599474	2.5189605 *	0.0000000
25 H	6.0554480	2.4022274 *	4.7818742	5.9761641

26 H	6.4678609	4.7797227	6.8520918	7.3472964
27 H	5.2526494	5.9686040	7.3468984	6.9642626
28 H	4.7224557	7.1960821	8.0267891	7.0024393
29 H	6.2510842	10.9496836	10.6896451	8.6834891
30 H	7.9719448	12.3879696	12.4585759	10.5745231
31 H	8.0304557	11.7595374	12.2468223	10.6679315
32 H	6.3966056	9.4627817	10.1874152	8.9070884
33 H	4.3763247	8.9795975	8.5640954	6.6048987
34 H	1.0439970 *	5.8570849	5.1910508	3.2283132
35 H	1.0391788 *	5.8220588	4.5867930	2.2143373 *

H H H H

1 CO	6.4874498	6.2735900	4.5219226	3.8775066
2 C	2.6821704 *	4.6690179	5.3920968	6.3997760
3 C	4.0817023	5.9303353	6.2671481	6.9284658
4 C	4.8915668	6.2527243	6.0069368	6.2613043
5 C	4.6721919	5.4679454	4.8007086	4.8842506
6 C	3.5169989	4.0163109	3.5043983	4.0383277
7 C	2.1972081 *	3.4839050	3.9509179	5.0271679
8 C	1.1051560 *	2.1845685 *	3.4318024	4.9888680
9 C	2.1813182 *	1.1041560 *	2.1822868 *	3.9986024
10 C	3.4539114	2.1974755 *	1.1043085 *	2.6627240 *
11 C	3.9639696	3.4739261	2.1876515 *	2.6585626 *
12 N	5.4105183	4.6666451	2.6908358 *	2.0961211 *
13 C	6.2452152	5.0114692	2.6489765 *	1.1085476 *
14 C	7.6802273	6.3617432	3.9003402	2.1777505 *
15 C	8.5000115	7.4149787	5.0131352	3.5334458
16 C	9.8815949	8.6876492	6.2348936	4.6752262
17 C	10.5255388	9.0596984	6.5584587	4.8550158
18 C	9.9194639	8.2586251	5.7848972	3.9992419
19 C	8.5359945	6.9060134	4.4423494	2.5841157 *
20 O	8.0916136	7.4079820	5.2359249	4.1431812
21 N	6.0554480	6.4678609	5.2526494	4.7224557
22 H	2.4022274 *	4.7797227	5.9686040	7.1960821
23 H	4.7818742	6.8520918	7.3468984	8.0267891
24 H	5.9761641	7.3472964	6.9642626	7.0024393
25 H	0.0000000	2.5287802 *	4.3494352	6.0197483
26 H	2.5287802 *	0.0000000	2.5014730 *	4.4905839
27 H	4.3494352	2.5014730 *	0.0000000	2.1622113 *
28 H	6.0197483	4.4905839	2.1622113 *	0.0000000
29 H	10.5725737	9.5259809	7.1240185	5.6718890
30 H	11.6206437	10.1217407	7.6215997	5.9346806
31 H	10.6269245	8.8141945	6.4067150	4.6577877
32 H	8.2204075	6.4213424	4.0795991	2.2678355 *
33 H	8.8914187	8.2722408	6.1317543	5.1008378

34 H	6.3274289	6.5912826	5.2927914	4.4552083
35 H	6.7612342	7.3975704	6.2700457	5.7284943

H H H H

1 CO	4.6139178	6.4188725	6.6748286	5.2797843
2 C	9.9228433	11.4112209	10.8812100	8.6499917
3 C	9.7691433	11.4580585	11.1787408	9.0977521
4 C	8.5563900	10.3195333	10.2131284	8.2953223
5 C	7.3852981	9.0187026	8.8239294	6.8966165
6 C	7.5287787	8.8962713	8.3809585	6.2333327
7 C	8.9221871	10.2329636	9.5650632	7.2903716
8 C	9.4869982	10.5413449	9.6007685	7.2190608
9 C	8.8535578	9.6484403	8.5242172	6.1258350
10 C	7.4586320	8.2333771	7.1892909	4.8384791
11 C	6.6984312	7.7898123	7.0815123	4.8761949
12 N	5.2668676	6.4023989	5.9184507	3.9706155
13 C	4.7950937	5.4489118	4.6576509	2.6408619 *
14 C	3.5027794	3.9873786	3.4937150	2.1971652 *
15 C	2.1937938 *	3.4398932	3.9292479	3.4501482
16 C	1.1068697 *	2.1920543 *	3.4745730	3.9511133
17 C	2.2010593 *	1.1051251 *	2.1976915 *	3.4571333
18 C	3.4740432	2.2005053 *	1.1042374 *	2.1861268 *
19 C	3.9521652	3.4607110	2.1879094 *	1.1058098 *
20 O	2.6837963 *	4.6489719	5.3947296	4.6926280
21 N	6.2510842	7.9719448	8.0304557	6.3966056
22 H	10.9496836	12.3879696	11.7595374	9.4627817
23 H	10.6896451	12.4585759	12.2468223	10.1874152
24 H	8.6834891	10.5745231	10.6679315	8.9070884
25 H	10.5725737	11.6206437	10.6269245	8.2204075
26 H	9.5259809	10.1217407	8.8141945	6.4213424
27 H	7.1240185	7.6215997	6.4067150	4.0795991
28 H	5.6718890	5.9346806	4.6577877	2.2678355 *
29 H	0.0000000	2.5215831 *	4.3874668	5.0579657
30 H	2.5215831 *	0.0000000	2.5405320 *	4.3744180
31 H	4.3874668	2.5405320 *	0.0000000	2.5154444 *
32 H	5.0579657	4.3744180	2.5154444 *	0.0000000
33 H	2.3036047 *	4.6286736	5.8151592	5.4658708
34 H	6.3044395	7.7889646	7.6722894	6.0140411
35 H	6.5961339	8.4894745	8.7737113	7.2990046

H H H

1 CO	2.6577212 *	2.4990190 *	2.6223399 *
2 C	7.9454628	4.7797233	4.7390334
3 C	7.6919171	4.3344419	3.9186781

4 C	6.4923037	3.0688136	2.4871992 *
5 C	5.4282756	2.1127128 *	2.0892909 *
6 C	5.7271885	2.9557018 *	3.4244759
7 C	7.0954409	4.2429798	4.5644250
8 C	7.8376993	5.3674748	5.8897672
9 C	7.4550448	5.5425071	6.3016125
10 C	6.1708051	4.6669324	5.5540360
11 C	5.1865089	3.3178054	4.1504306
12 N	3.8902226	2.9831307 *	3.8811698
13 C	4.0170515	3.8249102	4.9345117
14 C	3.3303656	4.5266528	5.5100469
15 C	2.0453021 *	4.6766201	5.2975181
16 C	2.5069247 *	5.8766791	6.4193135
17 C	3.9275746	6.8093072	7.5743800
18 C	4.7294061	6.7342812	7.7532863
19 C	4.4866789	5.7052826	6.8366369
20 O	0.9917243 *	4.0136366	4.2215756
21 N	4.3763247	1.0439970 *	1.0391788 *
22 H	8.9795975	5.8570849	5.8220588
23 H	8.5640954	5.1910508	4.5867930
24 H	6.6048987	3.2283132	2.2143373 *
25 H	8.8914187	6.3274289	6.7612342
26 H	8.2722408	6.5912826	7.3975704
27 H	6.1317543	5.2927914	6.2700457
28 H	5.1008378	4.4552083	5.7284943
29 H	2.3036047 *	6.3044395	6.5961339
30 H	4.6286736	7.7889646	8.4894745
31 H	5.8151592	7.6722894	8.7737113
32 H	5.4658708	6.0140411	7.2990046
33 H	0.0000000	4.7187415	4.6565939
34 H	4.7187415	0.0000000	1.6669118 *
35 H	4.6565939	1.6669118 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.79 , TOTAL = 8543.6 SECONDS (142.4 MIN)

WALL CLOCK TIME: STEP = 0.80 , TOTAL = 7901.8 SECONDS (131.7 MIN)

CPU UTILIZATION: STEP = 98.54% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.96 , TOTAL = 8544.6 SECONDS (142.4 MIN)

WALL CLOCK TIME: STEP = 0.95 , TOTAL = 7902.7 SECONDS (131.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636948786	-284.636948786	0.004083109	0.000354259	198409461
11311866						
2	1	-284.636960103	-0.000011318	0.000943022	0.000023337	148985687
15471106						
3	2	-284.636960075	0.000000028	0.000424435	0.000048060	132197498
16796238						
4	3	-284.636960284	-0.000000208	0.000325194	0.000023131	125451638
17300159						
5	4	-284.636960254	0.000000030	0.000104020	0.000036375	121064642
17618235						
6	5	-284.636960299	-0.000000045	0.000099681	0.000010425	113301654
18197555						
7	6	-284.636960273	0.000000026	0.000050298	0.000011655	111673749
18307107						
8	7	-284.636960283	-0.000000010	0.000063421	0.000008073	129461497
17016645						
9	8	-284.636960285	-0.000000002	0.000090909	0.000007441	152800095
15220750						

-----DISABLING FDIFF OPTION-----

10	9	-284.636960288	-0.000000003	0.000160563	0.000006543	198409207
11311874						
11	10	-284.636960293	-0.000000005	0.000135979	0.000006990	198409473
11311863						
12	11	-284.636960297	-0.000000003	0.000109432	0.000008071	198409342
11311861						
13	12	-284.636960300	-0.000000003	0.000090487	0.000006469	198409097
11311875						
14	13	-284.636960301	-0.000000002	0.000042413	0.000003165	198409036
11311879						
15	14	-284.636960302	-0.000000001	0.000016855	0.000002082	198409174
11311868						
16	15	-284.636960302	0.000000000	0.000008425	0.000001293	198409120
11311874						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 52.6 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 17.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
TIME TO SOLVE SCF EQUATIONS= 2.2 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369603019 AFTER 16 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6024626472
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998585595

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 55.75 , TOTAL = 8600.4 SECONDS (143.3 MIN)
WALL CLOCK TIME: STEP = 51.25 , TOTAL = 7954.0 SECONDS (132.6
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.85 , TOTAL = 8604.2 SECONDS (143.4 MIN)
WALL CLOCK TIME: STEP = 3.81 , TOTAL = 7957.8 SECONDS (132.6
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.89 , TOTAL = 8607.1 SECONDS (143.5 MIN)
WALL CLOCK TIME: STEP = 2.72 , TOTAL = 7960.5 SECONDS (132.7
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH= 97 ENERGY= -284.6369603

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000751	-0.0000211	0.0000999
2 C	6.0	-0.0000133	0.0000613	0.0000694
3 C	6.0	0.0000279	-0.0000112	0.0000217
4 C	6.0	-0.0000210	0.0000440	0.0000134
5 C	6.0	-0.0000263	0.0001054	-0.0000050
6 C	6.0	0.0000090	0.0000396	0.0000017
7 C	6.0	0.0000460	-0.0000541	-0.0000299
8 C	6.0	0.0000089	0.0000452	-0.0000014
9 C	6.0	0.0000047	0.0000375	-0.0000126
10 C	6.0	-0.0000031	-0.0000271	-0.0000139
11 C	6.0	-0.0000159	-0.0000778	0.0000163
12 N	7.0	-0.0000077	0.0000018	0.0000105
13 C	6.0	0.0000165	-0.0000839	-0.0000270
14 C	6.0	0.0000407	0.0000191	-0.0000089
15 C	6.0	0.0000582	0.0000049	-0.0000248
16 C	6.0	0.0000515	0.0000209	-0.0000772
17 C	6.0	-0.0000186	-0.0000619	-0.0000028
18 C	6.0	-0.0001209	0.0000251	0.0000179
19 C	6.0	-0.0000078	0.0000860	0.0000888
20 O	8.0	0.0000025	-0.0000217	-0.0000313
21 N	7.0	-0.0000462	-0.0000077	-0.0000330
22 H	1.0	0.0000159	-0.0000240	0.0000294
23 H	1.0	0.0000164	0.0000494	0.0000522
24 H	1.0	0.0000308	0.0000083	-0.0000168
25 H	1.0	0.0000999	-0.0000004	0.0000164
26 H	1.0	-0.0000365	-0.0001050	0.0000119
27 H	1.0	-0.0000829	-0.0000781	-0.0000418
28 H	1.0	0.0000844	0.0000393	-0.0001291
29 H	1.0	0.0000685	0.0000062	0.0000722
30 H	1.0	0.0000193	0.0000720	0.0000724
31 H	1.0	-0.0000565	0.0000182	0.0000323
32 H	1.0	0.0000331	-0.0001006	-0.0000381
33 H	1.0	-0.0000257	0.0000303	-0.0001154
34 H	1.0	-0.0001359	-0.0001171	0.0000066
35 H	1.0	-0.0000908	0.0000770	-0.0000240

MAXIMUM GRADIENT = 0.0001359 RMS GRADIENT = 0.0000529
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000027975
 PREDICTED ENERGY CHANGE WAS -0.0000019923 RATIO= 1.404

GDIIS STEP HAS LENGTH = 0.020510
RADIUS OF STEP TAKEN= 0.02051 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8607.1 SECONDS (143.5 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 7960.5 SECONDS (132.7 MIN)
CPU UTILIZATION: STEP = 81.44%, TOTAL = 100.00%

1NSERCH= 98

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1628414894	-1.7190176494	0.8935082451
C	6.0	4.9801297882	0.6177566260	0.5601372323
C	6.0	5.1754548180	-0.7227220664	0.2001971603
C	6.0	4.0347282999	-1.5366267216	-0.0948662509
C	6.0	2.7294576465	-1.0178629733	-0.0032703297
C	6.0	2.4668858401	0.3486582567	0.4311460611
C	6.0	3.6532929637	1.1756100448	0.6789701706
C	6.0	3.5126385284	2.5625107714	1.0566859519
C	6.0	2.2471877889	3.1430043169	1.2209632682
C	6.0	1.0775520515	2.3393414597	1.0437837953
C	6.0	1.1640659075	0.9854400040	0.6435420711
N	7.0	-0.0492736584	0.1862403506	0.5969432511
C	6.0	-1.2454690753	0.7064080639	0.3284416472
C	6.0	-2.5467801421	0.0390902642	0.4415166938
C	6.0	-2.8136741686	-1.2842337322	0.9360887724
C	6.0	-4.1116217320	-1.8126158424	1.0547200495
C	6.0	-5.2237029318	-1.0048845265	0.6660221978
C	6.0	-5.0139818669	0.3089409231	0.1608785613
C	6.0	-3.6973021692	0.8185498502	0.0540515119
O	8.0	-1.6907567307	-2.1361524907	1.3383244578
N	7.0	1.6157923652	-1.9430854541	-0.4285740093
H	1.0	5.8465226338	1.2732212031	0.7629923937
H	1.0	6.1909138310	-1.1488626843	0.1196076218
H	1.0	4.1929613905	-2.5801215304	-0.4314767595
H	1.0	4.4282600040	3.1571200407	1.2281583023
H	1.0	2.1439419516	4.1992020871	1.5261836085
H	1.0	0.0948690358	2.7860889313	1.2772906065
H	1.0	-1.2910248923	1.7558106854	-0.0254536581
H	1.0	-4.2799661857	-2.8358375566	1.4414953027
H	1.0	-6.2466431506	-1.4128357901	0.7589267529
H	1.0	-5.8733168817	0.9330882076	-0.1414310832

H	1.0	-3.5361739241	1.8433263384	-0.3289813313
H	1.0	-2.0078882994	-2.9493346141	1.8090442290
H	1.0	1.2414224592	-1.6554130393	-1.3597007974
H	1.0	2.0046540156	-2.8986967536	-0.5529786962

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C	
1	CO	0.0000000	5.3645053	5.1574778	4.0002073
2	C	5.3645053	0.0000000	1.4016390 *	2.4421673 *
3	C	5.1574778	1.4016390 *	0.0000000	1.4320476 *
4	C	4.0002073	2.4421673 *	1.4320476 *	0.0000000
5	C	2.8077301 *	2.8386977 *	2.4721265 *	1.4075643 *
6	C	3.1301250	2.5308986 *	2.9219068 *	2.5078115 *
7	C	4.5396198	1.4442360 *	2.4798922 *	2.8461455 *
8	C	5.4386812	2.4863950 *	3.7803817	4.2897061
9	C	5.3000928	3.7792246	4.9558603	5.1793489
10	C	4.1628784	4.2927708	5.1846580	5.0064503
11	C	2.8946545 *	3.8346435	4.3824209	3.8918851
12	N	1.9398329 *	5.0480155	5.3180267	4.4861947
13	C	2.8610014 *	6.2305396	6.5792950	5.7524672
14	C	3.2614857	7.5500529	7.7634725	6.7887292
15	C	3.0084042	8.0313316	8.0425751	6.9301650
16	C	4.2785261	9.4239731	9.3897747	8.2316910
17	C	5.4384370	10.3325882	10.4134092	9.3048509
18	C	5.6079285	10.0068498	10.2416060	9.2385432
19	C	4.6951726	8.6944963	9.0068138	8.0841405
20	O	1.9513301 *	7.2588097	7.1019702	5.9325075
21	N	1.9771631 *	4.3421456	3.8152112	2.4754435 *
22	H	6.4245435	1.1051790 *	2.1796468 *	3.4516323
23	H	6.1042325	2.1865517 *	1.1041954 *	2.2012487 *
24	H	4.3288511	3.4393832	2.1941372 *	1.1078022 *
25	H	6.4871029	2.6831286 *	4.0826681	4.8924963
26	H	6.2729867	4.6694709	5.9307375	6.2532078
27	H	4.5219348	5.3927494	6.2677138	6.0075932
28	H	3.8771962	6.4004269	6.9288818	6.2616778
29	H	4.6136880	9.9223728	9.7678587	8.5546771
30	H	6.4182048	11.4106640	11.4565596	10.3175038
31	H	6.6738274	10.8806680	11.1773778	10.2113182
32	H	5.2789668	8.6498544	9.0970935	8.2944230
33	H	2.6578100 *	7.9445771	7.6906834	6.4910580
34	H	2.4988664 *	4.7781807	4.3335672	3.0686274
35	H	2.6222587 *	4.7389796	3.9186882	2.4872281 *

	C	C	C	C
1 CO	2.8077301 *	3.1301250	4.5396198	5.4386812
2 C	2.8386977 *	2.5308986 *	1.4442360 *	2.4863950 *
3 C	2.4721265 *	2.9219068 *	2.4798922 *	3.7803817
4 C	1.4075643 *	2.5078115 *	2.8461455 *	4.2897061
5 C	0.0000000	1.4577523 *	2.4759337 *	3.8152268
6 C	1.4577523 *	0.0000000	1.4672518 *	2.5270619 *
7 C	2.4759337 *	1.4672518 *	0.0000000	1.4442806 *
8 C	3.8152268	2.5270619 *	1.4442806 *	0.0000000
9 C	4.3639602	2.9121209 *	2.4782107 *	1.4019006 *
10 C	3.8853489	2.5036759 *	2.8498774 *	2.4453256 *
11 C	2.6233643 *	1.4655862 *	2.4967321 *	2.8589567 *
12 N	3.0873077	2.5268413 *	3.8333511	4.3064188
13 C	4.3454788	3.7309666	4.9336488	5.1589771
14 C	5.3994139	5.0232247	6.3078497	6.5926200
15 C	5.6284686	5.5502808	6.9237710	7.4050131
16 C	6.9678794	6.9524609	8.3285402	8.7903971
17 C	7.9812834	7.8123236	9.1408851	9.4447123
18 C	7.8580029	7.4858536	8.7258918	8.8647788
19 C	6.6842307	6.1935622	7.3857474	7.4853136
20 O	4.7527616	4.9278037	6.3215019	7.0165575
21 N	1.5090296 *	2.5914413 *	3.8864282	5.1092485
22 H	3.9436429	3.5195005	2.1970080 *	2.6824501 *
23 H	3.4661129	4.0259172	3.4864853	4.6717842
24 H	2.1830840 *	3.5073075	3.9534610	5.3966781
25 H	4.6725613	3.5170548	2.1973992 *	1.1051360 *
26 H	5.4680733	4.0162281	3.4839661	2.1846091 *
27 H	4.8011398	3.5047814	3.9514567	3.4321716
28 H	4.8844690	4.0386204	5.0278350	4.9896867
29 H	7.3840640	7.5287337	8.9224300	9.4876199
30 H	9.0170579	8.8958355	10.2330435	10.5420880
31 H	8.8223029	8.3802377	9.5649449	9.6013885
32 H	6.8956966	6.2328607	7.2904215	7.2196300
33 H	5.4274776	5.7270380	7.0951539	7.8372635
34 H	2.1120186 *	2.9538441 *	4.2412251	5.3654663
35 H	2.0892715 *	3.4245400	4.5646122	5.8898069

	C	C	C	N
1 CO	5.3000928	4.1628784	2.8946545 *	1.9398329 *
2 C	3.7792246	4.2927708	3.8346435	5.0480155
3 C	4.9558603	5.1846580	4.3824209	5.3180267
4 C	5.1793489	5.0064503	3.8918851	4.4861947
5 C	4.3639602	3.8853489	2.6233643 *	3.0873077
6 C	2.9121209 *	2.5036759 *	1.4655862 *	2.5268413 *

7 C	2.4782107 *	2.8498774 *	2.4967321 *	3.8333511
8 C	1.4019006 *	2.4453256 *	2.8589567 *	4.3064188
9 C	0.0000000	1.4301449 *	2.4822675 *	3.7954696
10 C	1.4301449 *	0.0000000	1.4144707 *	2.4708798 *
11 C	2.4822675 *	1.4144707 *	0.0000000	1.4536452 *
12 N	3.7954696	2.4708798 *	1.4536452 *	0.0000000
13 C	4.3511203	2.9282440 *	2.4460184 *	1.3317474 *
14 C	5.7640219	4.3347047	3.8349407	2.5066610 *
15 C	6.7300753	5.3182269	4.5890542	3.1494799
16 C	8.0635145	6.6457801	5.9859054	4.5505667
17 C	8.5631273	7.1436941	6.6907016	5.3102042
18 C	7.8664020	6.4814222	6.2336899	4.9853320
19 C	6.4885848	5.1079947	4.8998215	3.7420127
20 O	6.5871600	5.2707052	4.2868490	2.9389830 *
21 N	5.3840452	4.5603421	3.1511507	2.8910481 *
22 H	4.0817934	4.8947458	4.6928123	5.9974589
23 H	5.9317857	6.2584454	5.4862515	6.3992413
24 H	6.2666388	6.0069364	4.8003232	5.1678781
25 H	2.1811298 *	3.4539831	3.9639543	5.4104405
26 H	1.1042522 *	2.1974937 *	3.4738278	4.6666416
27 H	2.1824384 *	1.1044341 *	2.1879570 *	2.6912566 *
28 H	3.9996013	2.6634439 *	2.6586645 *	2.0959187 *
29 H	8.8543167	7.4594674	6.6989833	5.2673506
30 H	9.6495762	8.2343071	7.7899711	6.4023958
31 H	8.5253999	7.1900530	7.0812202	5.9179775
32 H	6.1268886	4.8391097	4.8758615	3.9701063
33 H	7.4544017	6.1705478	5.1867273	3.8906542
34 H	5.5404152	4.6649389	3.3155800	2.9809461 *
35 H	6.3014161	5.5539367	4.1502733	3.8804351

C C C C

1 CO	2.8610014 *	3.2614857	3.0084042	4.2785261
2 C	6.2305396	7.5500529	8.0313316	9.4239731
3 C	6.5792950	7.7634725	8.0425751	9.3897747
4 C	5.7524672	6.7887292	6.9301650	8.2316910
5 C	4.3454788	5.3994139	5.6284686	6.9678794
6 C	3.7309666	5.0232247	5.5502808	6.9524609
7 C	4.9336488	6.3078497	6.9237710	8.3285402
8 C	5.1589771	6.5926200	7.4050131	8.7903971
9 C	4.3511203	5.7640219	6.7300753	8.0635145
10 C	2.9282440 *	4.3347047	5.3182269	6.6457801
11 C	2.4460184 *	3.8349407	4.5890542	5.9859054
12 N	1.3317474 *	2.5066610 *	3.1494799	4.5505667
13 C	0.0000000	1.4668025 *	2.6059848 *	3.8843008
14 C	1.4668025 *	0.0000000	1.4377136 *	2.5007125 *

15 C	2.6059848 *	1.4377136 *	0.0000000	1.4063886 *
16 C	3.8843008	2.5007125 *	1.4063886 *	0.0000000
17 C	4.3438264	2.8820482 *	2.4411494 *	1.4283699 *
18 C	3.7931183	2.4977313 *	2.8249797 *	2.4726928 *
19 C	2.4696865 *	1.4427014 *	2.4455034 *	2.8453525 *
20 O	3.0493106	2.5037415 *	1.4657772 *	2.4587995 *
21 N	3.9723678	4.6918108	4.6815130	5.9178084
22 H	7.1278649	8.4896382	9.0315861	10.4293880
23 H	7.6671658	8.8239534	9.0425423	10.3661585
24 H	6.3996311	7.2833031	7.2555153	8.4713604
25 H	6.2455329	7.6806315	8.5003846	9.8822030
26 H	5.0122154	6.3628536	7.4158100	8.6888612
27 H	2.6498855 *	3.9016445	5.0143363	6.2363601
28 H	1.1084056 *	2.1776390 *	3.5333971	4.6750625
29 H	4.7952649	3.5027277	2.1938374 *	1.1067600 *
30 H	5.4486929	3.9872076	3.4399420	2.1921757 *
31 H	4.6571600	3.4935522	3.9292466	3.4746565
32 H	2.6404766 *	2.1972335 *	3.4502232	3.9511622
33 H	4.0172032	3.3303482	2.0454591 *	2.5073550 *
34 H	3.8226500	4.5239590	4.6746372	5.8744551
35 H	4.9332527	5.5077370	5.2952903	6.4166265

C C C O

1 CO	5.4384370	5.6079285	4.6951726	1.9513301 *
2 C	10.3325882	10.0068498	8.6944963	7.2588097
3 C	10.4134092	10.2416060	9.0068138	7.1019702
4 C	9.3048509	9.2385432	8.0841405	5.9325075
5 C	7.9812834	7.8580029	6.6842307	4.7527616
6 C	7.8123236	7.4858536	6.1935622	4.9278037
7 C	9.1408851	8.7258918	7.3857474	6.3215019
8 C	9.4447123	8.8647788	7.4853136	7.0165575
9 C	8.5631273	7.8664020	6.4885848	6.5871600
10 C	7.1436941	6.4814222	5.1079947	5.2707052
11 C	6.6907016	6.2336899	4.8998215	4.2868490
12 N	5.3102042	4.9853320	3.7420127	2.9389830 *
13 C	4.3438264	3.7931183	2.4696865 *	3.0493106
14 C	2.8820482 *	2.4977313 *	1.4427014 *	2.5037415 *
15 C	2.4411494 *	2.8249797 *	2.4455034 *	1.4657772 *
16 C	1.4283699 *	2.4726928 *	2.8453525 *	2.4587995 *
17 C	0.0000000	1.4231270 *	2.4554674 *	3.7700751
18 C	1.4231270 *	0.0000000	1.4158950 *	4.2905345
19 C	2.4554674 *	1.4158950 *	0.0000000	3.7955036
20 O	3.7700751	4.2905345	3.7955036	0.0000000
21 N	6.9897824	7.0265912	6.0073730	3.7539941
22 H	11.3026131	10.9198414	9.5809141	8.2924916

23 H	11.4285946	11.2994063	10.0822530	8.0362145
24 H	9.6103820	9.6677490	8.6048221	6.1601497
25 H	10.5260946	9.9200374	8.5365214	8.0915534
26 H	9.0611581	8.2603912	6.9076852	7.4078960
27 H	6.5599037	5.7864493	4.4438819	5.2364726
28 H	4.8544344	3.9985698	2.5835923 *	4.1433143
29 H	2.2009967 *	3.4739588	3.9520937	2.6840658 *
30 H	1.1051978 *	2.2003705 *	3.4605015	4.6491924
31 H	2.1976618 *	1.1042679 *	2.1877780 *	5.3947868
32 H	3.4568904	2.1859135 *	1.1058225 *	4.6927311
33 H	3.9279574	4.7296309	4.4867663	0.9916727 *
34 H	6.8062168	6.7305967	5.7017707	4.0134929
35 H	7.5711051	7.7498246	6.8336456	4.2207300

N H H H

1 CO	1.9771631 *	6.4245435	6.1042325	4.3288511
2 C	4.3421456	1.1051790 *	2.1865517 *	3.4393832
3 C	3.8152112	2.1796468 *	1.1041954 *	2.1941372 *
4 C	2.4754435 *	3.4516323	2.2012487 *	1.1078022 *
5 C	1.5090296 *	3.9436429	3.4661129	2.1830840 *
6 C	2.5914413 *	3.5195005	4.0259172	3.5073075
7 C	3.8864282	2.1970080 *	3.4864853	3.9534610
8 C	5.1092485	2.6824501 *	4.6717842	5.3966781
9 C	5.3840452	4.0817934	5.9317857	6.2666388
10 C	4.5603421	4.8947458	6.2584454	6.0069364
11 C	3.1511507	4.6928123	5.4862515	4.8003232
12 N	2.8910481 *	5.9974589	6.3992413	5.1678781
13 C	3.9723678	7.1278649	7.6671658	6.3996311
14 C	4.6918108	8.4896382	8.8239534	7.2833031
15 C	4.6815130	9.0315861	9.0425423	7.2555153
16 C	5.9178084	10.4293880	10.3661585	8.4713604
17 C	6.9897824	11.3026131	11.4285946	9.6103820
18 C	7.0265912	10.9198414	11.2994063	9.6677490
19 C	6.0073730	9.5809141	10.0822530	8.6048221
20 O	3.7539941	8.2924916	8.0362145	6.1601497
21 N	0.0000000	5.4464243	4.6757918	2.6547361 *
22 H	5.4464243	0.0000000	2.5296323 *	4.3599623
23 H	4.6757918	2.5296323 *	0.0000000	2.5187318 *
24 H	2.6547361 *	4.3599623	2.5187318 *	0.0000000
25 H	6.0553144	2.4035230 *	4.7830242	5.9770975
26 H	6.4674350	4.7804737	6.8526078	7.3477985
27 H	5.2524539	5.9694883	7.3475054	6.9649452
28 H	4.7216443	7.1971609	8.0273020	7.0028043
29 H	6.2493307	10.9494523	10.6879652	8.6812394
30 H	7.9692669	12.3878803	12.4567746	10.5718948

31 H	8.0275515	11.7596050	12.2453388	10.6656799
32 H	6.3944968	9.4632141	10.1867887	8.9060052
33 H	4.3761323	8.9786398	8.5624910	6.6035437
34 H	1.0439853 *	5.8557384	5.1906080	3.2292828
35 H	1.0391741 *	5.8220816	4.5868358	2.2147104 *

H H H H

1 CO	6.4871029	6.2729867	4.5219348	3.8771962
2 C	2.6831286 *	4.6694709	5.3927494	6.4004269
3 C	4.0826681	5.9307375	6.2677138	6.9288818
4 C	4.8924963	6.2532078	6.0075932	6.2616778
5 C	4.6725613	5.4680733	4.8011398	4.8844690
6 C	3.5170548	4.0162281	3.5047814	4.0386204
7 C	2.1973992 *	3.4839661	3.9514567	5.0278350
8 C	1.1051360 *	2.1846091 *	3.4321716	4.9896867
9 C	2.1811298 *	1.1042522 *	2.1824384 *	3.9996013
10 C	3.4539831	2.1974937 *	1.1044341 *	2.6634439 *
11 C	3.9639543	3.4738278	2.1879570 *	2.6586645 *
12 N	5.4104405	4.6666416	2.6912566 *	2.0959187 *
13 C	6.2455329	5.0122154	2.6498855 *	1.1084056 *
14 C	7.6806315	6.3628536	3.9016445	2.1776390 *
15 C	8.5003846	7.4158100	5.0143363	3.5333971
16 C	9.8822030	8.6888612	6.2363601	4.6750625
17 C	10.5260946	9.0611581	6.5599037	4.8544344
18 C	9.9200374	8.2603912	5.7864493	3.9985698
19 C	8.5365214	6.9076852	4.4438819	2.5835923 *
20 O	8.0915534	7.4078960	5.2364726	4.1433143
21 N	6.0553144	6.4674350	5.2524539	4.7216443
22 H	2.4035230 *	4.7804737	5.9694883	7.1971609
23 H	4.7830242	6.8526078	7.3475054	8.0273020
24 H	5.9770975	7.3477985	6.9649452	7.0028043
25 H	0.0000000	2.5284112 *	4.3495236	6.0204178
26 H	2.5284112 *	0.0000000	2.5015068 *	4.4918523
27 H	4.3495236	2.5015068 *	0.0000000	2.1631731 *
28 H	6.0204178	4.4918523	2.1631731 *	0.0000000
29 H	10.5732803	9.5270956	7.1254617	5.6717672
30 H	11.6214557	10.1235157	7.6232832	5.9341154
31 H	10.6275387	8.8161714	6.4082467	4.6570079
32 H	8.2208847	6.4230447	4.0808558	2.2672632 *
33 H	8.8910192	8.2715949	6.1318377	5.1007517
34 H	6.3256164	6.5893390	5.2910536	4.4530835
35 H	6.7615998	7.3974648	6.2700839	5.7274970

H H H H

1 CO	4.6136880	6.4182048	6.6738274	5.2789668
2 C	9.9223728	11.4106640	10.8806680	8.6498544
3 C	9.7678587	11.4565596	11.1773778	9.0970935
4 C	8.5546771	10.3175038	10.2113182	8.2944230
5 C	7.3840640	9.0170579	8.8223029	6.8956966
6 C	7.5287337	8.8958355	8.3802377	6.2328607
7 C	8.9224300	10.2330435	9.5649449	7.2904215
8 C	9.4876199	10.5420880	9.6013885	7.2196300
9 C	8.8543167	9.6495762	8.5253999	6.1268886
10 C	7.4594674	8.2343071	7.1900530	4.8391097
11 C	6.6989833	7.7899711	7.0812202	4.8758615
12 N	5.2673506	6.4023958	5.9179775	3.9701063
13 C	4.7952649	5.4486929	4.6571600	2.6404766 *
14 C	3.5027277	3.9872076	3.4935522	2.1972335 *
15 C	2.1938374 *	3.4399420	3.9292466	3.4502232
16 C	1.1067600 *	2.1921757 *	3.4746565	3.9511622
17 C	2.2009967 *	1.1051978 *	2.1976618 *	3.4568904
18 C	3.4739588	2.2003705 *	1.1042679 *	2.1859135 *
19 C	3.9520937	3.4605015	2.1877780 *	1.1058225 *
20 O	2.6840658 *	4.6491924	5.3947868	4.6927311
21 N	6.2493307	7.9692669	8.0275515	6.3944968
22 H	10.9494523	12.3878803	11.7596050	9.4632141
23 H	10.6879652	12.4567746	12.2453388	10.1867887
24 H	8.6812394	10.5718948	10.6656799	8.9060052
25 H	10.5732803	11.6214557	10.6275387	8.2208847
26 H	9.5270956	10.1235157	8.8161714	6.4230447
27 H	7.1254617	7.6232832	6.4082467	4.0808558
28 H	5.6717672	5.9341154	4.6570079	2.2672632 *
29 H	0.0000000	2.5216368 *	4.3873937	5.0579036
30 H	2.5216368 *	0.0000000	2.5403496 *	4.3741032
31 H	4.3873937	2.5403496 *	0.0000000	2.5151433 *
32 H	5.0579036	4.3741032	2.5151433 *	0.0000000
33 H	2.3044114 *	4.6293216	5.8154191	5.4659317
34 H	6.3028433	7.7857917	7.6683789	6.0107393
35 H	6.5938099	8.4860346	8.7700840	7.2964191

H H H

1 CO	2.6578100 *	2.4988664 *	2.6222587 *
2 C	7.9445771	4.7781807	4.7389796
3 C	7.6906834	4.3335672	3.9186882
4 C	6.4910580	3.0686274	2.4872281 *
5 C	5.4274776	2.1120186 *	2.0892715 *
6 C	5.7270380	2.9538441 *	3.4245400
7 C	7.0951539	4.2412251	4.5646122
8 C	7.8372635	5.3654663	5.8898069

9 C	7.4544017	5.5404152	6.3014161
10 C	6.1705478	4.6649389	5.5539367
11 C	5.1867273	3.3155800	4.1502733
12 N	3.8906542	2.9809461 *	3.8804351
13 C	4.0172032	3.8226500	4.9332527
14 C	3.3303482	4.5239590	5.5077370
15 C	2.0454591 *	4.6746372	5.2952903
16 C	2.5073550 *	5.8744551	6.4166265
17 C	3.9279574	6.8062168	7.5711051
18 C	4.7296309	6.7305967	7.7498246
19 C	4.4867663	5.7017707	6.8336456
20 O	0.9916727 *	4.0134929	4.2207300
21 N	4.3761323	1.0439853 *	1.0391741 *
22 H	8.9786398	5.8557384	5.8220816
23 H	8.5624910	5.1906080	4.5868358
24 H	6.6035437	3.2292828	2.2147104 *
25 H	8.8910192	6.3256164	6.7615998
26 H	8.2715949	6.5893390	7.3974648
27 H	6.1318377	5.2910536	6.2700839
28 H	5.1007517	4.4530835	5.7274970
29 H	2.3044114 *	6.3028433	6.5938099
30 H	4.6293216	7.7857917	8.4860346
31 H	5.8154191	7.6683789	8.7700840
32 H	5.4659317	6.0107393	7.2964191
33 H	0.0000000	4.7194490	4.6564163
34 H	4.7194490	0.0000000	1.6670565 *
35 H	4.6564163	1.6670565 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.74 , TOTAL = 8607.9 SECONDS (143.5 MIN)
WALL CLOCK TIME: STEP = 0.74 , TOTAL = 7961.3 SECONDS (132.7 MIN)
CPU UTILIZATION: STEP = 99.46%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.35 , TOTAL = 8609.2 SECONDS (143.5 MIN)
WALL CLOCK TIME: STEP = 1.35 , TOTAL = 7962.6 SECONDS (132.7 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
1	0	-284.636954316	-284.636954316	0.002832915	0.000336135
2	1	-284.636962275	-0.000007958	0.000564069	0.000021615
3	2	-284.636962276	-0.000000002	0.000168332	0.000042907
4	3	-284.636962365	-0.000000089	0.000188116	0.000020739
5	4	-284.636962349	0.000000016	0.000075795	0.000032166
6	5	-284.636962382	-0.000000033	0.000064467	0.000009038
7	6	-284.636962378	0.000000004	0.000036014	0.000009820
8	7	-284.636962389	-0.000000010	0.000068268	0.000007226
9	8	-284.636962391	-0.000000002	0.000156021	0.000006089
10	9	-284.636962374	0.000000017	0.000230101	0.000005419
11	10	-284.636962379	-0.000000005	0.000233919	0.000006748
12	11	-284.636962383	-0.000000004	0.000071699	0.000007819
13	12	-284.636962385	-0.000000002	0.000084222	0.000004621
14	13	-284.636962387	-0.000000002	0.000050504	0.000002709
15	14	-284.636962387	-0.000000001	0.000043570	0.000001541
16	15	-284.636962387	0.000000000	0.000016413	0.000001424
17	16	-284.636962388	0.000000000	0.000022970	0.000001351

-----START SECOND ORDER SCF-----

11310481

15552518

16981865

17590285

17848295

18338398

18523740

17107516

15322440

-----DISABLING FDIFF OPTION-----

11310483

11310473

11310462

11310463

11310470

11310468

11310461

11310463

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 55.4 SECONDS (3.3 SEC/ITER)

OF THE ABOVE TIME, DFT PART= 18.4 SECONDS (1.1 SEC/ITER)

FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 2.6 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6369623876 AFTER 17 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6025552199
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998599104

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 58.96 , TOTAL = 8668.2 SECONDS (144.5 MIN)
WALL CLOCK TIME: STEP = 54.37 , TOTAL = 8017.0 SECONDS (133.6
MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.98 , TOTAL = 8672.1 SECONDS (144.5 MIN)
WALL CLOCK TIME: STEP = 3.95 , TOTAL = 8020.9 SECONDS (133.7
MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.93 , TOTAL = 8675.1 SECONDS (144.6 MIN)
WALL CLOCK TIME: STEP = 2.75 , TOTAL = 8023.7 SECONDS (133.7
MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 98 ENERGY= -284.6369624

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ	

1	CO	27.0	0.0000694	0.0000176	0.0000794
2	C	6.0	-0.0000353	-0.0000414	0.0000142
3	C	6.0	-0.0000144	0.0000098	-0.0000437
4	C	6.0	0.0000120	-0.0000492	-0.0000132
5	C	6.0	-0.0000444	-0.0000081	0.0000609
6	C	6.0	-0.0000239	0.0000751	-0.0000355
7	C	6.0	0.0000382	0.0000541	-0.0000247
8	C	6.0	0.0000439	0.0000331	-0.0000168
9	C	6.0	0.0000195	-0.0000490	0.0000279
10	C	6.0	-0.0000280	-0.0000530	0.0000183
11	C	6.0	-0.0000467	-0.0000145	-0.0000765
12	N	7.0	0.0000075	0.0000363	-0.0000166
13	C	6.0	-0.0000101	-0.0000300	-0.0000365
14	C	6.0	0.0000300	-0.0000199	0.0000242
15	C	6.0	0.0000782	0.0000316	-0.0000732
16	C	6.0	0.0000463	-0.0000940	-0.0000420
17	C	6.0	0.0000554	0.0000662	0.0000522
18	C	6.0	-0.0000083	-0.0000136	0.0000036
19	C	6.0	-0.0000494	0.0000075	0.0000275
20	O	8.0	0.0000141	-0.0000893	0.0000199
21	N	7.0	-0.0000697	0.0000190	0.0000343
22	H	1.0	0.0000685	-0.0000043	0.0000750
23	H	1.0	0.0000317	0.0000090	0.0000681
24	H	1.0	0.0000584	0.0000123	-0.0000139
25	H	1.0	0.0000669	0.0000259	0.0000052
26	H	1.0	-0.0000493	-0.0000446	0.0000269
27	H	1.0	-0.0001514	-0.0000221	-0.0000271
28	H	1.0	0.0000912	-0.0000499	-0.0000933
29	H	1.0	0.0000680	0.0000687	0.0000416
30	H	1.0	-0.0000290	0.0000571	0.0000363
31	H	1.0	-0.0000674	0.0000413	0.0000342
32	H	1.0	0.0000105	-0.0000707	-0.0000011
33	H	1.0	-0.0000079	0.0000637	-0.0001306
34	H	1.0	-0.0000868	-0.0000481	0.0000128
35	H	1.0	-0.0000878	0.0000732	-0.0000179

MAXIMUM GRADIENT = 0.0001514 RMS GRADIENT = 0.0000501
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000020856
 PREDICTED ENERGY CHANGE WAS -0.0000014741 RATIO= 1.415
 GDIIS STEP HAS LENGTH = 0.017987
 RADIUS OF STEP TAKEN= 0.01799 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 8675.1 SECONDS (144.6 MIN)

WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8023.7 SECONDS (133.7 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 99

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1627063018	-1.7179126401	0.8942133733
C	6.0	4.9800598149	0.6171004042	0.5593798135
C	6.0	5.1748391612	-0.7234793237	0.1994190170
C	6.0	4.0338146546	-1.5371303176	-0.0950998952
C	6.0	2.7288530198	-1.0177490875	-0.0031302224
C	6.0	2.4667541376	0.3489807115	0.4310346354
C	6.0	3.6534720651	1.1754776126	0.6786907556
C	6.0	3.5130553545	2.5623183878	1.0569234823
C	6.0	2.2478392798	3.1432222098	1.2216592680
C	6.0	1.0779611382	2.3401445586	1.0440417049
C	6.0	1.1641126909	0.9863592334	0.6434399314
N	7.0	-0.0493126523	0.1872338240	0.5971494308
C	6.0	-1.2457053405	0.7070685528	0.3292478078
C	6.0	-2.5466703397	0.0391020823	0.4420026293
C	6.0	-2.8133469990	-1.2841704156	0.9370447015
C	6.0	-4.1111339636	-1.8131033314	1.0548868689
C	6.0	-5.2231872135	-1.0061104530	0.6647094584
C	6.0	-5.0135655835	0.3076077252	0.1593165979
C	6.0	-3.6971477997	0.8179532178	0.0534801019
O	8.0	-1.6902705393	-2.1351988783	1.3404468840
N	7.0	1.6148751201	-1.9422224967	-0.4285866576
H	1.0	5.8467365526	1.2720406577	0.7623382017
H	1.0	6.1899542919	-1.1502279737	0.1183974721
H	1.0	4.1914768485	-2.5808200762	-0.4315778219
H	1.0	4.4286643556	3.1569344425	1.2283271146
H	1.0	2.1452025197	4.1993861068	1.5273296439
H	1.0	0.0956133346	2.7874201556	1.2776745366
H	1.0	-1.2919783928	1.7565801391	-0.0242947207
H	1.0	-4.2793766369	-2.8363992210	1.4416922042
H	1.0	-6.2459374701	-1.4147412081	0.7562829842
H	1.0	-5.8728245044	0.9312077303	-0.1438892334
H	1.0	-3.5365510686	1.8431576248	-0.3288339934
H	1.0	-2.0068174882	-2.9480032193	1.8121388670
H	1.0	1.2406155219	-1.6529529245	-1.3592192989

H 1.0 2.0032168286 -2.8979688101 -0.5537486426

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3638880	5.1568510	3.9996128
2 C	5.3638880	0.0000000	1.4016650 *	2.4422190 *
3 C	5.1568510	1.4016650 *	0.0000000	1.4320287 *
4 C	3.9996128	2.4422190 *	1.4320287 *	0.0000000
5 C	2.8072341 *	2.8385000 *	2.4719363 *	1.4075298 *
6 C	3.1297315	2.5308232 *	2.9219071 *	2.5079695 *
7 C	4.5391192	1.4442490 *	2.4799792 *	2.8463405 *
8 C	5.4379859	2.4866694 *	3.7806489	4.2899683
9 C	5.2995879	3.7795416	4.9561764	5.1796971
10 C	4.1626876	4.2930353	5.1849386	5.0067928
11 C	2.8946137 *	3.8346930	4.3825369	3.8921241
12 N	1.9397892 *	5.0478510	5.3178332	4.4860416
13 C	2.8606543 *	6.2306666	6.5792640	5.7523761
14 C	3.2607234	7.5498031	7.7628658	6.7879136
15 C	3.0077999	8.0308562	8.0417401	6.9291366
16 C	4.2779186	9.4234400	9.3887381	8.2303596
17 C	5.4375715	10.3320936	10.4122682	9.3032992
18 C	5.6068348	10.0064172	10.2405244	9.2370382
19 C	4.6942435	8.6942630	9.0060793	8.0830857
20 O	1.9510959 *	7.2579973	7.1010301	5.9315792
21 N	1.9770961 *	4.3417369	3.8148486	2.4751932 *
22 H	6.4238160	1.1051097 *	2.1795468 *	3.4515688
23 H	6.1034314	2.1867235 *	1.1041457 *	2.2009572 *
24 H	4.3282010	3.4395575	2.1942819 *	1.1078642 *
25 H	6.4864601	2.6837072 *	4.0832634	4.8930164
26 H	6.2726033	4.6697017	5.9309905	6.2535393
27 H	4.5221198	5.3929632	6.2679809	6.0079677
28 H	3.8770949	6.4013712	6.9296805	6.2623968
29 H	4.6133335	9.9218092	9.7667738	8.5533022
30 H	6.4172933	11.4100905	11.4552206	10.3156743
31 H	6.6725653	10.8801815	11.1761676	10.2096314
32 H	5.2784061	8.6501330	9.0969773	8.2940590
33 H	2.6575446 *	7.9432880	7.6893149	6.4897888
34 H	2.4988131 *	4.7767780	4.3325962	3.0681222
35 H	2.6223283 *	4.7388143	3.9185271	2.4870801 *

	C	C	C	C
1 CO	2.8072341 *	3.1297315	4.5391192	5.4379859

2 C	2.8385000 *	2.5308232 *	1.4442490 *	2.4866694 *
3 C	2.4719363 *	2.9219071 *	2.4799792 *	3.7806489
4 C	1.4075298 *	2.5079695 *	2.8463405 *	4.2899683
5 C	0.0000000	1.4577878 *	2.4758925 *	3.8151763
6 C	1.4577878 *	0.0000000	1.4672185 *	2.5269244 *
7 C	2.4758925 *	1.4672185 *	0.0000000	1.4443352 *
8 C	3.8151763	2.5269244 *	1.4443352 *	0.0000000
9 C	4.3640767	2.9121807 *	2.4784344 *	1.4019126 *
10 C	3.8855454	2.5038485 *	2.8501205 *	2.4452425 *
11 C	2.6235311 *	1.4656883 *	2.4967816 *	2.8586968 *
12 N	3.0871547	2.5267268 *	3.8332609	4.3061450
13 C	4.3454097	3.7310780	4.9339089	5.1591925
14 C	5.3987243	5.0230041	6.3078631	6.5928009
15 C	5.6276896	5.5500177	6.9236092	7.4049452
16 C	6.9668795	6.9521515	8.3284000	8.7904825
17 C	7.9800432	7.8119187	9.1408206	9.4450755
18 C	7.8567172	7.4853674	8.7258518	8.8652514
19 C	6.6832997	6.1932358	7.3858191	7.4857690
20 O	4.7521097	4.9273759	6.3209244	7.0158146
21 N	1.5088443 *	2.5911887 *	3.8861285	5.1088861
22 H	3.9433839	3.5193867	2.1969821 *	2.6828464 *
23 H	3.4657671	4.0258649	3.4866283	4.6722178
24 H	2.1831232 *	3.5074922	3.9537220	5.3970145
25 H	4.6726682	3.5170117	2.1975428 *	1.1051187 *
26 H	5.4682223	4.0163267	3.4841193	2.1845581 *
27 H	4.8014295	3.5050100	3.9516451	3.4319545
28 H	4.8851239	4.0393974	5.0288517	4.9906509
29 H	7.3831080	7.5285028	8.9222988	9.4876865
30 H	9.0156073	8.8953638	10.2329645	10.5425485
31 H	8.8208334	8.3796240	9.5648644	9.6019380
32 H	6.8953723	6.2329478	7.2909077	7.2204201
33 H	5.4265696	5.7262898	7.0941297	7.8360060
34 H	2.1112348 *	2.9523149 *	4.2396902	5.3637898
35 H	2.0892474 *	3.4245213	4.5645608	5.8897040

C C C N

1 CO	5.2995879	4.1626876	2.8946137 *	1.9397892 *
2 C	3.7795416	4.2930353	3.8346930	5.0478510
3 C	4.9561764	5.1849386	4.3825369	5.3178332
4 C	5.1796971	5.0067928	3.8921241	4.4860416
5 C	4.3640767	3.8855454	2.6235311 *	3.0871547
6 C	2.9121807 *	2.5038485 *	1.4656883 *	2.5267268 *
7 C	2.4784344 *	2.8501205 *	2.4967816 *	3.8332609
8 C	1.4019126 *	2.4452425 *	2.8586968 *	4.3061450
9 C	0.0000000	1.4300687 *	2.4821077 *	3.7953639

10 C	1.4300687 *	0.0000000	1.4144393 *	2.4709277 *
11 C	2.4821077 *	1.4144393 *	0.0000000	1.4536662 *
12 N	3.7953639	2.4709277 *	1.4536662 *	0.0000000
13 C	4.3515626	2.9287017 *	2.4462099 *	1.3316737 *
14 C	5.7646118	4.3353432	3.8350729	2.5065532 *
15 C	6.7304099	5.3187768	4.5893022	3.1496738
16 C	8.0640881	6.6465249	5.9861930	4.5507433
17 C	8.5640756	7.1446334	6.6908884	5.3101425
18 C	7.8674826	6.4823331	6.2336817	4.9849769
19 C	6.4895601	5.1088104	4.8998231	3.7416687
20 O	6.5866948	5.2706415	4.2868925	2.9392053 *
21 N	5.3838372	4.5602169	3.1510345	2.8907161 *
22 H	4.0822001	4.8950405	4.6928368	5.9972902
23 H	5.9322147	6.2587532	5.4863247	6.3989421
24 H	6.2670232	6.0072728	4.8005588	5.1676588
25 H	2.1808784 *	3.4537398	3.9636836	5.4101557
26 H	1.1042875 *	2.1975783 *	3.4738077	4.6667438
27 H	2.1821570 *	1.1043763 *	2.1880962 *	2.6916699 *
28 H	4.0006858	2.6643017 *	2.6592279 *	2.0960102 *
29 H	8.8548763	7.4602815	6.6994227	5.2677368
30 H	9.6506916	8.2353787	7.7901772	6.4023282
31 H	8.5266002	7.1909460	7.0810602	5.9174256
32 H	6.1280804	4.8399904	4.8760291	3.9699321
33 H	7.4534420	6.1701166	5.1865078	3.8907243
34 H	5.5388383	4.6633622	3.3139803	2.9795269 *
35 H	6.3014207	5.5539953	4.1503446	3.8801957

C C C C

1 CO	2.8606543 *	3.2607234	3.0077999	4.2779186
2 C	6.2306666	7.5498031	8.0308562	9.4234400
3 C	6.5792640	7.7628658	8.0417401	9.3887381
4 C	5.7523761	6.7879136	6.9291366	8.2303596
5 C	4.3454097	5.3987243	5.6276896	6.9668795
6 C	3.7310780	5.0230041	5.5500177	6.9521515
7 C	4.9339089	6.3078631	6.9236092	8.3284000
8 C	5.1591925	6.5928009	7.4049452	8.7904825
9 C	4.3515626	5.7646118	6.7304099	8.0640881
10 C	2.9287017 *	4.3353432	5.3187768	6.6465249
11 C	2.4462099 *	3.8350729	4.5893022	5.9861930
12 N	1.3316737 *	2.5065532 *	3.1496738	4.5507433
13 C	0.0000000	1.4667661 *	2.6061370 *	3.8843918
14 C	1.4667661 *	0.0000000	1.4377876 *	2.5007676 *
15 C	2.6061370 *	1.4377876 *	0.0000000	1.4063811 *
16 C	3.8843918	2.5007676 *	1.4063811 *	0.0000000
17 C	4.3437172	2.8819802 *	2.4410681 *	1.4283341 *

18 C	3.7927848	2.4975145 *	2.8248151 *	2.4726189 *
19 C	2.4693953 *	1.4426217 *	2.4455498 *	2.8454628 *
20 O	3.0493681	2.5036388 *	1.4657024 *	2.4588350 *
21 N	3.9718984	4.6906325	4.6805056	5.9164639
22 H	7.1280778	8.4895248	9.0311563	10.4289445
23 H	7.6670100	8.8231421	9.0414356	10.3647882
24 H	6.3993763	7.2821537	7.2541013	8.4694931
25 H	6.2456911	7.6807863	8.5002933	9.8822827
26 H	5.0129770	6.3639272	7.4165384	8.6899354
27 H	2.6507568 *	3.9029813	5.0155686	6.2378821
28 H	1.1084259 *	2.1774793 *	3.5333978	4.6749236
29 H	4.7955039	3.5028785	2.1939294 *	1.1068236 *
30 H	5.4485555	3.9871054	3.4398257	2.1920864 *
31 H	4.6566435	3.4931967	3.9289593	3.4744584
32 H	2.6404061 *	2.1974233 *	3.4504570	3.9513381
33 H	4.0171890	3.3303922	2.0456342 *	2.5079027 *
34 H	3.8213105	4.5222765	4.6736967	5.8732256
35 H	4.9326942	5.5063036	5.2939680	6.4148209

C C C O

1 CO	5.4375715	5.6068348	4.6942435	1.9510959 *
2 C	10.3320936	10.0064172	8.6942630	7.2579973
3 C	10.4122682	10.2405244	9.0060793	7.1010301
4 C	9.3032992	9.2370382	8.0830857	5.9315792
5 C	7.9800432	7.8567172	6.6832997	4.7521097
6 C	7.8119187	7.4853674	6.1932358	4.9273759
7 C	9.1408206	8.7258518	7.3858191	6.3209244
8 C	9.4450755	8.8652514	7.4857690	7.0158146
9 C	8.5640756	7.8674826	6.4895601	6.5866948
10 C	7.1446334	6.4823331	5.1088104	5.2706415
11 C	6.6908884	6.2336817	4.8998231	4.2868925
12 N	5.3101425	4.9849769	3.7416687	2.9392053 *
13 C	4.3437172	3.7927848	2.4693953 *	3.0493681
14 C	2.8819802 *	2.4975145 *	1.4426217 *	2.5036388 *
15 C	2.4410681 *	2.8248151 *	2.4455498 *	1.4657024 *
16 C	1.4283341 *	2.4726189 *	2.8454628 *	2.4588350 *
17 C	0.0000000	1.4231018 *	2.4555256 *	3.7700082
18 C	1.4231018 *	0.0000000	1.4158424 *	4.2902987
19 C	2.4555256 *	1.4158424 *	0.0000000	3.7953850
20 O	3.7700082	4.2902987	3.7953850	0.0000000
21 N	6.9878966	7.0244994	6.0057094	3.7537591
22 H	11.3023323	10.9197037	9.5809396	8.2915600
23 H	11.4271180	11.2980448	10.0813064	8.0350181
24 H	9.6081973	9.6656597	8.6033331	6.1590261
25 H	10.5264831	9.9205419	8.5369738	8.0907732

26 H	9.0628073	8.2622854	6.9093689	7.4076140
27 H	6.5617254	5.7882556	4.4455021	5.2369361
28 H	4.8540281	3.9979301	2.5830039 *	4.1433199
29 H	2.2010083 *	3.4739459	3.9522671	2.6842882 *
30 H	1.1051619 *	2.2003625 *	3.4605180	4.6491298
31 H	2.1975127 *	1.1041452 *	2.1875444 *	5.3944287
32 H	3.4569059	2.1858125 *	1.1058931 *	4.6928212
33 H	3.9284317	4.7298370	4.4869282	0.9916381 *
34 H	6.8040751	6.7278920	5.6993511	4.0138326
35 H	7.5686646	7.7472200	6.8316148	4.2203843

N H H H

1 CO	1.9770961 *	6.4238160	6.1034314	4.3282010
2 C	4.3417369	1.1051097 *	2.1867235 *	3.4395575
3 C	3.8148486	2.1795468 *	1.1041457 *	2.1942819 *
4 C	2.4751932 *	3.4515688	2.2009572 *	1.1078642 *
5 C	1.5088443 *	3.9433839	3.4657671	2.1831232 *
6 C	2.5911887 *	3.5193867	4.0258649	3.5074922
7 C	3.8861285	2.1969821 *	3.4866283	3.9537220
8 C	5.1088861	2.6828464 *	4.6722178	5.3970145
9 C	5.3838372	4.0822001	5.9322147	6.2670232
10 C	4.5602169	4.8950405	6.2587532	6.0072728
11 C	3.1510345	4.6928368	5.4863247	4.8005588
12 N	2.8907161 *	5.9972902	6.3989421	5.1676588
13 C	3.9718984	7.1280778	7.6670100	6.3993763
14 C	4.6906325	8.4895248	8.8231421	7.2821537
15 C	4.6805056	9.0311563	9.0414356	7.2541013
16 C	5.9164639	10.4289445	10.3647882	8.4694931
17 C	6.9878966	11.3023323	11.4271180	9.6081973
18 C	7.0244994	10.9197037	11.2980448	9.6656597
19 C	6.0057094	9.5809396	10.0813064	8.6033331
20 O	3.7537591	8.2915600	8.0350181	6.1590261
21 N	0.0000000	5.4459564	4.6752322	2.6545607 *
22 H	5.4459564	0.0000000	2.5297912 *	4.3600294
23 H	4.6752322	2.5297912 *	0.0000000	2.5185271 *
24 H	2.6545607 *	4.3600294	2.5185271 *	0.0000000
25 H	6.0550949	2.4043500 *	4.7839036	5.9777395
26 H	6.4673188	4.7807863	6.8529904	7.3481802
27 H	5.2525235	5.9697039	7.3477880	6.9653173
28 H	4.7216936	7.1982512	8.0280266	7.0033707
29 H	6.2481756	10.9489254	10.6864949	8.6792753
30 H	7.9670903	12.3875582	12.4550499	10.5693127
31 H	8.0251666	11.7594867	12.2438475	10.6633609
32 H	6.3934533	9.4637687	10.1865244	8.9053102
33 H	4.3759688	8.9771467	8.5608308	6.6021164

34 H	1.0439465 *	5.8543099	5.1896087	3.2294022
35 H	1.0391948 *	5.8218302	4.5864092	2.2144956 *

	H	H	H	H
--	---	---	---	---

1 CO	6.4864601	6.2726033	4.5221198	3.8770949
2 C	2.6837072 *	4.6697017	5.3929632	6.4013712
3 C	4.0832634	5.9309905	6.2679809	6.9296805
4 C	4.8930164	6.2535393	6.0079677	6.2623968
5 C	4.6726682	5.4682223	4.8014295	4.8851239
6 C	3.5170117	4.0163267	3.5050100	4.0393974
7 C	2.1975428 *	3.4841193	3.9516451	5.0288517
8 C	1.1051187 *	2.1845581 *	3.4319545	4.9906509
9 C	2.1808784 *	1.1042875 *	2.1821570 *	4.0006858
10 C	3.4537398	2.1975783 *	1.1043763 *	2.6643017 *
11 C	3.9636836	3.4738077	2.1880962 *	2.6592279 *
12 N	5.4101557	4.6667438	2.6916699 *	2.0960102 *
13 C	6.2456911	5.0129770	2.6507568 *	1.1084259 *
14 C	7.6807863	6.3639272	3.9029813	2.1774793 *
15 C	8.5002933	7.4165384	5.0155686	3.5333978
16 C	9.8822827	8.6899354	6.2378821	4.6749236
17 C	10.5264831	9.0628073	6.5617254	4.8540281
18 C	9.9205419	8.2622854	5.7882556	3.9979301
19 C	8.5369738	6.9093689	4.4455021	2.5830039 *
20 O	8.0907732	7.4076140	5.2369361	4.1433199
21 N	6.0550949	6.4673188	5.2525235	4.7216936
22 H	2.4043500 *	4.7807863	5.9697039	7.1982512
23 H	4.7839036	6.8529904	7.3477880	8.0280266
24 H	5.9777395	7.3481802	6.9653173	7.0033707
25 H	0.0000000	2.5279054 *	4.3490582	6.0212795
26 H	2.5279054 *	0.0000000	2.5013579 *	4.4932229
27 H	4.3490582	2.5013579 *	0.0000000	2.1640624 *
28 H	6.0212795	4.4932229	2.1640624 *	0.0000000
29 H	10.5733415	9.5281072	7.1270459	5.6717833
30 H	11.6219692	10.1254219	7.6253050	5.9336575
31 H	10.6281471	8.8183173	6.4100404	4.6561458
32 H	8.2216432	6.4249109	4.0822934	2.2667921 *
33 H	8.8896865	8.2707654	6.1319613	5.1006458
34 H	6.3240864	6.5878915	5.2897214	4.4520749
35 H	6.7616894	7.3975329	6.2703038	5.7274304

	H	H	H	H
--	---	---	---	---

1 CO	4.6133335	6.4172933	6.6725653	5.2784061
2 C	9.9218092	11.4100905	10.8801815	8.6501330
3 C	9.7667738	11.4552206	11.1761676	9.0969773

4 C	8.5533022	10.3156743	10.2096314	8.2940590
5 C	7.3831080	9.0156073	8.8208334	6.8953723
6 C	7.5285028	8.8953638	8.3796240	6.2329478
7 C	8.9222988	10.2329645	9.5648644	7.2909077
8 C	9.4876865	10.5425485	9.6019380	7.2204201
9 C	8.8548763	9.6506916	8.5266002	6.1280804
10 C	7.4602815	8.2353787	7.1909460	4.8399904
11 C	6.6994227	7.7901772	7.0810602	4.8760291
12 N	5.2677368	6.4023282	5.9174256	3.9699321
13 C	4.7955039	5.4485555	4.6566435	2.6404061 *
14 C	3.5028785	3.9871054	3.4931967	2.1974233 *
15 C	2.1939294 *	3.4398257	3.9289593	3.4504570
16 C	1.1068236 *	2.1920864 *	3.4744584	3.9513381
17 C	2.2010083 *	1.1051619 *	2.1975127 *	3.4569059
18 C	3.4739459	2.2003625 *	1.1041452 *	2.1858125 *
19 C	3.9522671	3.4605180	2.1875444 *	1.1058931 *
20 O	2.6842882 *	4.6491298	5.3944287	4.6928212
21 N	6.2481756	7.9670903	8.0251666	6.3934533
22 H	10.9489254	12.3875582	11.7594867	9.4637687
23 H	10.6864949	12.4550499	12.2438475	10.1865244
24 H	8.6792753	10.5693127	10.6633609	8.9053102
25 H	10.5733415	11.6219692	10.6281471	8.2216432
26 H	9.5281072	10.1254219	8.8183173	6.4249109
27 H	7.1270459	7.6253050	6.4100404	4.0822934
28 H	5.6717833	5.9336575	4.6561458	2.2667921 *
29 H	0.0000000	2.5215588 *	4.3872550	5.0581425
30 H	2.5215588 *	0.0000000	2.5402755 *	4.3740323
31 H	4.3872550	2.5402755 *	0.0000000	2.5147626 *
32 H	5.0581425	4.3740323	2.5147626 *	0.0000000
33 H	2.3052573 *	4.6298879	5.8155252	5.4661752
34 H	6.3020603	7.7833521	7.6652425	6.0088105
35 H	6.5921586	8.4832007	8.7671321	7.2950596

H H H

1 CO	2.6575446 *	2.4988131 *	2.6223283 *
2 C	7.9432880	4.7767780	4.7388143
3 C	7.6893149	4.3325962	3.9185271
4 C	6.4897888	3.0681222	2.4870801 *
5 C	5.4265696	2.1112348 *	2.0892474 *
6 C	5.7262898	2.9523149 *	3.4245213
7 C	7.0941297	4.2396902	4.5645608
8 C	7.8360060	5.3637898	5.8897040
9 C	7.4534420	5.5388383	6.3014207
10 C	6.1701166	4.6633622	5.5539953
11 C	5.1865078	3.3139803	4.1503446

12 N	3.8907243	2.9795269 *	3.8801957
13 C	4.0171890	3.8213105	4.9326942
14 C	3.3303922	4.5222765	5.5063036
15 C	2.0456342 *	4.6736967	5.2939680
16 C	2.5079027 *	5.8732256	6.4148209
17 C	3.9284317	6.8040751	7.5686646
18 C	4.7298370	6.7278920	7.7472200
19 C	4.4869282	5.6993511	6.8316148
20 O	0.9916381 *	4.0138326	4.2203843
21 N	4.3759688	1.0439465 *	1.0391948 *
22 H	8.9771467	5.8543099	5.8218302
23 H	8.5608308	5.1896087	4.5864092
24 H	6.6021164	3.2294022	2.2144956 *
25 H	8.8896865	6.3240864	6.7616894
26 H	8.2707654	6.5878915	7.3975329
27 H	6.1319613	5.2897214	6.2703038
28 H	5.1006458	4.4520749	5.7274304
29 H	2.3052573 *	6.3020603	6.5921586
30 H	4.6298879	7.7833521	8.4832007
31 H	5.8155252	7.6652425	8.7671321
32 H	5.4661752	6.0088105	7.2950596
33 H	0.0000000	4.7202213	4.6562112
34 H	4.7202213	0.0000000	1.6674556 *
35 H	4.6562112	1.6674556 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.83 , TOTAL = 8675.9 SECONDS (144.6 MIN)
WALL CLOCK TIME: STEP = 0.83 , TOTAL = 8024.5 SECONDS (133.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.10 , TOTAL = 8677.0 SECONDS (144.6 MIN)
WALL CLOCK TIME: STEP = 1.10 , TOTAL = 8025.6 SECONDS (133.8 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636958535	-284.636958535	0.003676335	0.000280089	198441957
11309459						
2	1	-284.636963871	-0.000005336	0.000639095	0.000020557	145030887
15784213						
3	2	-284.636963886	-0.000000015	0.000174955	0.000042998	127088671
17149075						
4	3	-284.636963913	-0.000000027	0.000220766	0.000026905	118205029
17848838						
5	4	-284.636963895	0.000000019	0.000124503	0.000028866	118243520
17838648						
6	5	-284.636963922	-0.000000027	0.000039322	0.000007803	111391282
18310001						
7	6	-284.636963908	0.000000014	0.000033943	0.000006843	105891827
18714957						
8	7	-284.636963916	-0.000000008	0.000063352	0.000006164	124823220
17340107						
9	8	-284.636963918	-0.000000002	0.000131377	0.000004844	151414768
15325292						

-----DISABLING FDIFF OPTION-----

10	9	-284.636963928	-0.000000010	0.000198663	0.000005903	198442733
11309439						
11	10	-284.636963931	-0.000000004	0.000142890	0.000005804	198443043
11309439						
12	11	-284.636963934	-0.000000002	0.000058399	0.000004276	198443095
11309444						
13	12	-284.636963935	-0.000000001	0.000043406	0.000003090	198443040
11309443						
14	13	-284.636963936	-0.000000001	0.000046589	0.000001854	198442965
11309448						
15	14	-284.636963936	0.000000000	0.000035300	0.000001823	198442968
11309449						
16	15	-284.636963937	0.000000000	0.000011107	0.000001831	198443020
11309445						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 53.5 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 17.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369639367 AFTER 16 ITERATIONS

DFT EXCHANGE + CORRELATION ENERGY IS -46.6028251521
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998604543

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 55.85 , TOTAL = 8732.9 SECONDS (145.5 MIN)
WALL CLOCK TIME: STEP = 51.26 , TOTAL = 8076.9 SECONDS (134.6
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.79 , TOTAL = 8736.7 SECONDS (145.6 MIN)
WALL CLOCK TIME: STEP = 3.77 , TOTAL = 8080.7 SECONDS (134.7
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.87 , TOTAL = 8739.5 SECONDS (145.7 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 8083.4 SECONDS (134.7
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH= 99 ENERGY= -284.6369639

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000146	0.0000495	0.0000855

2 C	6.0	-0.0000338	-0.0000141	-0.0000188
3 C	6.0	0.0000140	0.0000283	-0.0000439
4 C	6.0	0.0000047	-0.0000740	-0.0000246
5 C	6.0	-0.0000456	-0.0000456	0.0000640
6 C	6.0	-0.0000157	0.0000513	-0.0000474
7 C	6.0	0.0000760	0.0000296	-0.0000436
8 C	6.0	-0.0000054	0.0000135	0.0000028
9 C	6.0	-0.0000558	-0.0000641	0.0000566
10 C	6.0	-0.0000297	-0.0000475	0.0000135
11 C	6.0	-0.0000409	0.0000862	-0.0001080
12 N	7.0	-0.0000165	0.0000336	-0.0000382
13 C	6.0	-0.0000198	-0.0000763	-0.0000109
14 C	6.0	0.0000344	0.0000026	-0.0000018
15 C	6.0	0.0000849	-0.0000244	-0.0000466
16 C	6.0	0.0000305	-0.0000270	-0.0000334
17 C	6.0	0.0000437	0.0000682	0.0000953
18 C	6.0	0.0000118	0.0000102	-0.0000117
19 C	6.0	-0.0000082	-0.0000477	-0.0000369
20 O	8.0	-0.0000120	-0.0000838	0.0000305
21 N	7.0	-0.0000353	0.0000076	0.0000275
22 H	1.0	0.0000335	-0.0000461	0.0000871
23 H	1.0	-0.0000189	-0.0000184	0.0000543
24 H	1.0	0.0000581	-0.0000342	-0.0000242
25 H	1.0	0.0000320	0.0000485	-0.0000037
26 H	1.0	-0.0000389	-0.0000182	0.0000356
27 H	1.0	-0.0000920	-0.0000004	-0.0000212
28 H	1.0	0.0000613	-0.0000434	-0.0000957
29 H	1.0	0.0000525	0.0000235	0.0000424
30 H	1.0	-0.0000022	0.0000471	0.0000099
31 H	1.0	0.0000049	-0.0000005	0.0000560
32 H	1.0	-0.0000121	0.0000004	0.0000292
33 H	1.0	0.0000289	0.0000757	-0.0001431
34 H	1.0	-0.0000396	0.0000505	0.0000451
35 H	1.0	-0.0000636	0.0000393	0.0000185

MAXIMUM GRADIENT = 0.0001431 RMS GRADIENT = 0.0000469
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000015491
 PREDICTED ENERGY CHANGE WAS -0.0000011242 RATIO= 1.378
 GDIIS STEP HAS LENGTH = 0.015427
 RADIUS OF STEP TAKEN= 0.01543 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8739.6 SECONDS (145.7 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8083.4 SECONDS (134.7 MIN)

CPU UTILIZATION: STEP = 81.14%, TOTAL = 100.00%

INSERCH= 100

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1624875651	-1.7171361467	0.8945996411
C	6.0	4.9800648980	0.6165807752	0.5586706987
C	6.0	5.1744699543	-0.7241269958	0.1987631837
C	6.0	4.0332125515	-1.5374179882	-0.0952884880
C	6.0	2.7285643600	-1.0175598301	-0.0031999892
C	6.0	2.4667149336	0.3491013537	0.4310577741
C	6.0	3.6535548619	1.1753059349	0.6785703848
C	6.0	3.5134817115	2.5620575187	1.0572145819
C	6.0	2.2486089139	3.1435562296	1.2219031303
C	6.0	1.0785358196	2.3409100069	1.0438600589
C	6.0	1.1642548126	0.9869319721	0.6435946960
N	7.0	-0.0494081182	0.1880161009	0.5974074211
C	6.0	-1.2459821597	0.7078195412	0.3301666608
C	6.0	-2.5468036891	0.0392985038	0.4427379497
C	6.0	-2.8134267824	-1.2839008678	0.9381526696
C	6.0	-4.1109986611	-1.8135117519	1.0551100081
C	6.0	-5.2229564355	-1.0073059544	0.6632373268
C	6.0	-5.0133628428	0.3065180890	0.1582371423
C	6.0	-3.6972531509	0.8177043728	0.0534653838
O	8.0	-1.6900513467	-2.1343025069	1.3421877354
N	7.0	1.6144084352	-1.9416971670	-0.4284648108
H	1.0	5.8469243123	1.2712539315	0.7614935424
H	1.0	6.1893522818	-1.1512767837	0.1169590701
H	1.0	4.1901892440	-2.5812530159	-0.4314889096
H	1.0	4.4289975240	3.1565398296	1.2288770462
H	1.0	2.1464408977	4.1996710814	1.5279982541
H	1.0	0.0964904143	2.7887667289	1.2775227264
H	1.0	-1.2930905480	1.7575126683	-0.0226970092
H	1.0	-4.2791482833	-2.8369870459	1.4414604763
H	1.0	-6.2455083175	-1.4166382544	0.7535993936
H	1.0	-5.8725946919	0.9295752407	-0.1459881180
H	1.0	-3.5370995874	1.8431410163	-0.3285261353
H	1.0	-2.0058994689	-2.9470482421	1.8144749478
H	1.0	1.2403857662	-1.6514352334	-1.3587928245
H	1.0	2.0024418261	-2.8975581112	-0.5539886190

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C	
1	CO	0.0000000	5.3635934	5.1565709	3.9993361
2	C	5.3635934	0.0000000	1.4017218 *	2.4421103 *
3	C	5.1565709	1.4017218 *	0.0000000	1.4319138 *
4	C	3.9993361	2.4421103 *	1.4319138 *	0.0000000
5	C	2.8071696 *	2.8381982 *	2.4717092 *	1.4074231 *
6	C	3.1294843	2.5307624 *	2.9219372 *	2.5079694 *
7	C	4.5387708	1.4443610 *	2.4801700 *	2.8463782 *
8	C	5.4375641	2.4868237 *	3.7808504	4.2899980
9	C	5.2995623	3.7797267	4.9564556	5.1798961
10	C	4.1628310	4.2930932	5.1851053	5.0069154
11	C	2.8945683 *	3.8346810	4.3826274	3.8921986
12	N	1.9398010 *	5.0478478	5.3178778	4.4860609
13	C	2.8605562 *	6.2309069	6.5795093	5.7525647
14	C	3.2602915	7.5498640	7.7627578	6.7876447
15	C	3.0075997	8.0308374	8.0415507	6.9288341
16	C	4.2775853	9.4233348	9.3882915	8.2296914
17	C	5.4369472	10.3319692	10.4116474	9.3023139
18	C	5.6059641	10.0062522	10.2399125	9.2360653
19	C	4.6936683	8.6943391	9.0058773	8.0826251
20	O	1.9509647 *	7.2575277	7.1005399	5.9311347
21	N	1.9771195 *	4.3412977	3.8144371	2.4748862 *
22	H	6.4234736	1.1050698 *	2.1795425 *	3.4514147
23	H	6.1031156	2.1869626 *	1.1041445 *	2.2007027 *
24	H	4.3275385	3.4395437	2.1942979 *	1.1078195 *
25	H	6.4859514	2.6840722 *	4.0836796	4.8931892
26	H	6.2726288	4.6698562	5.9312405	6.2537315
27	H	4.5226261	5.3929991	6.2681752	6.0081833
28	H	3.8772832	6.4025146	6.9308671	6.2634928
29	H	4.6131607	9.9216671	9.7662363	8.5525329
30	H	6.4165872	11.4098848	11.4544017	10.3144220
31	H	6.6715907	10.8800152	11.1754741	10.2085084
32	H	5.2781204	8.6506450	9.0972712	8.2941066
33	H	2.6572084 *	7.9423041	7.6882773	6.4888464
34	H	2.4987915 *	4.7755380	4.3316163	3.0674622
35	H	2.6224484 *	4.7385042	3.9181884	2.4868487 *

	C	C	C	C	
1	CO	2.8071696 *	3.1294843	4.5387708	5.4375641
2	C	2.8381982 *	2.5307624 *	1.4443610 *	2.4868237 *
3	C	2.4717092 *	2.9219372 *	2.4801700 *	3.7808504
4	C	1.4074231 *	2.5079694 *	2.8463782 *	4.2899980
5	C	0.0000000	1.4577063 *	2.4756976 *	3.8150013

6 C	1.4577063 *	0.0000000	1.4671283 *	2.5268494 *
7 C	2.4756976 *	1.4671283 *	0.0000000	1.4443240 *
8 C	3.8150013	2.5268494 *	1.4443240 *	0.0000000
9 C	4.3641863	2.9123847 *	2.4785263 *	1.4018439 *
10 C	3.8856465	2.5039708 *	2.8500513 *	2.4450043 *
11 C	2.6236225 *	1.4657429 *	2.4966623 *	2.8584907 *
12 N	3.0872761	2.5267560 *	3.8331793	4.3060050
13 C	4.3456976	3.7313506	4.9341050	5.1593889
14 C	5.3986404	5.0230950	6.3079772	6.5930989
15 C	5.6276770	5.5501115	6.9236502	7.4050890
16 C	6.9665760	6.9521689	8.3284515	8.7908084
17 C	7.9794064	7.8118368	9.1409235	9.4456829
18 C	7.8559965	7.4851725	8.7258811	8.8658162
19 C	6.6830035	6.1932760	7.3860012	7.4863194
20 O	4.7519835	4.9270842	6.3204449	7.0152522
21 N	1.5087158 *	2.5909387 *	3.8857886	5.1085741
22 H	3.9430437	3.5192852	2.1970325 *	2.6830168 *
23 H	3.4654540	4.0258939	3.4869274	4.6726026
24 H	2.1828685 *	3.5073248	3.9537252	5.3970190
25 H	4.6725362	3.5169275	2.1975979 *	1.1050097 *
26 H	5.4683575	4.0165584	3.4842079	2.1845402 *
27 H	4.8016857	3.5052010	3.9515449	3.4315831
28 H	4.8862169	4.0405016	5.0299147	4.9916569
29 H	7.3827770	7.5285286	8.9223470	9.4880140
30 H	9.0147651	8.8952068	10.2330472	10.5432485
31 H	8.8199581	8.3793805	9.5649258	9.6026624
32 H	6.8955051	6.2333708	7.2914853	7.2213444
33 H	5.4260497	5.7256200	7.0932014	7.8350021
34 H	2.1104752 *	2.9512023 *	4.2384784	5.3626093
35 H	2.0892620 *	3.4244216	4.5643836	5.8895348

C C C N

1 CO	5.2995623	4.1628310	2.8945683 *	1.9398010 *
2 C	3.7797267	4.2930932	3.8346810	5.0478478
3 C	4.9564556	5.1851053	4.3826274	5.3178778
4 C	5.1798961	5.0069154	3.8921986	4.4860609
5 C	4.3641863	3.8856465	2.6236225 *	3.0872761
6 C	2.9123847 *	2.5039708 *	1.4657429 *	2.5267560 *
7 C	2.4785263 *	2.8500513 *	2.4966623 *	3.8331793
8 C	1.4018439 *	2.4450043 *	2.8584907 *	4.3060050
9 C	0.0000000	1.4300389 *	2.4821951 *	3.7955361
10 C	1.4300389 *	0.0000000	1.4145023 *	2.4711393 *
11 C	2.4821951 *	1.4145023 *	0.0000000	1.4537460 *
12 N	3.7955361	2.4711393 *	1.4537460 *	0.0000000
13 C	4.3520310	2.9291170 *	2.4465043 *	1.3316917 *

14	C	5.7653705	4.3361100	3.8354019	2.5065961 *
15	C	6.7310546	5.3195677	4.5897056	3.1499914
16	C	8.0650450	6.6476022	5.9866626	4.5510574
17	C	8.5653986	7.1459239	6.6913256	5.3102477
18	C	7.8686978	6.4833871	6.2338989	4.9847527
19	C	6.4906170	5.1097160	4.9001174	3.7415443
20	O	6.5866005	5.2708255	4.2868637	2.9393148 *
21	N	5.3838394	4.5602219	3.1510028	2.8907400 *
22	H	4.0823237	4.8950407	4.6927745	5.9972548
23	H	5.9326175	6.2589902	5.4864275	6.3989583
24	H	6.2671270	6.0072232	4.8004196	5.1673654
25	H	2.1804384 *	3.4532705	3.9633696	5.4098987
26	H	1.1043148 *	2.1976815 *	3.4739821	4.6670256
27	H	2.1818761 *	1.1043492 *	2.1882856 *	2.6921640 *
28	H	4.0017223	2.6650531 *	2.6601288 *	2.0963289 *
29	H	8.8558860	7.4614665	6.6999689	5.2681848
30	H	9.6521868	8.2368102	7.7906252	6.4024190
31	H	8.5280001	7.1920665	7.0812415	5.9170980
32	H	6.1293828	4.8410028	4.8765609	3.9699853
33	H	7.4530159	6.1700965	5.1862355	3.8907249
34	H	5.5379101	4.6623767	3.3130550	2.9789040 *
35	H	6.3015436	5.5541220	4.1504249	3.8802795

C C C C

1	CO	2.8605562 *	3.2602915	3.0075997	4.2775853
2	C	6.2309069	7.5498640	8.0308374	9.4233348
3	C	6.5795093	7.7627578	8.0415507	9.3882915
4	C	5.7525647	6.7876447	6.9288341	8.2296914
5	C	4.3456976	5.3986404	5.6276770	6.9665760
6	C	3.7313506	5.0230950	5.5501115	6.9521689
7	C	4.9341050	6.3079772	6.9236502	8.3284515
8	C	5.1593889	6.5930989	7.4050890	8.7908084
9	C	4.3520310	5.7653705	6.7310546	8.0650450
10	C	2.9291170 *	4.3361100	5.3195677	6.6476022
11	C	2.4465043 *	3.8354019	4.5897056	5.9866626
12	N	1.3316917 *	2.5065961 *	3.1499914	4.5510574
13	C	0.0000000	1.4668774 *	2.6064305 *	3.8847103
14	C	1.4668774 *	0.0000000	1.4378387 *	2.5009221 *
15	C	2.6064305 *	1.4378387 *	0.0000000	1.4063639 *
16	C	3.8847103	2.5009221 *	1.4063639 *	0.0000000
17	C	4.3438365	2.8819775 *	2.4408843 *	1.4282794 *
18	C	3.7925928	2.4972507 *	2.8244326 *	2.4724823 *
19	C	2.4692849 *	1.4425612 *	2.4455194 *	2.8456591 *
20	O	3.0494330	2.5035127 *	1.4657420 *	2.4589238 *
21	N	3.9720643	4.6903118	4.6803914	5.9158864

22 H	7.1283114	8.4896401	9.0311520	10.4289127
23 H	7.6671960	8.8229260	9.0411271	10.3641648
24 H	6.3992247	7.2813897	7.2532529	8.4681240
25 H	6.2457430	7.6809512	8.5002791	9.8824664
26 H	5.0136176	6.3649850	7.4173962	8.6912336
27 H	2.6514255 *	3.9042854	5.0169125	6.2396634
28 H	1.1084167 *	2.1773117 *	3.5333908	4.6748786
29 H	4.7959070	3.5030677	2.1940225 *	1.1068165 *
30 H	5.4486584	3.9870795	3.4396021	2.1919281 *
31 H	4.6563336	3.4928608	3.9285298	3.4742458
32 H	2.6404640 *	2.1975855 *	3.4505896	3.9515717
33 H	4.0173006	3.3305415	2.0459962 *	2.5085818 *
34 H	3.8210853	4.5218246	4.6738032	5.8728622
35 H	4.9328224	5.5058356	5.2936722	6.4139309

C C C O

1 CO	5.4369472	5.6059641	4.6936683	1.9509647 *
2 C	10.3319692	10.0062522	8.6943391	7.2575277
3 C	10.4116474	10.2399125	9.0058773	7.1005399
4 C	9.3023139	9.2360653	8.0826251	5.9311347
5 C	7.9794064	7.8559965	6.6830035	4.7519835
6 C	7.8118368	7.4851725	6.1932760	4.9270842
7 C	9.1409235	8.7258811	7.3860012	6.3204449
8 C	9.4456829	8.8658162	7.4863194	7.0152522
9 C	8.5653986	7.8686978	6.4906170	6.5866005
10 C	7.1459239	6.4833871	5.1097160	5.2708255
11 C	6.6913256	6.2338989	4.9001174	4.2868637
12 N	5.3102477	4.9847527	3.7415443	2.9393148 *
13 C	4.3438365	3.7925928	2.4692849 *	3.0494330
14 C	2.8819775 *	2.4972507 *	1.4425612 *	2.5035127 *
15 C	2.4408843 *	2.8244326 *	2.4455194 *	1.4657420 *
16 C	1.4282794 *	2.4724823 *	2.8456591 *	2.4589238 *
17 C	0.0000000	1.4230560 *	2.4556578 *	3.7699487
18 C	1.4230560 *	0.0000000	1.4157801 *	4.2899584
19 C	2.4556578 *	1.4157801 *	0.0000000	3.7952614
20 O	3.7699487	4.2899584	3.7952614	0.0000000
21 N	6.9867345	7.0232502	6.0050231	3.7538995
22 H	11.3023780	10.9197285	9.5811447	8.2910206
23 H	11.4262828	11.2972428	10.0809665	8.0344587
24 H	9.6064065	9.6639728	8.6023159	6.1581591
25 H	10.5270022	9.9210414	8.5374290	8.0900316
26 H	9.0646808	8.2641198	6.9109121	7.4075920
27 H	6.5638426	5.7900742	4.4470095	5.2376067
28 H	4.8537175	3.9973176	2.5824481 *	4.1432733
29 H	2.2009403 *	3.4738103	3.9524551	2.6845937 *

30 H	1.1051383 *	2.2004332 *	3.4606472	4.6490501
31 H	2.1973585 *	1.1040981 *	2.1873289 *	5.3940414
32 H	3.4569866	2.1857497 *	1.1059326 *	4.6928594
33 H	3.9290462	4.7300796	4.4872257	0.9916506 *
34 H	6.8028157	6.7263908	5.6983683	4.0144637
35 H	7.5671046	7.7456365	6.8307173	4.2204916

N H H H

1 CO	1.9771195 *	6.4234736	6.1031156	4.3275385
2 C	4.3412977	1.1050698 *	2.1869626 *	3.4395437
3 C	3.8144371	2.1795425 *	1.1041445 *	2.1942979 *
4 C	2.4748862 *	3.4514147	2.2007027 *	1.1078195 *
5 C	1.5087158 *	3.9430437	3.4654540	2.1828685 *
6 C	2.5909387 *	3.5192852	4.0258939	3.5073248
7 C	3.8857886	2.1970325 *	3.4869274	3.9537252
8 C	5.1085741	2.6830168 *	4.6726026	5.3970190
9 C	5.3838394	4.0823237	5.9326175	6.2671270
10 C	4.5602219	4.8950407	6.2589902	6.0072232
11 C	3.1510028	4.6927745	5.4864275	4.8004196
12 N	2.8907400 *	5.9972548	6.3989583	5.1673654
13 C	3.9720643	7.1283114	7.6671960	6.3992247
14 C	4.6903118	8.4896401	8.8229260	7.2813897
15 C	4.6803914	9.0311520	9.0411271	7.2532529
16 C	5.9158864	10.4289127	10.3641648	8.4681240
17 C	6.9867345	11.3023780	11.4262828	9.6064065
18 C	7.0232502	10.9197285	11.2972428	9.6639728
19 C	6.0050231	9.5811447	10.0809665	8.6023159
20 O	3.7538995	8.2910206	8.0344587	6.1581591
21 N	0.0000000	5.4454794	4.6746511	2.6539947 *
22 H	5.4454794	0.0000000	2.5300863 *	4.3600216
23 H	4.6746511	2.5300863 *	0.0000000	2.5183884 *
24 H	2.6539947 *	4.3600216	2.5183884 *	0.0000000
25 H	6.0548092	2.4048423 *	4.7846102	5.9779688
26 H	6.4673959	4.7808717	6.8533792	7.3482943
27 H	5.2527857	5.9696416	7.3480485	6.9653573
28 H	4.7225365	7.1993899	8.0291662	7.0041670
29 H	6.2475736	10.9488513	10.6857581	8.6777311
30 H	7.9656295	12.3875645	12.4539747	10.5671446
31 H	8.0236659	11.7595660	12.2429429	10.6614749
32 H	6.3932013	9.4644124	10.1867002	8.9048782
33 H	4.3758586	8.9760617	8.5597025	6.6007329
34 H	1.0438655 *	5.8530269	5.1884749	3.2288998
35 H	1.0392287 *	5.8214717	4.5858356	2.2138866 *

H H H H

1	CO	6.4859514	6.2726288	4.5226261	3.8772832
2	C	2.6840722 *	4.6698562	5.3929991	6.4025146
3	C	4.0836796	5.9312405	6.2681752	6.9308671
4	C	4.8931892	6.2537315	6.0081833	6.2634928
5	C	4.6725362	5.4683575	4.8016857	4.8862169
6	C	3.5169275	4.0165584	3.5052010	4.0405016
7	C	2.1975979 *	3.4842079	3.9515449	5.0299147
8	C	1.1050097 *	2.1845402 *	3.4315831	4.9916569
9	C	2.1804384 *	1.1043148 *	2.1818761 *	4.0017223
10	C	3.4532705	2.1976815 *	1.1043492 *	2.6650531 *
11	C	3.9633696	3.4739821	2.1882856 *	2.6601288 *
12	N	5.4098987	4.6670256	2.6921640 *	2.0963289 *
13	C	6.2457430	5.0136176	2.6514255 *	1.1084167 *
14	C	7.6809512	6.3649850	3.9042854	2.1773117 *
15	C	8.5002791	7.4173962	5.0169125	3.5333908
16	C	9.8824664	8.6912336	6.2396634	4.6748786
17	C	10.5270022	9.0646808	6.5638426	4.8537175
18	C	9.9210414	8.2641198	5.7900742	3.9973176
19	C	8.5374290	6.9109121	4.4470095	2.5824481 *
20	O	8.0900316	7.4075920	5.2376067	4.1432733
21	N	6.0548092	6.4673959	5.2527857	4.7225365
22	H	2.4048423 *	4.7808717	5.9696416	7.1993899
23	H	4.7846102	6.8533792	7.3480485	8.0291662
24	H	5.9779688	7.3482943	6.9653573	7.0041670
25	H	0.0000000	2.5273823 *	4.3483608	6.0221264
26	H	2.5273823 *	0.0000000	2.5011370 *	4.4943487
27	H	4.3483608	2.5011370 *	0.0000000	2.1644841 *
28	H	6.0221264	4.4943487	2.1644841 *	0.0000000
29	H	10.5735216	9.5294408	7.1289687	5.6718362
30	H	11.6226039	10.1275582	7.6276389	5.9333222
31	H	10.6288488	8.8204699	6.4119383	4.6553775
32	H	8.2224829	6.4267059	4.0836965	2.2663716 *
33	H	8.8884538	8.2704049	6.1325308	5.1006069
34	H	6.3229664	6.5871044	5.2890500	4.4524802
35	H	6.7615741	7.3977069	6.2706758	5.7282186

H H H H

1	CO	4.6131607	6.4165872	6.6715907	5.2781204
2	C	9.9216671	11.4098848	10.8800152	8.6506450
3	C	9.7662363	11.4544017	11.1754741	9.0972712
4	C	8.5525329	10.3144220	10.2085084	8.2941066
5	C	7.3827770	9.0147651	8.8199581	6.8955051
6	C	7.5285286	8.8952068	8.3793805	6.2333708
7	C	8.9223470	10.2330472	9.5649258	7.2914853

8 C	9.4880140	10.5432485	9.6026624	7.2213444
9 C	8.8558860	9.6521868	8.5280001	6.1293828
10 C	7.4614665	8.2368102	7.1920665	4.8410028
11 C	6.6999689	7.7906252	7.0812415	4.8765609
12 N	5.2681848	6.4024190	5.9170980	3.9699853
13 C	4.7959070	5.4486584	4.6563336	2.6404640 *
14 C	3.5030677	3.9870795	3.4928608	2.1975855 *
15 C	2.1940225 *	3.4396021	3.9285298	3.4505896
16 C	1.1068165 *	2.1919281 *	3.4742458	3.9515717
17 C	2.2009403 *	1.1051383 *	2.1973585 *	3.4569866
18 C	3.4738103	2.2004332 *	1.1040981 *	2.1857497 *
19 C	3.9524551	3.4606472	2.1873289 *	1.1059326 *
20 O	2.6845937 *	4.6490501	5.3940414	4.6928594
21 N	6.2475736	7.9656295	8.0236659	6.3932013
22 H	10.9488513	12.3875645	11.7595660	9.4644124
23 H	10.6857581	12.4539747	12.2429429	10.1867002
24 H	8.6777311	10.5671446	10.6614749	8.9048782
25 H	10.5735216	11.6226039	10.6288488	8.2224829
26 H	9.5294408	10.1275582	8.8204699	6.4267059
27 H	7.1289687	7.6276389	6.4119383	4.0836965
28 H	5.6718362	5.9333222	4.6553775	2.2663716 *
29 H	0.0000000	2.5213321 *	4.3870327	5.0583681
30 H	2.5213321 *	0.0000000	2.5402835 *	4.3740867
31 H	4.3870327	2.5402835 *	0.0000000	2.5144502 *
32 H	5.0583681	4.3740867	2.5144502 *	0.0000000
33 H	2.3062770 *	4.6305394	5.8157508	5.4665291
34 H	6.3017623	7.7817698	7.6633544	6.0081510
35 H	6.5911957	8.4812494	8.7652504	7.2946268

H H H

1 CO	2.6572084 *	2.4987915 *	2.6224484 *
2 C	7.9423041	4.7755380	4.7385042
3 C	7.6882773	4.3316163	3.9181884
4 C	6.4888464	3.0674622	2.4868487 *
5 C	5.4260497	2.1104752 *	2.0892620 *
6 C	5.7256200	2.9512023 *	3.4244216
7 C	7.0932014	4.2384784	4.5643836
8 C	7.8350021	5.3626093	5.8895348
9 C	7.4530159	5.5379101	6.3015436
10 C	6.1700965	4.6623767	5.5541220
11 C	5.1862355	3.3130550	4.1504249
12 N	3.8907249	2.9789040 *	3.8802795
13 C	4.0173006	3.8210853	4.9328224
14 C	3.3305415	4.5218246	5.5058356
15 C	2.0459962 *	4.6738032	5.2936722

16 C	2.5085818 *	5.8728622	6.4139309
17 C	3.9290462	6.8028157	7.5671046
18 C	4.7300796	6.7263908	7.7456365
19 C	4.4872257	5.6983683	6.8307173
20 O	0.9916506 *	4.0144637	4.2204916
21 N	4.3758586	1.0438655 *	1.0392287 *
22 H	8.9760617	5.8530269	5.8214717
23 H	8.5597025	5.1884749	4.5858356
24 H	6.6007329	3.2288998	2.2138866 *
25 H	8.8884538	6.3229664	6.7615741
26 H	8.2704049	6.5871044	7.3977069
27 H	6.1325308	5.2890500	6.2706758
28 H	5.1006069	4.4524802	5.7282186
29 H	2.3062770 *	6.3017623	6.5911957
30 H	4.6305394	7.7817698	8.4812494
31 H	5.8157508	7.6633544	8.7652504
32 H	5.4665291	6.0081510	7.2946268
33 H	0.0000000	4.7208695	4.6560572
34 H	4.7208695	0.0000000	1.6677114 *
35 H	4.6560572	1.6677114 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.41 , TOTAL = 8740.0 SECONDS (145.7 MIN)
WALL CLOCK TIME: STEP = 0.41 , TOTAL = 8083.8 SECONDS (134.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.96 , TOTAL = 8740.9 SECONDS (145.7 MIN)
WALL CLOCK TIME: STEP = 0.96 , TOTAL = 8084.8 SECONDS (134.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.636961116 -284.636961116 0.003376401 0.000217775 198446805
11309256

2	1	-284.636965282	-0.000004166	0.000942198	0.000026830	143355608
15900804						
3	2	-284.636965196	0.000000086	0.000572908	0.000054576	130175933
16914416						
4	3	-284.636965370	-0.000000174	0.000077157	0.000005706	124528334
17333527						
5	4	-284.636965337	0.000000034	0.000070649	0.000013586	112143129
18286636						
6	5	-284.636965356	-0.000000019	0.000032591	0.000004742	105370727
18794356						
7	6	-284.636965367	-0.000000011	0.000024535	0.000006237	101136089
19065170						
8	7	-284.636965386	-0.000000019	0.000046372	0.000003929	94180309
19592301						
9	8	-284.636965382	0.000000004	0.000074529	0.000003301	126198622
17245647						
10	9	-284.636965383	-0.000000002	0.000146301	0.000003395	151395810
15369725						

-----DISABLING FDIFF OPTION-----

11	10	-284.636965384	-0.000000001	0.000144606	0.000004562	198447147
11309282						
12	11	-284.636965386	-0.000000001	0.000044991	0.000003149	198447263
11309271						
13	12	-284.636965386	-0.000000001	0.000059069	0.000002412	198447333
11309263						
14	13	-284.636965387	-0.000000001	0.000040002	0.000002067	198447333
11309263						
15	14	-284.636965387	0.000000000	0.000024372	0.000001109	198447296
11309267						
16	15	-284.636965387	0.000000000	0.000009076	0.000001022	198447324
11309265						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 52.5 SECONDS (3.3 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 17.4 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.5
 TIME TO SOLVE SCF EQUATIONS= 1.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369653871 AFTER 16 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6030297188
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998608281

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 55.32 , TOTAL = 8796.3 SECONDS (146.6 MIN)
WALL CLOCK TIME: STEP = 50.82 , TOTAL = 8135.6 SECONDS (135.6 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.93 , TOTAL = 8800.2 SECONDS (146.7 MIN)
WALL CLOCK TIME: STEP = 3.92 , TOTAL = 8139.5 SECONDS (135.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.85 , TOTAL = 8803.0 SECONDS (146.7 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 8142.2 SECONDS (135.7 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH=100 ENERGY= -284.6369654

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000163	0.0000564	0.0000953
2 C	6.0	0.0000097	0.0000032	-0.0000655
3 C	6.0	-0.0000282	-0.0000471	-0.0000205
4 C	6.0	0.0000117	-0.0000585	-0.0000210
5 C	6.0	0.0000181	-0.0000110	-0.0000052
6 C	6.0	0.0000271	-0.0000173	-0.0000529

7 C	6.0	-0.0000387	0.0000525	-0.0000411
8 C	6.0	-0.0000484	-0.0000019	0.0000289
9 C	6.0	-0.0000280	-0.0000291	0.0000568
10 C	6.0	-0.0000007	-0.0000005	-0.0000318
11 C	6.0	0.0000099	0.0000655	-0.0000784
12 N	7.0	-0.0000105	-0.0000362	-0.0000423
13 C	6.0	-0.0000002	-0.0000002	-0.0000517
14 C	6.0	-0.0000132	-0.0000184	-0.0000430
15 C	6.0	0.0000057	-0.0000142	-0.0000073
16 C	6.0	-0.0000010	0.0000053	0.0000389
17 C	6.0	0.0000402	0.0000573	0.0000293
18 C	6.0	0.0001108	-0.0000140	0.0000437
19 C	6.0	-0.0000036	-0.0000501	-0.0000569
20 O	8.0	-0.0000273	-0.0000577	0.0000239
21 N	7.0	-0.0000104	-0.0000026	0.0000058
22 H	1.0	0.0000131	-0.0000684	0.0000945
23 H	1.0	-0.0000345	-0.0000479	0.0000185
24 H	1.0	0.0000289	-0.0000145	-0.0000052
25 H	1.0	-0.0000596	0.0000448	-0.0000080
26 H	1.0	-0.0000326	0.0000009	0.0000587
27 H	1.0	-0.0000487	0.0000270	-0.0000058
28 H	1.0	0.0000037	-0.0000486	-0.0000840
29 H	1.0	0.0000362	0.0000143	0.0000132
30 H	1.0	0.0000206	0.0000293	0.0000161
31 H	1.0	0.0000391	-0.0000208	0.0000546
32 H	1.0	-0.0000242	0.0000374	0.0000342
33 H	1.0	0.0000691	0.0000434	-0.0001387
34 H	1.0	0.0000230	0.0001214	0.0001061
35 H	1.0	-0.0000409	0.0000001	0.0000409

MAXIMUM GRADIENT = 0.0001387 RMS GRADIENT = 0.0000440
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000014504
 PREDICTED ENERGY CHANGE WAS -0.0000009884 RATIO= 1.467
 GDIIS STEP HAS LENGTH = 0.013422
 RADIUS OF STEP TAKEN= 0.01342 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8803.0 SECONDS (146.7 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8142.2 SECONDS (135.7
 MIN)
 CPU UTILIZATION: STEP = 81.71% , TOTAL = 100.00%

INSERCH= 101

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1623270261	-1.7167880713	0.8950546741
C	6.0	4.9801865628	0.6162832153	0.5579782075
C	6.0	5.1743983476	-0.7245029544	0.1983078777
C	6.0	4.0328382223	-1.5375287066	-0.0951578554
C	6.0	2.7283554133	-1.0173954606	-0.0030707178
C	6.0	2.4666667438	0.3492408355	0.4312625054
C	6.0	3.6537688538	1.1751765495	0.6783467318
C	6.0	3.5139875086	2.5619919084	1.0569455990
C	6.0	2.2493148060	3.1439583356	1.2215342124
C	6.0	1.0791187447	2.3415528231	1.0437060940
C	6.0	1.1643887088	0.9873020341	0.6441364371
N	7.0	-0.0494630570	0.1885789970	0.5981444270
C	6.0	-1.2462078162	0.7084108991	0.3316047883
C	6.0	-2.5469976638	0.0395371396	0.4438801262
C	6.0	-2.8136763926	-1.2837418158	0.9391125495
C	6.0	-4.1111176275	-1.8139688544	1.0548498594
C	6.0	-5.2230130676	-1.0083157265	0.6617368215
C	6.0	-5.0134356371	0.3058479268	0.1574958231
C	6.0	-3.6974333647	0.8177206255	0.0540853448
O	8.0	-1.6900837515	-2.1338734863	1.3432367119
N	7.0	1.6141393115	-1.9413736277	-0.4280728445
H	1.0	5.8471175357	1.2709774444	0.7600958561
H	1.0	6.1890775528	-1.1519247430	0.1158161949
H	1.0	4.1891657108	-2.5816135342	-0.4309469168
H	1.0	4.4294929736	3.1562867274	1.2287970008
H	1.0	2.1475444149	4.2000778275	1.5278719951
H	1.0	0.0974030799	2.7898437981	1.2774597224
H	1.0	-1.2940076425	1.7584136842	-0.0204319840
H	1.0	-4.2793526669	-2.8377710530	1.4403605202
H	1.0	-6.2454198249	-1.4182170164	0.7508343339
H	1.0	-5.8724769505	0.9285985400	-0.1475249838
H	1.0	-3.5373343071	1.8431998925	-0.3279286335
H	1.0	-2.0054905723	-2.9468669573	1.8155649826
H	1.0	1.2401873387	-1.6507307431	-1.3582863097
H	1.0	2.0020284864	-2.8972814532	-0.5539121513

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3636380	5.1566408	3.9991889
2 C	5.3636380	0.0000000	1.4017091 *	2.4419176 *

3 C	5.1566408	1.4017091 *	0.0000000	1.4318843 *
4 C	3.9991889	2.4419176 *	1.4318843 *	0.0000000
5 C	2.8071838 *	2.8380320 *	2.4717333 *	1.4073713 *
6 C	3.1294664	2.5308399 *	2.9221574 *	2.5079695 *
7 C	4.5387870	1.4443802 *	2.4802285 *	2.8461856 *
8 C	5.4376277	2.4868636 *	3.7809088	4.2898272
9 C	5.2999021	3.7798292	4.9566217	5.1798605
10 C	4.1632602	4.2931127	5.1852397	5.0068696
11 C	2.8946832 *	3.8347609	4.3828320	3.8922139
12 N	1.9399573 *	5.0479619	5.3181121	4.4861230
13 C	2.8606007 *	6.2311892	6.5799083	5.7527992
14 C	3.2601652	7.5501097	7.7629904	6.7876313
15 C	3.0076680	8.0311679	8.0418205	6.9288445
16 C	4.2775352	9.4236309	9.3883655	8.2293957
17 C	5.4367507	10.3322490	10.4116032	9.3018137
18 C	5.6056729	10.0064600	10.2398852	9.2356344
19 C	4.6934757	8.6945714	9.0060342	8.0824855
20 O	1.9509621 *	7.2575822	7.1005846	5.9309731
21 N	1.9770847 *	4.3409883	3.8142590	2.4746773 *
22 H	6.4235348	1.1050092 *	2.1794722 *	3.4511991
23 H	6.1031144	2.1871178 *	1.1041142 *	2.2005837 *
24 H	4.3268503	3.4395102	2.1944258 *	1.1078383 *
25 H	6.4859037	2.6841906 *	4.0837875	4.8930660
26 H	6.2730254	4.6699186	5.9313642	6.2536939
27 H	4.5232930	5.3929207	6.2682599	6.0081513
28 H	3.8776351	6.4034782	6.9320270	6.2645117
29 H	4.6132938	9.9221044	9.7663711	8.5522491
30 H	6.4163201	11.4101106	11.4542032	10.3137058
31 H	6.6711245	10.8800543	11.1752315	10.2078301
32 H	5.2779443	8.6509142	9.0974891	8.2940352
33 H	2.6570409 *	7.9421187	7.6879924	6.4883365
34 H	2.4987381 *	4.7748315	4.3311545	3.0671171
35 H	2.6225123 *	4.7382341	3.9180010	2.4866788 *

C C C C

1 CO	2.8071838 *	3.1294664	4.5387870	5.4376277
2 C	2.8380320 *	2.5308399 *	1.4443802 *	2.4868636 *
3 C	2.4717333 *	2.9221574 *	2.4802285 *	3.7809088
4 C	1.4073713 *	2.5079695 *	2.8461856 *	4.2898272
5 C	0.0000000	1.4576766 *	2.4754983 *	3.8148219
6 C	1.4576766 *	0.0000000	1.4671168 *	2.5267820 *
7 C	2.4754983 *	1.4671168 *	0.0000000	1.4443451 *
8 C	3.8148219	2.5267820 *	1.4443451 *	0.0000000
9 C	4.3641726	2.9124246 *	2.4786378 *	1.4018457 *
10 C	3.8856475	2.5039336 *	2.8500429 *	2.4448629 *

11 C	2.6236770 *	1.4657304 *	2.4966940 *	2.8584391 *
12 N	3.0874115	2.5267709 *	3.8332406	4.3060152
13 C	4.3459830	3.7315375	4.9343562	5.1595873
14 C	5.3987241	5.0232366	6.3082610	6.5934944
15 C	5.6278563	5.5503664	6.9240253	7.4055981
16 C	6.9664996	6.9523798	8.3288779	8.7915451
17 C	7.9791173	7.8119942	9.1413988	9.4466113
18 C	7.8557039	7.4852363	8.7262507	8.8665744
19 C	6.6829394	6.1933728	7.3863151	7.4868419
20 O	4.7520176	4.9270811	6.3204946	7.0153740
21 N	1.5085887 *	2.5907865 *	3.8855036	5.1083269
22 H	3.9428100	3.5192581	2.1969613 *	2.6829711 *
23 H	3.4653759	4.0260833	3.4870663	4.6727945
24 H	2.1826184 *	3.5071805	3.9535622	5.3968849
25 H	4.6723645	3.5168530	2.1976217 *	1.1049296 *
26 H	5.4683777	4.0166325	3.4843124	2.1845512 *
27 H	4.8017433	3.5051395	3.9514332	3.4312668
28 H	4.8872101	4.0413448	5.0308001	4.9923239
29 H	7.3827660	7.5288845	8.9229384	9.4889724
30 H	9.0143038	8.8953070	10.2335175	10.5442780
31 H	8.8194148	8.3792582	9.5651568	9.6033556
32 H	6.8954627	6.2334833	7.2918317	7.2218888
33 H	5.4258266	5.7254529	7.0930759	7.8350282
34 H	2.1100633 *	2.9506987 *	4.2378063	5.3619534
35 H	2.0892459 *	3.4243780	4.5641672	5.8893589

C C C N

1 CO	5.2999021	4.1632602	2.8946832 *	1.9399573 *
2 C	3.7798292	4.2931127	3.8347609	5.0479619
3 C	4.9566217	5.1852397	4.3828320	5.3181121
4 C	5.1798605	5.0068696	3.8922139	4.4861230
5 C	4.3641726	3.8856475	2.6236770 *	3.0874115
6 C	2.9124246 *	2.5039336 *	1.4657304 *	2.5267709 *
7 C	2.4786378 *	2.8500429 *	2.4966940 *	3.8332406
8 C	1.4018457 *	2.4448629 *	2.8584391 *	4.3060152
9 C	0.0000000	1.4299777 *	2.4822609 *	3.7956899
10 C	1.4299777 *	0.0000000	1.4145395 *	2.4713394 *
11 C	2.4822609 *	1.4145395 *	0.0000000	1.4537915 *
12 N	3.7956899	2.4713394 *	1.4537915 *	0.0000000
13 C	4.3523033	2.9294000 *	2.4467186 *	1.3317157 *
14 C	5.7660030	4.3367946	3.8357202	2.5067290 *
15 C	6.7318772	5.3204845	4.5901692	3.1503751
16 C	8.0662213	6.6488374	5.9872173	4.5514630
17 C	8.5668219	7.1473341	6.6919131	5.3105763
18 C	7.8698534	6.4844955	6.2343173	4.9848718

19	C	6.4913891	5.1104661	4.9004318	3.7415915
20	O	6.5870465	5.2713985	4.2870142	2.9394871 *
21	N	5.3837954	4.5602455	3.1510394	2.8909156 *
22	H	4.0822993	4.8949340	4.6927463	5.9972892
23	H	5.9328707	6.2591568	5.4866120	6.3991390
24	H	6.2670478	6.0070426	4.8002332	5.1671046
25	H	2.1802251 *	3.4529781	3.9632346	5.4098114
26	H	1.1043498 *	2.1977409 *	3.4741203	4.6672645
27	H	2.1815703 *	1.1042514 *	2.1883129 *	2.6925114 *
28	H	4.0021679	2.6653649 *	2.6608226 *	2.0966423 *
29	H	8.8573399	7.4629717	6.7007072	5.2687844
30	H	9.6537826	8.2383559	7.7912238	6.4027328
31	H	8.5291057	7.1930629	7.0815007	5.9170214
32	H	6.1300992	4.8416295	4.8768505	3.9699657
33	H	7.4534820	6.1707345	5.1863345	3.8909096
34	H	5.5374051	4.6619565	3.3128023	2.9789058 *
35	H	6.3015822	5.5542354	4.1505361	3.8805137

C C C C

1	CO	2.8606007 *	3.2601652	3.0076680	4.2775352
2	C	6.2311892	7.5501097	8.0311679	9.4236309
3	C	6.5799083	7.7629904	8.0418205	9.3883655
4	C	5.7527992	6.7876313	6.9288445	8.2293957
5	C	4.3459830	5.3987241	5.6278563	6.9664996
6	C	3.7315375	5.0232366	5.5503664	6.9523798
7	C	4.9343562	6.3082610	6.9240253	8.3288779
8	C	5.1595873	6.5934944	7.4055981	8.7915451
9	C	4.3523033	5.7660030	6.7318772	8.0662213
10	C	2.9294000 *	4.3367946	5.3204845	6.6488374
11	C	2.4467186 *	3.8357202	4.5901692	5.9872173
12	N	1.3317157 *	2.5067290 *	3.1503751	4.5514630
13	C	0.0000000	1.4669874 *	2.6066637 *	3.8849957
14	C	1.4669874 *	0.0000000	1.4378595 *	2.5010477 *
15	C	2.6066637 *	1.4378595 *	0.0000000	1.4063746 *
16	C	3.8849957	2.5010477 *	1.4063746 *	0.0000000
17	C	4.3440899	2.8821026 *	2.4408400 *	1.4282599 *
18	C	3.7926740	2.4972492 *	2.8242983 *	2.4724573 *
19	C	2.4693060 *	1.4425712 *	2.4454946 *	2.8457782 *
20	O	3.0494271	2.5033692 *	1.4657765 *	2.4590468 *
21	N	3.9724116	4.6903486	4.6805157	5.9155607
22	H	7.1284886	8.4898532	9.0314998	10.4292963
23	H	7.6675212	8.8230504	9.0412815	10.3640777
24	H	6.3991430	7.2809100	7.2526775	8.4670877
25	H	6.2458490	7.6812528	8.5006631	9.8831031
26	H	5.0140151	6.3658356	7.4183979	8.6927187

27 H	2.6518474 *	3.9053677	5.0182629	6.2414976
28 H	1.1084767 *	2.1771785 *	3.5333877	4.6748537
29 H	4.7963229	3.5032741	2.1941885 *	1.1068389 *
30 H	5.4488917	3.9871788	3.4395342	2.1918693 *
31 H	4.6562232	3.4927071	3.9282938	3.4741571
32 H	2.6404528 *	2.1976476 *	3.4506287	3.9517321
33 H	4.0174251	3.3306694	2.0462938 *	2.5091455 *
34 H	3.8214450	4.5219000	4.6740276	5.8725069
35 H	4.9331731	5.5058271	5.2937365	6.4134419

C C C O

1 CO	5.4367507	5.6056729	4.6934757	1.9509621 *
2 C	10.3322490	10.0064600	8.6945714	7.2575822
3 C	10.4116032	10.2398852	9.0060342	7.1005846
4 C	9.3018137	9.2356344	8.0824855	5.9309731
5 C	7.9791173	7.8557039	6.6829394	4.7520176
6 C	7.8119942	7.4852363	6.1933728	4.9270811
7 C	9.1413988	8.7262507	7.3863151	6.3204946
8 C	9.4466113	8.8665744	7.4868419	7.0153740
9 C	8.5668219	7.8698534	6.4913891	6.5870465
10 C	7.1473341	6.4844955	5.1104661	5.2713985
11 C	6.6919131	6.2343173	4.9004318	4.2870142
12 N	5.3105763	4.9848718	3.7415915	2.9394871 *
13 C	4.3440899	3.7926740	2.4693060 *	3.0494271
14 C	2.8821026 *	2.4972492 *	1.4425712 *	2.5033692 *
15 C	2.4408400 *	2.8242983 *	2.4454946 *	1.4657765 *
16 C	1.4282599 *	2.4724573 *	2.8457782 *	2.4590468 *
17 C	0.0000000	1.4230980 *	2.4558181 *	3.7700016
18 C	1.4230980 *	0.0000000	1.4158282 *	4.2898589
19 C	2.4558181 *	1.4158282 *	0.0000000	3.7951642
20 O	3.7700016	4.2898589	3.7951642	0.0000000
21 N	6.9860529	7.0226523	6.0048216	3.7539957
22 H	11.3027715	10.9199916	9.5813540	8.2911077
23 H	11.4260433	11.2970412	10.0809926	8.0344239
24 H	9.6051202	9.6628966	8.6016960	6.1574161
25 H	10.5278841	9.9217734	8.5379020	8.0900007
26 H	9.0665689	8.2657482	6.9120296	7.4081320
27 H	6.5659697	5.7918242	4.4482242	5.2385521
28 H	4.8535790	3.9969676	2.5820363 *	4.1432316
29 H	2.2008309 *	3.4737530	3.9525951	2.6849988 *
30 H	1.1051122 *	2.2005080 *	3.4607963	4.6491065
31 H	2.1973495 *	1.1039964 *	2.1871797 *	5.3938408
32 H	3.4571798	2.1858552 *	1.1059720 *	4.6927860
33 H	3.9295994	4.7304419	4.4874938	0.9917327 *
34 H	6.8019225	6.7255926	5.6980825	4.0147406

35 H	7.5661892	7.7448613	6.8304295	4.2206230
	N	H	H	H
1 CO	1.9770847 *	6.4235348	6.1031144	4.3268503
2 C	4.3409883	1.1050092 *	2.1871178 *	3.4395102
3 C	3.8142590	2.1794722 *	1.1041142 *	2.1944258 *
4 C	2.4746773 *	3.4511991	2.2005837 *	1.1078383 *
5 C	1.5085887 *	3.9428100	3.4653759	2.1826184 *
6 C	2.5907865 *	3.5192581	4.0260833	3.5071805
7 C	3.8855036	2.1969613 *	3.4870663	3.9535622
8 C	5.1083269	2.6829711 *	4.6727945	5.3968849
9 C	5.3837954	4.0822993	5.9328707	6.2670478
10 C	4.5602455	4.8949340	6.2591568	6.0070426
11 C	3.1510394	4.6927463	5.4866120	4.8002332
12 N	2.8909156 *	5.9972892	6.3991390	5.1671046
13 C	3.9724116	7.1284886	7.6675212	6.3991430
14 C	4.6903486	8.4898532	8.8230504	7.2809100
15 C	4.6805157	9.0314998	9.0412815	7.2526775
16 C	5.9155607	10.4292963	10.3640777	8.4670877
17 C	6.9860529	11.3027715	11.4260433	9.6051202
18 C	7.0226523	10.9199916	11.2970412	9.6628966
19 C	6.0048216	9.5813540	10.0809926	8.6016960
20 O	3.7539957	8.2911077	8.0344239	6.1574161
21 N	0.0000000	5.4450940	4.6743026	2.6534273 *
22 H	5.4450940	0.0000000	2.5303138 *	4.3600280
23 H	4.6743026	2.5303138 *	0.0000000	2.5184534 *
24 H	2.6534273 *	4.3600280	2.5184534 *	0.0000000
25 H	6.0545499	2.4049389 *	4.7849295	5.9779601
26 H	6.4674313	4.7807897	6.8535993	7.3482329
27 H	5.2529752	5.9694084	7.3481598	6.9651797
28 H	4.7235491	7.2001727	8.0302676	7.0049660
29 H	6.2472249	10.9494280	10.6857160	8.6765899
30 H	7.9646836	12.3879503	12.4535491	10.5655418
31 H	8.0227720	11.7596724	12.2425088	10.6601393
32 H	6.3930201	9.4646274	10.1867938	8.9044028
33 H	4.3756883	8.9759501	8.5593172	6.5995449
34 H	1.0438441 *	5.8521558	5.1878030	3.2284632
35 H	1.0392561 *	5.8211433	4.5854319	2.2132185 *

H H H H

1 CO	6.4859037	6.2730254	4.5232930	3.8776351
2 C	2.6841906 *	4.6699186	5.3929207	6.4034782
3 C	4.0837875	5.9313642	6.2682599	6.9320270
4 C	4.8930660	6.2536939	6.0081513	6.2645117

5 C	4.6723645	5.4683777	4.8017433	4.8872101
6 C	3.5168530	4.0166325	3.5051395	4.0413448
7 C	2.1976217 *	3.4843124	3.9514332	5.0308001
8 C	1.1049296 *	2.1845512 *	3.4312668	4.9923239
9 C	2.1802251 *	1.1043498 *	2.1815703 *	4.0021679
10 C	3.4529781	2.1977409 *	1.1042514 *	2.6653649 *
11 C	3.9632346	3.4741203	2.1883129 *	2.6608226 *
12 N	5.4098114	4.6672645	2.6925114 *	2.0966423 *
13 C	6.2458490	5.0140151	2.6518474 *	1.1084767 *
14 C	7.6812528	6.3658356	3.9053677	2.1771785 *
15 C	8.5006631	7.4183979	5.0182629	3.5333877
16 C	9.8831031	8.6927187	6.2414976	4.6748537
17 C	10.5278841	9.0665689	6.5659697	4.8535790
18 C	9.9217734	8.2657482	5.7918242	3.9969676
19 C	8.5379020	6.9120296	4.4482242	2.5820363 *
20 O	8.0900007	7.4081320	5.2385521	4.1432316
21 N	6.0545499	6.4674313	5.2529752	4.7235491
22 H	2.4049389 *	4.7807897	5.9694084	7.2001727
23 H	4.7849295	6.8535993	7.3481598	8.0302676
24 H	5.9779601	7.3482329	6.9651797	7.0049660
25 H	0.0000000	2.5271001 *	4.3478329	6.0227138
26 H	2.5271001 *	0.0000000	2.5009090 *	4.4948025
27 H	4.3478329	2.5009090 *	0.0000000	2.1643463 *
28 H	6.0227138	4.4948025	2.1643463 *	0.0000000
29 H	10.5743785	9.5312109	7.1310992	5.6719586
30 H	11.6236094	10.1297025	7.6299746	5.9331540
31 H	10.6295551	8.8221468	6.4136014	4.6547961
32 H	8.2230121	6.4278080	4.0846937	2.2658900 *
33 H	8.8882954	8.2709907	6.1336424	5.1006626
34 H	6.3223483	6.5867418	5.2888387	4.4535676
35 H	6.7613847	7.3978043	6.2709580	5.7292192

H H H H

1 CO	4.6132938	6.4163201	6.6711245	5.2779443
2 C	9.9221044	11.4101106	10.8800543	8.6509142
3 C	9.7663711	11.4542032	11.1752315	9.0974891
4 C	8.5522491	10.3137058	10.2078301	8.2940352
5 C	7.3827660	9.0143038	8.8194148	6.8954627
6 C	7.5288845	8.8953070	8.3792582	6.2334833
7 C	8.9229384	10.2335175	9.5651568	7.2918317
8 C	9.4889724	10.5442780	9.6033556	7.2218888
9 C	8.8573399	9.6537826	8.5291057	6.1300992
10 C	7.4629717	8.2383559	7.1930629	4.8416295
11 C	6.7007072	7.7912238	7.0815007	4.8768505
12 N	5.2687844	6.4027328	5.9170214	3.9699657

13 C	4.7963229	5.4488917	4.6562232	2.6404528 *
14 C	3.5032741	3.9871788	3.4927071	2.1976476 *
15 C	2.1941885 *	3.4395342	3.9282938	3.4506287
16 C	1.1068389 *	2.1918693 *	3.4741571	3.9517321
17 C	2.2008309 *	1.1051122 *	2.1973495 *	3.4571798
18 C	3.4737530	2.2005080 *	1.1039964 *	2.1858552 *
19 C	3.9525951	3.4607963	2.1871797 *	1.1059720 *
20 O	2.6849988 *	4.6491065	5.3938408	4.6927860
21 N	6.2472249	7.9646836	8.0227720	6.3930201
22 H	10.9494280	12.3879503	11.7596724	9.4646274
23 H	10.6857160	12.4535491	12.2425088	10.1867938
24 H	8.6765899	10.5655418	10.6601393	8.9044028
25 H	10.5743785	11.6236094	10.6295551	8.2230121
26 H	9.5312109	10.1297025	8.8221468	6.4278080
27 H	7.1310992	7.6299746	6.4136014	4.0846937
28 H	5.6719586	5.9331540	4.6547961	2.2658900 *
29 H	0.0000000	2.5211109 *	4.3869084	5.0585499
30 H	2.5211109 *	0.0000000	2.5404092 *	4.3742767
31 H	4.3869084	2.5404092 *	0.0000000	2.5143453 *
32 H	5.0585499	4.3742767	2.5143453 *	0.0000000
33 H	2.3071907 *	4.6311362	5.8160587	5.4667953
34 H	6.3013340	7.7805377	7.6621717	6.0078200
35 H	6.5906308	8.4799999	8.7641511	7.2943658

H H H

1 CO	2.6570409 *	2.4987381 *	2.6225123 *
2 C	7.9421187	4.7748315	4.7382341
3 C	7.6879924	4.3311545	3.9180010
4 C	6.4883365	3.0671171	2.4866788 *
5 C	5.4258266	2.1100633 *	2.0892459 *
6 C	5.7254529	2.9506987 *	3.4243780
7 C	7.0930759	4.2378063	4.5641672
8 C	7.8350282	5.3619534	5.8893589
9 C	7.4534820	5.5374051	6.3015822
10 C	6.1707345	4.6619565	5.5542354
11 C	5.1863345	3.3128023	4.1505361
12 N	3.8909096	2.9789058 *	3.8805137
13 C	4.0174251	3.8214450	4.9331731
14 C	3.3306694	4.5219000	5.5058271
15 C	2.0462938 *	4.6740276	5.2937365
16 C	2.5091455 *	5.8725069	6.4134419
17 C	3.9295994	6.8019225	7.5661892
18 C	4.7304419	6.7255926	7.7448613
19 C	4.4874938	5.6980825	6.8304295
20 O	0.9917327 *	4.0147406	4.2206230

21 N	4.3756883	1.0438441 *	1.0392561 *
22 H	8.9759501	5.8521558	5.8211433
23 H	8.5593172	5.1878030	4.5854319
24 H	6.5995449	3.2284632	2.2132185 *
25 H	8.8882954	6.3223483	6.7613847
26 H	8.2709907	6.5867418	7.3978043
27 H	6.1336424	5.2888387	6.2709580
28 H	5.1006626	4.4535676	5.7292192
29 H	2.3071907 *	6.3013340	6.5906308
30 H	4.6311362	7.7805377	8.4799999
31 H	5.8160587	7.6621717	8.7641511
32 H	5.4667953	6.0078200	7.2943658
33 H	0.0000000	4.7209878	4.6558662
34 H	4.7209878	0.0000000	1.6677255 *
35 H	4.6558662	1.6677255 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80, TOTAL = 8803.9 SECONDS (146.7 MIN)
WALL CLOCK TIME: STEP = 0.81, TOTAL = 8143.0 SECONDS (135.7 MIN)

CPU UTILIZATION: STEP = 99.18%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.93, TOTAL = 8804.8 SECONDS (146.7 MIN)
WALL CLOCK TIME: STEP = 0.92, TOTAL = 8143.9 SECONDS (135.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636963168	-284.636963168	0.001630556	0.000271532	198441871
11309805					
2 1	-284.636966659	-0.000003491	0.000426844	0.000020411	142155226
15985444					
3 2	-284.636966662	-0.000000003	0.000268381	0.000035390	124966886
17340215					

4 3	-284.636966713	-0.000000051	0.000064557	0.000009143	118944931
17768492					
5 4	-284.636966685	0.000000028	0.000068129	0.000016081	111863834
18318004					
6 5	-284.636966679	0.000000006	0.000039721	0.000004700	104178513
18873954					
7 6	-284.636966680	-0.000000001	0.000015114	0.000004920	129454508
17010315					
8 7	-284.636966677	0.000000004	0.000027703	0.000001447	121934756
17544380					
9 8	-284.636966676	0.000000000	0.000016814	0.000002606	142039328
16046216					
10 9	-284.636966677	0.000000000	0.000007059	0.000001116	134884294
16582488					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 32.2 SECONDS (3.2 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 10.9 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.3
TIME TO SOLVE SCF EQUATIONS= 0.8 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369666766 AFTER 10 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6029969008
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998617959

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 33.79 , TOTAL = 8838.6 SECONDS (147.3 MIN)
WALL CLOCK TIME: STEP = 31.05 , TOTAL = 8175.0 SECONDS (136.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.97, TOTAL = 8842.5 SECONDS (147.4 MIN)
WALL CLOCK TIME: STEP = 3.94, TOTAL = 8178.9 SECONDS (136.3 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.84, TOTAL = 8845.4 SECONDS (147.4 MIN)
WALL CLOCK TIME: STEP = 2.67, TOTAL = 8181.6 SECONDS (136.4 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH=101 ENERGY= -284.6369667

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000072	0.0000240	0.0000943
2 C	6.0	0.0000156	-0.0000016	-0.0000662
3 C	6.0	0.0000174	-0.0000492	0.0000097
4 C	6.0	0.0000105	-0.0000007	-0.0000038
5 C	6.0	0.0000289	-0.0000152	-0.0000835
6 C	6.0	-0.0000050	-0.0000139	-0.0000458
7 C	6.0	-0.0000283	0.0000062	-0.0000495
8 C	6.0	-0.0000470	0.0000110	0.0000336
9 C	6.0	-0.0000670	-0.0000090	0.0000231
10 C	6.0	0.0000121	0.0000552	-0.0000599
11 C	6.0	0.0000403	0.0000176	-0.0000191
12 N	7.0	0.0000025	-0.0000474	-0.0000500
13 C	6.0	0.0000393	0.0000073	-0.0000779
14 C	6.0	-0.0000203	-0.0000473	-0.0000667
15 C	6.0	-0.0000480	0.0000116	0.0000432
16 C	6.0	-0.0000073	0.0000411	0.0000876
17 C	6.0	0.0000126	-0.0000282	-0.0000108
18 C	6.0	0.0000493	0.0000171	0.0000392
19 C	6.0	0.0000131	-0.0000057	-0.0000240
20 O	8.0	-0.0000240	0.0000157	-0.0000212
21 N	7.0	0.0000211	0.0000214	0.0000396
22 H	1.0	-0.0000185	-0.0000917	0.0000749
23 H	1.0	-0.0000599	-0.0000587	-0.0000076

24 H	1.0	-0.0000028	-0.0000330	0.0000055
25 H	1.0	-0.0001203	0.0000277	0.0000003
26 H	1.0	-0.0000259	0.0000210	0.0000900
27 H	1.0	0.0000262	0.0000202	-0.0000075
28 H	1.0	-0.0000482	-0.0000075	-0.0000839
29 H	1.0	0.0000079	-0.0000079	-0.0000077
30 H	1.0	0.0000397	0.0000277	0.0000225
31 H	1.0	0.0001038	-0.0000533	0.0000669
32 H	1.0	-0.0000121	0.0000546	0.0000041
33 H	1.0	0.0000782	-0.0000321	-0.0001083
34 H	1.0	0.0000549	0.0001437	0.0001241
35 H	1.0	-0.0000314	-0.0000208	0.0000350

MAXIMUM GRADIENT = 0.0001437 RMS GRADIENT = 0.0000472
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000012895
 PREDICTED ENERGY CHANGE WAS -0.0000009231 RATIO= 1.397
 GDIIS STEP HAS LENGTH = 0.028331
 RADIUS OF STEP TAKEN= 0.02833 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8845.4 SECONDS (147.4 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8181.6 SECONDS (136.4
 MIN)
 CPU UTILIZATION: STEP = 81.83% , TOTAL = 100.00%

INSERCH= 102

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1620183012	-1.7165031092	0.8960504494
C	6.0	4.9804992620	0.6160583971	0.5565437899
C	6.0	5.1743621440	-0.7249776781	0.1976202040
C	6.0	4.0322818960	-1.5377871124	-0.0942372457
C	6.0	2.7279606668	-1.0172286417	-0.0019263903
C	6.0	2.4666294086	0.3495733922	0.4320188021
C	6.0	3.6542197932	1.1751907663	0.6777395507
C	6.0	3.5150572096	2.5622759664	1.0553191536
C	6.0	2.2507380079	3.1448386258	1.2201456076
C	6.0	1.0801673603	2.3425925918	1.0438650215
C	6.0	1.1645565695	0.9879068547	0.6455445848
N	7.0	-0.0495613281	0.1894405804	0.6003224858
C	6.0	-1.2466389732	0.7093990074	0.3352636404
C	6.0	-2.5473691324	0.0400023953	0.4465439859

C	6.0	-2.8141574221	-1.2839253473	0.9400606556
C	6.0	-4.1115218576	-1.8151619518	1.0529767505
C	6.0	-5.2233674259	-1.0098551843	0.6586640215
C	6.0	-5.0136757390	0.3051107170	0.1564952894
C	6.0	-3.6976989169	0.8180008408	0.0561157618
O	8.0	-1.6903655849	-2.1338829993	1.3444409333
N	7.0	1.6136712626	-1.9411640364	-0.4269699310
H	1.0	5.8475904285	1.2713280801	0.7562771066
H	1.0	6.1889356616	-1.1526769574	0.1141833314
H	1.0	4.1875615649	-2.5823614828	-0.4289875448
H	1.0	4.4308257395	3.1562583529	1.2268938661
H	1.0	2.1495148221	4.2010418342	1.5262962313
H	1.0	0.0988933419	2.7916216689	1.2778943661
H	1.0	-1.2953525229	1.7600506753	-0.0149069434
H	1.0	-4.2802273881	-2.8396603888	1.4366916083
H	1.0	-6.2456156714	-1.4208468817	0.7452677079
H	1.0	-5.8724630951	0.9278594471	-0.1496261420
H	1.0	-3.5372421567	1.8436468701	-0.3253540099
H	1.0	-2.0055299568	-2.9475538728	1.8159996946
H	1.0	1.2396851996	-1.6505238588	-1.3572006846
H	1.0	2.0016155314	-2.8969825609	-0.5531387084

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3641278	5.1569873	3.9989435
2 C	5.3641278	0.0000000	1.4017085 *	2.4416557 *
3 C	5.1569873	1.4017085 *	0.0000000	1.4318475 *
4 C	3.9989435	2.4416557 *	1.4318475 *	0.0000000
5 C	2.8070282 *	2.8378593 *	2.4718636 *	1.4073934 *
6 C	3.1297332	2.5310200 *	2.9225707 *	2.5080556 *
7 C	4.5392758	1.4444150 *	2.4803200 *	2.8458967 *
8 C	5.4383993	2.4867771 *	3.7808699	4.2894660
9 C	5.3009840	3.7797742	4.9566737	5.1796221
10 C	4.1642652	4.2931330	5.1854169	5.0067558
11 C	2.8951113 *	3.8350503	4.3832808	3.8923329
12 N	1.9403202 *	5.0483095	5.3186188	4.4863318
13 C	2.8607339 *	6.2317676	6.5807019	5.7533748
14 C	3.2600840	7.5506783	7.7635231	6.7877590
15 C	3.0077703	8.0320418	8.0423930	6.9287769
16 C	4.2775583	9.4245491	9.3887048	8.2288867
17 C	5.4367346	10.3330982	10.4118441	9.3012159
18 C	5.6055038	10.0070106	10.2400630	9.2351767
19 C	4.6932523	8.6949602	9.0063463	8.0823849

20	O	1.9510474 *	7.2583330	7.1010350	5.9307520
21	N	1.9769046 *	4.3407622	3.8141502	2.4744901 *
22	H	6.4243601	1.1050425 *	2.1795804 *	3.4510647
23	H	6.1035194	2.1873331 *	1.1041955 *	2.2006600 *
24	H	4.3255560	3.4394639	2.1946041 *	1.1078381 *
25	H	6.4865999	2.6840503 *	4.0836557	4.8926769
26	H	6.2741287	4.6697965	5.9313362	6.2534069
27	H	4.5247076	5.3929119	6.2684804	6.0081670
28	H	3.8781696	6.4048099	6.9338115	6.2662362
29	H	4.6138186	9.9235936	9.7671103	8.5519839
30	H	6.4162233	11.4109709	11.4542588	10.3127892
31	H	6.6709114	10.8803809	11.1751867	10.2071766
32	H	5.2774070	8.6508171	9.0974383	8.2936847
33	H	2.6570770 *	7.9429318	7.6882929	6.4878054
34	H	2.4985716 *	4.7742542	4.3307951	3.0669826
35	H	2.6225558 *	4.7377843	3.9175969	2.4862841 *

C C C C

1	CO	2.8070282 *	3.1297332	4.5392758	5.4383993
2	C	2.8378593 *	2.5310200 *	1.4444150 *	2.4867771 *
3	C	2.4718636 *	2.9225707 *	2.4803200 *	3.7808699
4	C	1.4073934 *	2.5080556 *	2.8458967 *	4.2894660
5	C	0.0000000	1.4576523 *	2.4751979 *	3.8144649
6	C	1.4576523 *	0.0000000	1.4671038 *	2.5266098 *
7	C	2.4751979 *	1.4671038 *	0.0000000	1.4442777 *
8	C	3.8144649	2.5266098 *	1.4442777 *	0.0000000
9	C	4.3639438	2.9122604 *	2.4786041 *	1.4018024 *
10	C	3.8855246	2.5037489 *	2.8500212 *	2.4448069 *
11	C	2.6237415 *	1.4657614 *	2.4969050 *	2.8585672 *
12	N	3.0876176	2.5268923 *	3.8334960	4.3062600
13	C	4.3465368	3.7319161	4.9348423	5.1599790
14	C	5.3988858	5.0235671	6.3088675	6.5943525
15	C	5.6279250	5.5509580	6.9250248	7.4071254
16	C	6.9662070	6.9529664	8.3300514	8.7935588
17	C	7.9787250	7.8125198	9.1425568	9.4486783
18	C	7.8553557	7.4855097	8.7270355	8.8680305
19	C	6.6828540	6.1935185	7.3867929	7.4876401
20	O	4.7519710	4.9275427	6.3213173	7.0166892
21	N	1.5086284 *	2.5909221 *	3.8853428	5.1081720
22	H	3.9426456	3.5193284	2.1968808 *	2.6826636 *
23	H	3.4655700	4.0265791	3.4873125	4.6729260
24	H	2.1823054 *	3.5070189	3.9532894	5.3965473
25	H	4.6720169	3.5167277	2.1975705 *	1.1049366 *
26	H	5.4681268	4.0164429	3.4842446	2.1845089 *
27	H	4.8017993	3.5050363	3.9513771	3.4310807

28 H	4.8888135	4.0424865	5.0319068	4.9928941
29 H	7.3827894	7.5299838	8.9247123	9.4917239
30 H	9.0136718	8.8958264	10.2347796	10.5466646
31 H	8.8188702	8.3793311	9.5657406	9.6046212
32 H	6.8950693	6.2331648	7.2917868	7.2220227
33 H	5.4255824	5.7259637	7.0940416	7.8366921
34 H	2.1101647 *	2.9507774 *	4.2374075	5.3614599
35 H	2.0892312 *	3.4244560	4.5638534	5.8890701

C C C N

1 CO	5.3009840	4.1642652	2.8951113 *	1.9403202 *
2 C	3.7797742	4.2931330	3.8350503	5.0483095
3 C	4.9566737	5.1854169	4.3832808	5.3186188
4 C	5.1796221	5.0067558	3.8923329	4.4863318
5 C	4.3639438	3.8855246	2.6237415 *	3.0876176
6 C	2.9122604 *	2.5037489 *	1.4657614 *	2.5268923 *
7 C	2.4786041 *	2.8500212 *	2.4969050 *	3.8334960
8 C	1.4018024 *	2.4448069 *	2.8585672 *	4.3062600
9 C	0.0000000	1.4300032 *	2.4824003 *	3.7960421
10 C	1.4300032 *	0.0000000	1.4145509 *	2.4716554 *
11 C	2.4824003 *	1.4145509 *	0.0000000	1.4538486 *
12 N	3.7960421	2.4716554 *	1.4538486 *	0.0000000
13 C	4.3527035	2.9297551 *	2.4469787 *	1.3317687 *
14 C	5.7671743	4.3379413	3.8362112	2.5069949 *
15 C	6.7339115	5.3224217	4.5910921	3.1510666
16 C	8.0689468	6.6513640	5.9883386	4.5522358
17 C	8.5696554	7.1499536	6.6930410	5.3113071
18 C	7.8719193	6.4864228	6.2350569	4.9852577
19 C	6.4925374	5.1115589	4.9007982	3.7416783
20 O	6.5888276	5.2730477	4.2877277	2.9400312 *
21 N	5.3838896	4.5605430	3.1514199	2.8915650 *
22 H	4.0819803	4.8947561	4.6929091	5.9975996
23 H	5.9330594	6.2594513	5.4871513	6.3997231
24 H	6.2667174	6.0066934	4.7999994	5.1667762
25 H	2.1801281 *	3.4528920	3.9633609	5.4100340
26 H	1.1043276 *	2.1977437 *	3.4742053	4.6675805
27 H	2.1814061 *	1.1042172 *	2.1883536 *	2.6930445 *
28 H	4.0022182	2.6652294 *	2.6614949 *	2.0969785 *
29 H	8.8608481	7.4661831	6.7023770	5.2700570
30 H	9.6570709	8.2413430	7.7924766	6.4035244
31 H	8.5309828	7.1947871	7.0820582	5.9172519
32 H	6.1304472	4.8419189	4.8766634	3.9695331
33 H	7.4557431	6.1727927	5.1872213	3.8915830
34 H	5.5371873	4.6621392	3.3132989	2.9798528 *
35 H	6.3016032	5.5545149	4.1508885	3.8812121

	C	C	C	C
1 CO	2.8607339 *	3.2600840	3.0077703	4.2775583
2 C	6.2317676	7.5506783	8.0320418	9.4245491
3 C	6.5807019	7.7635231	8.0423930	9.3887048
4 C	5.7533748	6.7877590	6.9287769	8.2288867
5 C	4.3465368	5.3988858	5.6279250	6.9662070
6 C	3.7319161	5.0235671	5.5509580	6.9529664
7 C	4.9348423	6.3088675	6.9250248	8.3300514
8 C	5.1599790	6.5943525	7.4071254	8.7935588
9 C	4.3527035	5.7671743	6.7339115	8.0689468
10 C	2.9297551 *	4.3379413	5.3224217	6.6513640
11 C	2.4469787 *	3.8362112	4.5910921	5.9883386
12 N	1.3317687 *	2.5069949 *	3.1510666	4.5522358
13 C	0.0000000	1.4670972 *	2.6069591 *	3.8853667
14 C	1.4670972 *	0.0000000	1.4378871 *	2.5011936 *
15 C	2.6069591 *	1.4378871 *	0.0000000	1.4064554 *
16 C	3.8853667	2.5011936 *	1.4064554 *	0.0000000
17 C	4.3445129	2.8823884 *	2.4410226 *	1.4283564 *
18 C	3.7928845	2.4974145 *	2.8243391 *	2.4724718 *
19 C	2.4692940 *	1.4425583 *	2.4454239 *	2.8457912 *
20 O	3.0495220	2.5032882 *	1.4658989 *	2.4593764 *
21 N	3.9733939	4.6906614	4.6804276	5.9147236
22 H	7.1288924	8.4904325	9.0326614	10.4306457
23 H	7.6683749	8.8236030	9.0418463	10.3643449
24 H	6.3992423	7.2802912	7.2515032	8.4651993
25 H	6.2462573	7.6821352	8.5021930	9.8851894
26 H	5.0143782	6.3671684	7.4206859	8.6959370
27 H	2.6522936 *	3.9070778	5.0209640	6.2450492
28 H	1.1085402 *	2.1769356 *	3.5333442	4.6747546
29 H	4.7970433	3.5036621	2.1946104 *	1.1069308 *
30 H	5.4493870	3.9875235	3.4397089	2.1919228 *
31 H	4.6562959	3.4928439	3.9284403	3.4743826
32 H	2.6400373 *	2.1974550 *	3.4504831	3.9517686
33 H	4.0176858	3.3308394	2.0466576 *	2.5099238 *
34 H	3.8230197	4.5225164	4.6739110	5.8712416
35 H	4.9342075	5.5062244	5.2937007	6.4125183

	C	C	C	O
1 CO	5.4367346	5.6055038	4.6932523	1.9510474 *
2 C	10.3330982	10.0070106	8.6949602	7.2583330
3 C	10.4118441	10.2400630	9.0063463	7.1010350
4 C	9.3012159	9.2351767	8.0823849	5.9307520
5 C	7.9787250	7.8553557	6.6828540	4.7519710

6 C	7.8125198	7.4855097	6.1935185	4.9275427
7 C	9.1425568	8.7270355	7.3867929	6.3213173
8 C	9.4486783	8.8680305	7.4876401	7.0166892
9 C	8.5696554	7.8719193	6.4925374	6.5888276
10 C	7.1499536	6.4864228	5.1115589	5.2730477
11 C	6.6930410	6.2350569	4.9007982	4.2877277
12 N	5.3113071	4.9852577	3.7416783	2.9400312 *
13 C	4.3445129	3.7928845	2.4692940 *	3.0495220
14 C	2.8823884 *	2.4974145 *	1.4425583 *	2.5032882 *
15 C	2.4410226 *	2.8243391 *	2.4454239 *	1.4658989 *
16 C	1.4283564 *	2.4724718 *	2.8457912 *	2.4593764 *
17 C	0.0000000	1.4231231 *	2.4559696 *	3.7703886
18 C	1.4231231 *	0.0000000	1.4159546 *	4.2900228
19 C	2.4559696 *	1.4159546 *	0.0000000	3.7951004
20 O	3.7703886	4.2900228	3.7951004	0.0000000
21 N	6.9850580	7.0219591	6.0047494	3.7538909
22 H	11.3039565	10.9206418	9.5816637	8.2922964
23 H	11.4261769	11.2971429	10.0812939	8.0349043
24 H	9.6031946	9.6614209	8.6008791	6.1559897
25 H	10.5300918	9.9233766	8.5387987	8.0912543
26 H	9.0700400	8.2683694	6.9134872	7.4100625
27 H	6.5697132	5.7947075	4.4499477	5.2408465
28 H	4.8533882	3.9965181	2.5814280 *	4.1432573
29 H	2.2006879 *	3.4736774	3.9526971	2.6858920 *
30 H	1.1051723 *	2.2007405 *	3.4611052	4.6494873
31 H	2.1975887 *	1.1041024 *	2.1872352 *	5.3941119
32 H	3.4574245	2.1861218 *	1.1059907 *	4.6925379
33 H	3.9304682	4.7310382	4.4877644	0.9918450 *
34 H	6.8003835	6.7246045	5.6981435	4.0146857
35 H	7.5650575	7.7441135	6.8304083	4.2206462

N H H H

1 CO	1.9769046 *	6.4243601	6.1035194	4.3255560
2 C	4.3407622	1.1050425 *	2.1873331 *	3.4394639
3 C	3.8141502	2.1795804 *	1.1041955 *	2.1946041 *
4 C	2.4744901 *	3.4510647	2.2006600 *	1.1078381 *
5 C	1.5086284 *	3.9426456	3.4655700	2.1823054 *
6 C	2.5909221 *	3.5193284	4.0265791	3.5070189
7 C	3.8853428	2.1968808 *	3.4873125	3.9532894
8 C	5.1081720	2.6826636 *	4.6729260	5.3965473
9 C	5.3838896	4.0819803	5.9330594	6.2667174
10 C	4.5605430	4.8947561	6.2594513	6.0066934
11 C	3.1514199	4.6929091	5.4871513	4.7999994
12 N	2.8915650 *	5.9975996	6.3997231	5.1667762
13 C	3.9733939	7.1288924	7.6683749	6.3992423

14 C	4.6906614	8.4904325	8.8236030	7.2802912
15 C	4.6804276	9.0326614	9.0418463	7.2515032
16 C	5.9147236	10.4306457	10.3643449	8.4651993
17 C	6.9850580	11.3039565	11.4261769	9.6031946
18 C	7.0219591	10.9206418	11.2971429	9.6614209
19 C	6.0047494	9.5816637	10.0812939	8.6008791
20 O	3.7538909	8.2922964	8.0349043	6.1559897
21 N	0.0000000	5.4448371	4.6741420	2.6525553 *
22 H	5.4448371	0.0000000	2.5307314 *	4.3602146
23 H	4.6741420	2.5307314 *	0.0000000	2.5188352 *
24 H	2.6525553 *	4.3602146	2.5188352 *	0.0000000
25 H	6.0543654	2.4045092 *	4.7849764	5.9776984
26 H	6.4675397	4.7803677	6.8537062	7.3478793
27 H	5.2536059	5.9691620	7.3484917	6.9649371
28 H	4.7255905	7.2010561	8.0321365	7.0064508
29 H	6.2464847	10.9515243	10.6863612	8.6746995
30 H	7.9632444	12.3892518	12.4534433	10.5631046
31 H	8.0218715	11.7600292	12.2423677	10.6585079
32 H	6.3927325	9.4642780	10.1867406	8.9035320
33 H	4.3751972	8.9773870	8.5596162	6.5975538
34 H	1.0438709 *	5.8512219	5.1872828	3.2279833
35 H	1.0392345 *	5.8207307	4.5849286	2.2119584 *

H H H H

1 CO	6.4865999	6.2741287	4.5247076	3.8781696
2 C	2.6840503 *	4.6697965	5.3929119	6.4048099
3 C	4.0836557	5.9313362	6.2684804	6.9338115
4 C	4.8926769	6.2534069	6.0081670	6.2662362
5 C	4.6720169	5.4681268	4.8017993	4.8888135
6 C	3.5167277	4.0164429	3.5050363	4.0424865
7 C	2.1975705 *	3.4842446	3.9513771	5.0319068
8 C	1.1049366 *	2.1845089 *	3.4310807	4.9928941
9 C	2.1801281 *	1.1043276 *	2.1814061 *	4.0022182
10 C	3.4528920	2.1977437 *	1.1042172 *	2.6652294 *
11 C	3.9633609	3.4742053	2.1883536 *	2.6614949 *
12 N	5.4100340	4.6675805	2.6930445 *	2.0969785 *
13 C	6.2462573	5.0143782	2.6522936 *	1.1085402 *
14 C	7.6821352	6.3671684	3.9070778	2.1769356 *
15 C	8.5021930	7.4206859	5.0209640	3.5333442
16 C	9.8851894	8.6959370	6.2450492	4.6747546
17 C	10.5300918	9.0700400	6.5697132	4.8533882
18 C	9.9233766	8.2683694	5.7947075	3.9965181
19 C	8.5387987	6.9134872	4.4499477	2.5814280 *
20 O	8.0912543	7.4100625	5.2408465	4.1432573
21 N	6.0543654	6.4675397	5.2536059	4.7255905

22 H	2.4045092 *	4.7803677	5.9691620	7.2010561
23 H	4.7849764	6.8537062	7.3484917	8.0321365
24 H	5.9776984	7.3478793	6.9649371	7.0064508
25 H	0.0000000	2.5269732 *	4.3475509	6.0233365
26 H	2.5269732 *	0.0000000	2.5006433 *	4.4945362
27 H	4.3475509	2.5006433 *	0.0000000	2.1631910 *
28 H	6.0233365	4.4945362	2.1631910 *	0.0000000
29 H	10.5772162	9.5352557	7.1353523	5.6722093
30 H	11.6261884	10.1337976	7.6342241	5.9330498
31 H	10.6310079	8.8246568	6.4162701	4.6540985
32 H	8.2232918	6.4284621	4.0854061	2.2648256 *
33 H	8.8898956	8.2734966	6.1364722	5.1007952
34 H	6.3218730	6.5865898	5.2894035	4.4564770
35 H	6.7610135	7.3978290	6.2716228	5.7312870

H H H H

1 CO	4.6138186	6.4162233	6.6709114	5.2774070
2 C	9.9235936	11.4109709	10.8803809	8.6508171
3 C	9.7671103	11.4542588	11.1751867	9.0974383
4 C	8.5519839	10.3127892	10.2071766	8.2936847
5 C	7.3827894	9.0136718	8.8188702	6.8950693
6 C	7.5299838	8.8958264	8.3793311	6.2331648
7 C	8.9247123	10.2347796	9.5657406	7.2917868
8 C	9.4917239	10.5466646	9.6046212	7.2220227
9 C	8.8608481	9.6570709	8.5309828	6.1304472
10 C	7.4661831	8.2413430	7.1947871	4.8419189
11 C	6.7023770	7.7924766	7.0820582	4.8766634
12 N	5.2700570	6.4035244	5.9172519	3.9695331
13 C	4.7970433	5.4493870	4.6562959	2.6400373 *
14 C	3.5036621	3.9875235	3.4928439	2.1974550 *
15 C	2.1946104 *	3.4397089	3.9284403	3.4504831
16 C	1.1069308 *	2.1919228 *	3.4743826	3.9517686
17 C	2.2006879 *	1.1051723 *	2.1975887 *	3.4574245
18 C	3.4736774	2.2007405 *	1.1041024 *	2.1861218 *
19 C	3.9526971	3.4611052	2.1872352 *	1.1059907 *
20 O	2.6858920 *	4.6494873	5.3941119	4.6925379
21 N	6.2464847	7.9632444	8.0218715	6.3927325
22 H	10.9515243	12.3892518	11.7600292	9.4642780
23 H	10.6863612	12.4534433	12.2423677	10.1867406
24 H	8.6746995	10.5631046	10.6585079	8.9035320
25 H	10.5772162	11.6261884	10.6310079	8.2232918
26 H	9.5352557	10.1337976	8.8246568	6.4284621
27 H	7.1353523	7.6342241	6.4162701	4.0854061
28 H	5.6722093	5.9330498	4.6540985	2.2648256 *
29 H	0.0000000	2.5206844 *	4.3870063	5.0586756

30 H	2.5206844 *	0.0000000	2.5409642 *	4.3747500
31 H	4.3870063	2.5409642 *	0.0000000	2.5145186 *
32 H	5.0586756	4.3747500	2.5145186 *	0.0000000
33 H	2.3086282 *	4.6320220	5.8168450	5.4669134
34 H	6.2999456	7.7783581	7.6608714	6.0077426
35 H	6.5897087	8.4783052	8.7631817	7.2941345

H H H

1 CO	2.6570770 *	2.4985716 *	2.6225558 *
2 C	7.9429318	4.7742542	4.7377843
3 C	7.6882929	4.3307951	3.9175969
4 C	6.4878054	3.0669826	2.4862841 *
5 C	5.4255824	2.1101647 *	2.0892312 *
6 C	5.7259637	2.9507774 *	3.4244560
7 C	7.0940416	4.2374075	4.5638534
8 C	7.8366921	5.3614599	5.8890701
9 C	7.4557431	5.5371873	6.3016032
10 C	6.1727927	4.6621392	5.5545149
11 C	5.1872213	3.3132989	4.1508885
12 N	3.8915830	2.9798528 *	3.8812121
13 C	4.0176858	3.8230197	4.9342075
14 C	3.3308394	4.5225164	5.5062244
15 C	2.0466576 *	4.6739110	5.2937007
16 C	2.5099238 *	5.8712416	6.4125183
17 C	3.9304682	6.8003835	7.5650575
18 C	4.7310382	6.7246045	7.7441135
19 C	4.4877644	5.6981435	6.8304083
20 O	0.9918450 *	4.0146857	4.2206462
21 N	4.3751972	1.0438709 *	1.0392345 *
22 H	8.9773870	5.8512219	5.8207307
23 H	8.5596162	5.1872828	4.5849286
24 H	6.5975538	3.2279833	2.2119584 *
25 H	8.8898956	6.3218730	6.7610135
26 H	8.2734966	6.5865898	7.3978290
27 H	6.1364722	5.2894035	6.2716228
28 H	5.1007952	4.4564770	5.7312870
29 H	2.3086282 *	6.2999456	6.5897087
30 H	4.6320220	7.7783581	8.4783052
31 H	5.8168450	7.6608714	8.7631817
32 H	5.4669134	6.0077426	7.2941345
33 H	0.0000000	4.7204776	4.6553828
34 H	4.7204776	0.0000000	1.6675469 *
35 H	4.6553828	1.6675469 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.78 , TOTAL = 8846.2 SECONDS (147.4 MIN)
WALL CLOCK TIME: STEP = 0.78 , TOTAL = 8182.4 SECONDS (136.4 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.11 , TOTAL = 8847.3 SECONDS (147.5 MIN)
WALL CLOCK TIME: STEP = 1.10 , TOTAL = 8183.5 SECONDS (136.4 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

		NONZERO BLOCKS				
ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD	
-----START SECOND ORDER SCF-----						
1	0	-284.636952955	-284.636952955	0.003649737	0.000635211	198421753
11311441						
2	1	-284.636969188	-0.000016233	0.000697505	0.000040706	147477881
15585641						
3	2	-284.636969253	-0.000000064	0.000450132	0.000058937	129465360
17053576						
4	3	-284.636969347	-0.000000094	0.000155673	0.000046016	124492322
17441107						
5	4	-284.636969360	-0.000000013	0.000237846	0.000026810	121559665
17646445						
6	5	-284.636969371	-0.000000011	0.000100858	0.000014718	116582703
17974328						
7	6	-284.636969385	-0.000000015	0.000104247	0.000006408	113849897
18198569						
8	7	-284.636969385	0.000000000	0.000087611	0.000006944	132646736
16740521						
9	8	-284.636969389	-0.000000003	0.000028640	0.000003815	128280770
17089101						
10	9	-284.636969391	-0.000000002	0.000015852	0.000003638	121207486
17612141						
11	10	-284.636969389	0.000000002	0.000064151	0.000003420	114344953
18203796						
12	11	-284.636969390	-0.000000001	0.000069575	0.000002491	145978284
15830364						

-----DISABLING FDIFF OPTION-----

13 12	-284.636969427	-0.000000037	0.000054529	0.000003342	198421196
11311484					
14 13	-284.636969428	-0.000000001	0.000022709	0.000001968	198421196
11311484					
15 14	-284.636969428	0.000000000	0.000015079	0.000001078	198420956
11311487					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 48.7 SECONDS (3.2 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 16.3 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.6 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369694279 AFTER 15 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6025471832
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998649931

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 51.28 , TOTAL = 8898.6 SECONDS (148.3 MIN)
WALL CLOCK TIME: STEP = 47.25 , TOTAL = 8230.8 SECONDS (137.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 4.08 , TOTAL = 8902.6 SECONDS (148.4 MIN)
WALL CLOCK TIME: STEP = 4.06 , TOTAL = 8234.8 SECONDS (137.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.86 , TOTAL = 8905.5 SECONDS (148.4 MIN)

WALL CLOCK TIME: STEP = 2.67 , TOTAL = 8237.5 SECONDS (137.3 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH=102 ENERGY= -284.6369694

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000322	-0.0000379	0.0000637
2 C	6.0	-0.0000022	-0.0000692	0.0000129
3 C	6.0	0.0000024	-0.0000328	-0.0000063
4 C	6.0	0.0000550	0.0000520	-0.0000054
5 C	6.0	0.0000363	0.0000147	-0.0000705
6 C	6.0	-0.0000021	0.0000519	-0.0000328
7 C	6.0	-0.0000219	-0.0000013	-0.0000248
8 C	6.0	-0.0001079	-0.0000202	-0.0000384
9 C	6.0	-0.0000157	0.0000498	-0.0000330
10 C	6.0	0.0000294	0.0000512	-0.0000633
11 C	6.0	0.0000232	-0.0000468	0.0000311
12 N	7.0	0.0000349	-0.0000102	-0.0000485
13 C	6.0	0.0000450	-0.0000046	-0.0001157
14 C	6.0	-0.0000243	-0.0000162	-0.0000735
15 C	6.0	-0.0000598	0.0000715	0.0000637
16 C	6.0	0.0000171	0.0000560	0.0001046
17 C	6.0	-0.0000488	-0.0000457	-0.0000447
18 C	6.0	0.0000303	-0.0000621	0.0000515
19 C	6.0	0.0000521	0.0000516	0.0000535
20 O	8.0	0.0000210	0.0000842	-0.0000475
21 N	7.0	0.0000465	-0.0000008	0.0000659
22 H	1.0	-0.0000080	-0.0000505	0.0000195
23 H	1.0	-0.0000088	-0.0000869	-0.0000287
24 H	1.0	-0.0000548	-0.0000453	0.0000358
25 H	1.0	-0.0001206	0.0000206	0.0000394
26 H	1.0	-0.0000211	0.0000001	0.0001188
27 H	1.0	0.0000529	0.0000226	-0.0000140
28 H	1.0	-0.0001064	0.0000431	-0.0000747
29 H	1.0	-0.0000583	-0.0000659	-0.0000070
30 H	1.0	0.0000068	-0.0000065	0.0000298

31 H	1.0	0.0000616	-0.0000008	0.0000372
32 H	1.0	0.0000340	0.0000431	-0.0000427
33 H	1.0	0.0000706	-0.0001316	-0.0000721
34 H	1.0	0.0000429	0.0001190	0.0001079
35 H	1.0	-0.0000336	0.0000040	0.0000082

MAXIMUM GRADIENT = 0.0001316 RMS GRADIENT = 0.0000530
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000027513
 PREDICTED ENERGY CHANGE WAS -0.0000016140 RATIO= 1.705
 GDIIS STEP HAS LENGTH = 0.035758
 RADIUS OF STEP TAKEN= 0.03576 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8905.5 SECONDS (148.4 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8237.5 SECONDS (137.3 MIN)
 CPU UTILIZATION: STEP = 81.23%, TOTAL = 100.00%

INSERCH= 103

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z

CO	27.0	0.1615139183	-1.7159290567	0.8971172276
C	6.0	4.9807937633	0.6159379426	0.5547562373
C	6.0	5.1740660341	-0.7255079006	0.1969354080
C	6.0	4.0313183608	-1.5381702748	-0.0929340801
C	6.0	2.7271470393	-1.0171603986	-0.0001905741
C	6.0	2.4664585968	0.3499411966	0.4331732229
C	6.0	3.6547516163	1.1752701304	0.6770633059
C	6.0	3.5165961515	2.5627850055	1.0532110343
C	6.0	2.2525619819	3.1458456933	1.2186196630
C	6.0	1.0813795229	2.3438241891	1.0445855667
C	6.0	1.1646916029	0.9887929651	0.6472512765
N	7.0	-0.0497274696	0.1905513805	0.6031435958
C	6.0	-1.2471777108	0.7106312079	0.3400377183
C	6.0	-2.5476938241	0.0403645884	0.4496280510
C	6.0	-2.8143961221	-1.2846226221	0.9404244864
C	6.0	-4.1117899970	-1.8168360810	1.0497508482
C	6.0	-5.2235881949	-1.0116135482	0.6549198973
C	6.0	-5.0139204966	0.3043378294	0.1551066412
C	6.0	-3.6979700084	0.8181242161	0.0582840280
O	8.0	-1.6906307359	-2.1340792054	1.3459581925
N	7.0	1.6128003775	-1.9410141626	-0.4257657020

H	1.0	5.8481622137	1.2719215221	0.7514675822
H	1.0	6.1885398255	-1.1533898965	0.1125012230
H	1.0	4.1856045352	-2.5832405887	-0.4266801417
H	1.0	4.4328844076	3.1564085542	1.2236789235
H	1.0	2.1520669459	4.2023322291	1.5238880384
H	1.0	0.1005320811	2.7937571102	1.2789330439
H	1.0	-1.2966474213	1.7620777668	-0.0078913844
H	1.0	-4.2810193054	-2.8419466938	1.4316824356
H	1.0	-6.2456751857	-1.4239257736	0.7388308968
H	1.0	-5.8725322293	0.9270892835	-0.1518234827
H	1.0	-3.5370715003	1.8442017341	-0.3216307392
H	1.0	-2.0059569234	-2.9481557019	1.8170046240
H	1.0	1.2387788721	-1.6508422594	-1.3561682588
H	1.0	2.0011462782	-2.8966553810	-0.5519818052

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3647249	5.1572151	3.9983980
2 C	5.3647249	0.0000000	1.4017371 *	2.4415545 *
3 C	5.1572151	1.4017371 *	0.0000000	1.4318927 *
4 C	3.9983980	2.4415545 *	1.4318927 *	0.0000000
5 C	2.8064056 *	2.8379393 *	2.4721109 *	1.4074500 *
6 C	3.1298297	2.5312878 *	2.9229330 *	2.5080949 *
7 C	4.5398421	1.4443681 *	2.4802815 *	2.8456032 *
8 C	5.4395162	2.4864725 *	3.7806461	4.2891050
9 C	5.3021410	3.7794704	4.9564507	5.1792039
10 C	4.1652726	4.2931288	5.1854984	5.0065928
11 C	2.8955690 *	3.8353894	4.3836851	3.8924243
12 N	1.9405440 *	5.0487067	5.3190402	4.4864170
13 C	2.8605846 *	6.2323912	6.5814394	5.7538764
14 C	3.2595430	7.5511894	7.7637613	6.7874551
15 C	3.0073146	8.0327988	8.0424445	6.9279090
16 C	4.2772194	9.4254172	9.3885789	8.2276119
17 C	5.4363632	10.3338457	10.4116675	9.2999916
18 C	5.6051030	10.0075535	10.2399903	9.2343222
19 C	4.6926201	8.6953036	9.0063893	8.0818865
20 O	1.9510888 *	7.2592355	7.1012948	5.9301113
21 N	1.9765917 *	4.3408302	3.8141611	2.4743260 *
22 H	6.4254520	1.1051415 *	2.1798247 *	3.4511667
23 H	6.1038606	2.1874097 *	1.1042505 *	2.2008780 *
24 H	4.3241154	3.4395184	2.1947946 *	1.1078640 *
25 H	6.4877517	2.6835896 *	4.0832374	4.8922178
26 H	6.2754251	4.6693828	5.9310109	6.2529248

27 H	4.5262315	5.3929846	6.2687074	6.0082190
28 H	3.8783768	6.4059720	6.9354285	6.2678616
29 H	4.6140846	9.9250767	9.7674230	8.5509792
30 H	6.4157924	11.4117717	11.4539045	10.3112308
31 H	6.6704974	10.8807516	11.1749740	10.2062348
32 H	5.2763067	8.6504748	9.0970454	8.2929649
33 H	2.6575374 *	7.9442256	7.6887917	6.4872658
34 H	2.4984058 *	4.7741596	4.3306881	3.0670397
35 H	2.6226418 *	4.7372439	3.9169093	2.4855191 *

C C C C

1 CO	2.8064056 *	3.1298297	4.5398421	5.4395162
2 C	2.8379393 *	2.5312878 *	1.4443681 *	2.4864725 *
3 C	2.4721109 *	2.9229330 *	2.4802815 *	3.7806461
4 C	1.4074500 *	2.5080949 *	2.8456032 *	4.2891050
5 C	0.0000000	1.4576452 *	2.4750504 *	3.8143012
6 C	1.4576452 *	0.0000000	1.4672050 *	2.5266408 *
7 C	2.4750504 *	1.4672050 *	0.0000000	1.4442201 *
8 C	3.8143012	2.5266408 *	1.4442201 *	0.0000000
9 C	4.3636394	2.9120027 *	2.4784243 *	1.4018210 *
10 C	3.8853990	2.5035652 *	2.8500588 *	2.4450559 *
11 C	2.6237944 *	1.4657961 *	2.4972107 *	2.8589700 *
12 N	3.0876548	2.5269522 *	3.8338363	4.3068222
13 C	4.3469847	3.7322736	4.9354216	5.1606813
14 C	5.3985778	5.0237270	6.3095219	6.5956448
15 C	5.6271657	5.5512638	6.9260598	7.4092327
16 C	6.9651215	6.9533047	8.3313123	8.7962133
17 C	7.9776808	7.8127986	9.1437338	9.4512318
18 C	7.8545911	7.4856845	8.7279344	8.8699994
19 C	6.6823512	6.1935383	7.3873511	7.4889042
20 O	4.7514613	4.9279738	6.3223671	7.0186499
21 N	1.5087705 *	2.5913288 *	3.8854890	5.1084261
22 H	3.9427936	3.5195566	2.1967994 *	2.6820846 *
23 H	3.4659051	4.0269993	3.4873300	4.6727052
24 H	2.1821088 *	3.5069026	3.9530314	5.3962236
25 H	4.6718384	3.5168151	2.1975415 *	1.1050033 *
26 H	5.4677816	4.0161446	3.4840032	2.1843974 *
27 H	4.8019117	3.5050184	3.9514837	3.4312960
28 H	4.8903114	4.0434681	5.0328778	4.9934341
29 H	7.3820391	7.5308450	8.9265862	9.4951131
30 H	9.0123887	8.8961399	10.2361167	10.5496275
31 H	8.8180260	8.3793848	9.5664928	9.6064218
32 H	6.8942839	6.2325691	7.2915828	7.2222420
33 H	5.4252386	5.7266860	7.0954724	7.8391607
34 H	2.1107979 *	2.9516224 *	4.2376723	5.3617362

35 H 2.0890314 * 3.4245343 4.5635008 5.8888642

C C C N

1 CO	5.3021410	4.1652726	2.8955690 *	1.9405440 *
2 C	3.7794704	4.2931288	3.8353894	5.0487067
3 C	4.9564507	5.1854984	4.3836851	5.3190402
4 C	5.1792039	5.0065928	3.8924243	4.4864170
5 C	4.3636394	3.8853990	2.6237944 *	3.0876548
6 C	2.9120027 *	2.5035652 *	1.4657961 *	2.5269522 *
7 C	2.4784243 *	2.8500588 *	2.4972107 *	3.8338363
8 C	1.4018210 *	2.4450559 *	2.8589700 *	4.3068222
9 C	0.0000000	1.4301030 *	2.4824988 *	3.7964605
10 C	1.4301030 *	0.0000000	1.4145406 *	2.4720149 *
11 C	2.4824988 *	1.4145406 *	0.0000000	1.4539425 *
12 N	3.7964605	2.4720149 *	1.4539425 *	0.0000000
13 C	4.3532004	2.9301682 *	2.4472163 *	1.3317638 *
14 C	5.7686928	4.3393633	3.8367143	2.5071815 *
15 C	6.7365055	5.3248046	4.5921137	3.1517122
16 C	8.0722799	6.6543317	5.9895591	4.5529567
17 C	8.5729252	7.1528609	6.6941619	5.3119409
18 C	7.8744520	6.4887102	6.2358586	4.9856692
19 C	6.4941125	5.1129965	4.9011721	3.7417099
20 O	6.5910994	5.2750815	4.2887513	2.9407898 *
21 N	5.3841844	4.5611600	3.1521321	2.8924427 *
22 H	4.0814414	4.8946002	4.6931780	5.9980384
23 H	5.9328616	6.2595826	5.4876184	6.4002255
24 H	6.2662664	6.0063968	4.7998612	5.1664781
25 H	2.1803539 *	3.4532525	3.9638252	5.4106545
26 H	1.1042879 *	2.1977613 *	3.4742246	4.6679819
27 H	2.1814758 *	1.1042736 *	2.1884590 *	2.6936869 *
28 H	4.0020033	2.6647981 *	2.6618360 *	2.0971095 *
29 H	8.8649161	7.4697647	6.7041529	5.2712761
30 H	9.6609028	8.2447047	7.7937882	6.4042732
31 H	8.5333552	7.1969036	7.0827147	5.9175602
32 H	6.1307833	4.8421338	4.8761699	3.9687952
33 H	7.4585455	6.1752189	5.1885354	3.8925280
34 H	5.5376443	4.6632342	3.3146422	2.9815905 *
35 H	6.3015918	5.5549639	4.1514486	3.8821699

C C C C

1 CO	2.8605846 *	3.2595430	3.0073146	4.2772194
2 C	6.2323912	7.5511894	8.0327988	9.4254172
3 C	6.5814394	7.7637613	8.0424445	9.3885789
4 C	5.7538764	6.7874551	6.9279090	8.2276119

5 C	4.3469847	5.3985778	5.6271657	6.9651215
6 C	3.7322736	5.0237270	5.5512638	6.9533047
7 C	4.9354216	6.3095219	6.9260598	8.3313123
8 C	5.1606813	6.5956448	7.4092327	8.7962133
9 C	4.3532004	5.7686928	6.7365055	8.0722799
10 C	2.9301682 *	4.3393633	5.3248046	6.6543317
11 C	2.4472163 *	3.8367143	4.5921137	5.9895591
12 N	1.3317638 *	2.5071815 *	3.1517122	4.5529567
13 C	0.0000000	1.4671774 *	2.6072353 *	3.8855871
14 C	1.4671774 *	0.0000000	1.4379160 *	2.5011474 *
15 C	2.6072353 *	1.4379160 *	0.0000000	1.4065683 *
16 C	3.8855871	2.5011474 *	1.4065683 *	0.0000000
17 C	4.3447806	2.8825706 *	2.4413630 *	1.4284152 *
18 C	3.7931023	2.4977387 *	2.8247879 *	2.4725708 *
19 C	2.4692758 *	1.4426349 *	2.4454895 *	2.8455701 *
20 O	3.0497383	2.5032320 *	1.4659068 *	2.4597549 *
21 N	3.9745632	4.6906170	4.6794652	5.9129945
22 H	7.1293878	8.4910681	9.0339105	10.4321639
23 H	7.6691748	8.8238587	9.0418767	10.3641397
24 H	6.3994196	7.2793219	7.2495098	8.4625044
25 H	6.2470597	7.6835771	8.5044733	9.8881178
26 H	5.0148122	6.3689686	7.4238035	8.7000630
27 H	2.6527834 *	3.9092221	5.0243980	6.2493001
28 H	1.1086216 *	2.1768641 *	3.5334470	4.6746400
29 H	4.7975715	3.5037931	2.1948978 *	1.1069607 *
30 H	5.4498024	3.9878378	3.4400176	2.1919206 *
31 H	4.6564671	3.4932184	3.9289784	3.4746396
32 H	2.6393940 *	2.1971656 *	3.4503022	3.9514791
33 H	4.0179471	3.3308334	2.0467802 *	2.5105966 *
34 H	3.8253956	4.5231025	4.6729736	5.8689512
35 H	4.9355673	5.5064739	5.2929552	6.4108928

C C C O

1 CO	5.4363632	5.6051030	4.6926201	1.9510888 *
2 C	10.3338457	10.0075535	8.6953036	7.2592355
3 C	10.4116675	10.2399903	9.0063893	7.1012948
4 C	9.2999916	9.2343222	8.0818865	5.9301113
5 C	7.9776808	7.8545911	6.6823512	4.7514613
6 C	7.8127986	7.4856845	6.1935383	4.9279738
7 C	9.1437338	8.7279344	7.3873511	6.3223671
8 C	9.4512318	8.8699994	7.4889042	7.0186499
9 C	8.5729252	7.8744520	6.4941125	6.5910994
10 C	7.1528609	6.4887102	5.1129965	5.2750815
11 C	6.6941619	6.2358586	4.9011721	4.2887513
12 N	5.3119409	4.9856692	3.7417099	2.9407898 *

13 C	4.3447806	3.7931023	2.4692758 *	3.0497383
14 C	2.8825706 *	2.4977387 *	1.4426349 *	2.5032320 *
15 C	2.4413630 *	2.8247879 *	2.4454895 *	1.4659068 *
16 C	1.4284152 *	2.4725708 *	2.8455701 *	2.4597549 *
17 C	0.0000000	1.4232013 *	2.4558961 *	3.7708423
18 C	1.4232013 *	0.0000000	1.4160073 *	4.2904848
19 C	2.4558961 *	1.4160073 *	0.0000000	3.7951312
20 O	3.7708423	4.2904848	3.7951312	0.0000000
21 N	6.9834000	7.0208581	6.0042844	3.7535233
22 H	11.3051984	10.9213875	9.5820184	8.2938326
23 H	11.4258910	11.2969864	10.0813136	8.0352036
24 H	9.6006655	9.6595986	8.5997221	6.1541964
25 H	10.5329653	9.9256374	8.5402876	8.0933090
26 H	9.0741735	8.2715959	6.9154748	7.4126982
27 H	6.5739254	5.7980876	4.4521599	5.2436941
28 H	4.8531996	3.9962099	2.5810420 *	4.1434491
29 H	2.2004353 *	3.4735999	3.9525041	2.6867337 *
30 H	1.1053073 *	2.2011017 *	3.4613197	4.6498765
31 H	2.1978471 *	1.1041918 *	2.1874047 *	5.3946643
32 H	3.4574081	2.1862164 *	1.1059198 *	4.6922186
33 H	3.9311306	4.7316450	4.4878582	0.9919858 *
34 H	6.7981819	6.7233125	5.6980664	4.0145294
35 H	7.5635166	7.7432224	6.8302224	4.2205351

N H H H

1 CO	1.9765917 *	6.4254520	6.1038606	4.3241154
2 C	4.3408302	1.1051415 *	2.1874097 *	3.4395184
3 C	3.8141611	2.1798247 *	1.1042505 *	2.1947946 *
4 C	2.4743260 *	3.4511667	2.2008780 *	1.1078640 *
5 C	1.5087705 *	3.9427936	3.4659051	2.1821088 *
6 C	2.5913288 *	3.5195566	4.0269993	3.5069026
7 C	3.8854890	2.1967994 *	3.4873300	3.9530314
8 C	5.1084261	2.6820846 *	4.6727052	5.3962236
9 C	5.3841844	4.0814414	5.9328616	6.2662664
10 C	4.5611600	4.8946002	6.2595826	6.0063968
11 C	3.1521321	4.6931780	5.4876184	4.7998612
12 N	2.8924427 *	5.9980384	6.4002255	5.1664781
13 C	3.9745632	7.1293878	7.6691748	6.3994196
14 C	4.6906170	8.4910681	8.8238587	7.2793219
15 C	4.6794652	9.0339105	9.0418767	7.2495098
16 C	5.9129945	10.4321639	10.3641397	8.4625044
17 C	6.9834000	11.3051984	11.4258910	9.6006655
18 C	7.0208581	10.9213875	11.2969864	9.6595986
19 C	6.0042844	9.5820184	10.0813136	8.5997221
20 O	3.7535233	8.2938326	8.0352036	6.1541964

21 N	0.0000000	5.4449172	4.6741282	2.6517498 *
22 H	5.4449172	0.0000000	2.5310611 *	4.3605510
23 H	4.6741282	2.5310611 *	0.0000000	2.5193133 *
24 H	2.6517498 *	4.3605510	2.5193133 *	0.0000000
25 H	6.0545239	2.4035986 *	4.7844963	5.9773242
26 H	6.4678175	4.7796507	6.8533850	7.3473798
27 H	5.2546182	5.9690414	7.3487666	6.9648430
28 H	4.7278320	7.2017487	8.0338331	7.0080141
29 H	6.2449102	10.9538542	10.6865865	8.6720332
30 H	7.9611120	12.3906681	12.4529186	10.5600200
31 H	8.0206774	11.7605069	12.2420472	10.6566447
32 H	6.3921736	9.4637021	10.1863409	8.9024157
33 H	4.3749008	8.9795105	8.5601573	6.5956590
34 H	1.0439065 *	5.8507343	5.1869627	3.2275527
35 H	1.0392272 *	5.8202702	4.5841877	2.2103817 *

H H H H

1 CO	6.4877517	6.2754251	4.5262315	3.8783768
2 C	2.6835896 *	4.6693828	5.3929846	6.4059720
3 C	4.0832374	5.9310109	6.2687074	6.9354285
4 C	4.8922178	6.2529248	6.0082190	6.2678616
5 C	4.6718384	5.4677816	4.8019117	4.8903114
6 C	3.5168151	4.0161446	3.5050184	4.0434681
7 C	2.1975415 *	3.4840032	3.9514837	5.0328778
8 C	1.1050033 *	2.1843974 *	3.4312960	4.9934341
9 C	2.1803539 *	1.1042879 *	2.1814758 *	4.0020033
10 C	3.4532525	2.1977613 *	1.1042736 *	2.6647981 *
11 C	3.9638252	3.4742246	2.1884590 *	2.6618360 *
12 N	5.4106545	4.6679819	2.6936869 *	2.0971095 *
13 C	6.2470597	5.0148122	2.6527834 *	1.1086216 *
14 C	7.6835771	6.3689686	3.9092221	2.1768641 *
15 C	8.5044733	7.4238035	5.0243980	3.5334470
16 C	9.8881178	8.7000630	6.2493001	4.6746400
17 C	10.5329653	9.0741735	6.5739254	4.8531996
18 C	9.9256374	8.2715959	5.7980876	3.9962099
19 C	8.5402876	6.9154748	4.4521599	2.5810420 *
20 O	8.0933090	7.4126982	5.2436941	4.1434491
21 N	6.0545239	6.4678175	5.2546182	4.7278320
22 H	2.4035986 *	4.7796507	5.9690414	7.2017487
23 H	4.7844963	6.8533850	7.3487666	8.0338331
24 H	5.9773242	7.3473798	6.9648430	7.0080141
25 H	0.0000000	2.5270952 *	4.3478553	6.0239903
26 H	2.5270952 *	0.0000000	2.5005764 *	4.4938648
27 H	4.3478553	2.5005764 *	0.0000000	2.1615712 *
28 H	6.0239903	4.4938648	2.1615712 *	0.0000000

29 H	10.5809097	9.5401764	7.1402018	5.6723795
30 H	11.6295389	10.1386965	7.6390383	5.9330505
31 H	10.6331314	8.8277640	6.4194245	4.6536699
32 H	8.2237501	6.4290758	4.0860274	2.2637749 *
33 H	8.8924922	8.2767480	6.1397378	5.1009474
34 H	6.3219919	6.5869926	5.2909194	4.4602982
35 H	6.7606142	7.3978130	6.2725894	5.7336962

H H H H

1 CO	4.6140846	6.4157924	6.6704974	5.2763067
2 C	9.9250767	11.4117717	10.8807516	8.6504748
3 C	9.7674230	11.4539045	11.1749740	9.0970454
4 C	8.5509792	10.3112308	10.2062348	8.2929649
5 C	7.3820391	9.0123887	8.8180260	6.8942839
6 C	7.5308450	8.8961399	8.3793848	6.2325691
7 C	8.9265862	10.2361167	9.5664928	7.2915828
8 C	9.4951131	10.5496275	9.6064218	7.2222420
9 C	8.8649161	9.6609028	8.5333552	6.1307833
10 C	7.4697647	8.2447047	7.1969036	4.8421338
11 C	6.7041529	7.7937882	7.0827147	4.8761699
12 N	5.2712761	6.4042732	5.9175602	3.9687952
13 C	4.7975715	5.4498024	4.6564671	2.6393940 *
14 C	3.5037931	3.9878378	3.4932184	2.1971656 *
15 C	2.1948978 *	3.4400176	3.9289784	3.4503022
16 C	1.1069607 *	2.1919206 *	3.4746396	3.9514791
17 C	2.2004353 *	1.1053073 *	2.1978471 *	3.4574081
18 C	3.4735999	2.2011017 *	1.1041918 *	2.1862164 *
19 C	3.9525041	3.4613197	2.1874047 *	1.1059198 *
20 O	2.6867337 *	4.6498765	5.3946643	4.6922186
21 N	6.2449102	7.9611120	8.0206774	6.3921736
22 H	10.9538542	12.3906681	11.7605069	9.4637021
23 H	10.6865865	12.4529186	12.2420472	10.1863409
24 H	8.6720332	10.5600200	10.6566447	8.9024157
25 H	10.5809097	11.6295389	10.6331314	8.2237501
26 H	9.5401764	10.1386965	8.8277640	6.4290758
27 H	7.1402018	7.6390383	6.4194245	4.0860274
28 H	5.6723795	5.9330505	4.6536699	2.2637749 *
29 H	0.0000000	2.5200594 *	4.3870305	5.0584140
30 H	2.5200594 *	0.0000000	2.5416083 *	4.3751309
31 H	4.3870305	2.5416083 *	0.0000000	2.5148174 *
32 H	5.0584140	4.3751309	2.5148174 *	0.0000000
33 H	2.3099053 *	4.6325961	5.8175779	5.4666958
34 H	6.2975402	7.7754463	7.6594336	6.0078571
35 H	6.5881349	8.4761544	8.7621894	7.2938772

	H	H	H
1 CO	2.6575374 *	2.4984058 *	2.6226418 *
2 C	7.9442256	4.7741596	4.7372439
3 C	7.6887917	4.3306881	3.9169093
4 C	6.4872658	3.0670397	2.4855191 *
5 C	5.4252386	2.1107979 *	2.0890314 *
6 C	5.7266860	2.9516224 *	3.4245343
7 C	7.0954724	4.2376723	4.5635008
8 C	7.8391607	5.3617362	5.8888642
9 C	7.4585455	5.5376443	6.3015918
10 C	6.1752189	4.6632342	5.5549639
11 C	5.1885354	3.3146422	4.1514486
12 N	3.8925280	2.9815905 *	3.8821699
13 C	4.0179471	3.8253956	4.9355673
14 C	3.3308334	4.5231025	5.5064739
15 C	2.0467802 *	4.6729736	5.2929552
16 C	2.5105966 *	5.8689512	6.4108928
17 C	3.9311306	6.7981819	7.5635166
18 C	4.7316450	6.7233125	7.7432224
19 C	4.4878582	5.6980664	6.8302224
20 O	0.9919858 *	4.0145294	4.2205351
21 N	4.3749008	1.0439065 *	1.0392272 *
22 H	8.9795105	5.8507343	5.8202702
23 H	8.5601573	5.1869627	4.5841877
24 H	6.5956590	3.2275527	2.2103817 *
25 H	8.8924922	6.3219919	6.7606142
26 H	8.2767480	6.5869926	7.3978130
27 H	6.1397378	5.2909194	6.2725894
28 H	5.1009474	4.4602982	5.7336962
29 H	2.3099053 *	6.2975402	6.5881349
30 H	4.6325961	7.7754463	8.4761544
31 H	5.8175779	7.6594336	8.7621894
32 H	5.4666958	6.0078571	7.2938772
33 H	0.0000000	4.7202075	4.6552793
34 H	4.7202075	0.0000000	1.6673243 *
35 H	4.6552793	1.6673243 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80 , TOTAL = 8906.3 SECONDS (148.4 MIN)
WALL CLOCK TIME: STEP = 0.80 , TOTAL = 8238.3 SECONDS (137.3 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.94, TOTAL = 8907.3 SECONDS (148.5 MIN)
WALL CLOCK TIME: STEP = 0.93, TOTAL = 8239.2 SECONDS (137.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636944771	-284.636944771	0.004999328	0.000757911	198404447
11313069						
2	1	-284.636971813	-0.000027043	0.000914117	0.000051435	149646323
15436679						
3	2	-284.636972023	-0.000000209	0.000458090	0.000038555	131314734
16907490						
4	3	-284.636972040	-0.000000017	0.000186237	0.000060643	126129738
17268727						
5	4	-284.636972108	-0.000000068	0.000244654	0.000030228	121467016
17690884						
6	5	-284.636972116	-0.000000009	0.000140994	0.000025094	118811598
17790418						
7	6	-284.636972135	-0.000000019	0.000045284	0.000005935	114741565
18102988						
8	7	-284.636972095	0.000000040	0.000041492	0.000005883	105656559
18724852						
9	8	-284.636972097	-0.000000002	0.000057625	0.000005796	125483133
17307459						
10	9	-284.636972098	-0.000000001	0.000069663	0.000005441	149598482
15448290						

-----DISABLING FDIFF OPTION-----

11	10	-284.636972122	-0.000000024	0.000206321	0.000004821	198404469
11313076						
12	11	-284.636972126	-0.000000004	0.000083912	0.000004445	198404407
11313081						
13	12	-284.636972127	-0.000000001	0.000042390	0.000004302	198404350
11313081						
14	13	-284.636972128	-0.000000001	0.000022788	0.000002992	198404395
11313073						
15	14	-284.636972128	0.000000000	0.000024021	0.000001133	198404397
11313073						

ENERGY CONVERGED

TIME TO FORM FOCK OPERATORS= 48.9 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 16.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.3 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369721279 AFTER 15 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6019811994
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998694718

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 51.40 , TOTAL = 8958.7 SECONDS (149.3 MIN)
WALL CLOCK TIME: STEP = 47.76 , TOTAL = 8287.0 SECONDS (138.1
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 4.06 , TOTAL = 8962.7 SECONDS (149.4 MIN)
WALL CLOCK TIME: STEP = 4.04 , TOTAL = 8291.0 SECONDS (138.2
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.85 , TOTAL = 8965.6 SECONDS (149.4 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 8293.7 SECONDS (138.2
MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH=103 ENERGY= -284.6369721

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000509	-0.0000340	-0.0000036
2 C	6.0	-0.0000540	-0.0000773	0.0001082
3 C	6.0	0.0000257	-0.0000163	-0.0000280
4 C	6.0	0.0000382	0.0000722	-0.0000247
5 C	6.0	0.0000177	0.0000238	0.0000368
6 C	6.0	-0.0000224	0.0000705	0.0000023
7 C	6.0	0.0000363	-0.0000091	0.0000050
8 C	6.0	-0.0000644	-0.0000228	-0.0001014
9 C	6.0	0.0000194	0.0000752	-0.0000736
10 C	6.0	0.0000214	-0.0000068	-0.0000184
11 C	6.0	0.0000048	-0.0000560	-0.0000143
12 N	7.0	0.0000209	0.0000284	-0.0000513
13 C	6.0	0.0000505	-0.0000573	-0.0000882
14 C	6.0	0.0000194	0.0000101	-0.0000132
15 C	6.0	0.0000345	0.0000126	0.0000507
16 C	6.0	-0.0000055	0.0000472	0.0000298
17 C	6.0	-0.0000453	-0.0000308	0.0000228
18 C	6.0	0.0000130	-0.0000368	0.0000016
19 C	6.0	0.0000164	0.0000946	0.0000471
20 O	8.0	0.0001038	0.0001792	-0.0000534
21 N	7.0	0.0000221	-0.0000028	0.0000448
22 H	1.0	0.0000347	0.0000278	-0.0000362
23 H	1.0	0.0000351	-0.0000852	-0.0000357
24 H	1.0	-0.0000952	-0.0000715	0.0000563
25 H	1.0	-0.0000653	0.0000191	0.0000709
26 H	1.0	-0.0000054	-0.0000299	0.0001159
27 H	1.0	0.0000117	0.0000392	-0.0000200
28 H	1.0	-0.0001238	0.0001049	-0.0000789
29 H	1.0	-0.0001098	-0.0000709	0.0000066
30 H	1.0	-0.0000677	-0.0000690	0.0000306
31 H	1.0	0.0000141	0.0000353	0.0000173
32 H	1.0	0.0000669	-0.0000157	-0.0000381
33 H	1.0	0.0000136	-0.0002311	-0.0000260
34 H	1.0	-0.0000083	0.0000491	0.0000818
35 H	1.0	-0.0000040	0.0000341	-0.0000236

MAXIMUM GRADIENT = 0.0002311 RMS GRADIENT = 0.0000579

HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0000027000
PREDICTED ENERGY CHANGE WAS -0.0000019429 RATIO= 1.390
GDIIS STEP HAS LENGTH = 0.022153
RADIUS OF STEP TAKEN= 0.02215 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 8965.6 SECONDS (149.4 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8293.8 SECONDS (138.2 MIN)
CPU UTILIZATION: STEP = 81.83%, TOTAL = 100.00%

INSERCH= 104

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1609616299	-1.7153969894	0.8972816785
C	6.0	4.9808138562	0.6159768594	0.5533775087
C	6.0	5.1735364134	-0.7257885371	0.1966457981
C	6.0	4.0305013134	-1.5385278609	-0.0920492295
C	6.0	2.7264374520	-1.0172448231	0.0006987434
C	6.0	2.4662582304	0.3500459910	0.4339076192
C	6.0	3.6549118653	1.1753176018	0.6767247920
C	6.0	3.5175976464	2.5630221809	1.0523898157
C	6.0	2.2536594782	3.1462839986	1.2181618517
C	6.0	1.0820395640	2.3445888221	1.0451652106
C	6.0	1.1647096068	0.9894235264	0.6482746996
N	7.0	-0.0499132792	0.1913383595	0.6047216728
C	6.0	-1.2475823147	0.7115250074	0.3430763293
C	6.0	-2.5478271857	0.0404892288	0.4511931639
C	6.0	-2.8144077817	-1.2851640420	0.9401706579
C	6.0	-4.1116936773	-1.8179176089	1.0474662561
C	6.0	-5.2233889356	-1.0126705111	0.6525068901
C	6.0	-5.0139679408	0.3038205388	0.1541529113
C	6.0	-3.6980365740	0.8179777916	0.0592430535
O	8.0	-1.6907664843	-2.1341449361	1.3470176100
N	7.0	1.6121525749	-1.9410751224	-0.4253663788
H	1.0	5.8482724775	1.2722314005	0.7486987266
H	1.0	6.1879541984	-1.1535954181	0.1116045244
H	1.0	4.1845021013	-2.5836256809	-0.4255911622
H	1.0	4.4343672641	3.1564023939	1.2215742328
H	1.0	2.1536851637	4.2031494709	1.5222749945
H	1.0	0.1014387875	2.7950183999	1.2796674139
H	1.0	-1.2971964938	1.7633290357	-0.0032470677

H	1.0	-4.2809889417	-2.8431997519	1.4286411091
H	1.0	-6.2452487539	-1.4256380040	0.7352251780
H	1.0	-5.8725890002	0.9264427675	-0.1532226836
H	1.0	-3.5371606105	1.8445750133	-0.3191750828
H	1.0	-2.0062830268	-2.9476986466	1.8189047808
H	1.0	1.2383456995	-1.6515150593	-1.3561146569
H	1.0	2.0009026773	-2.8966503962	-0.5511139611

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3651234	5.1571428	3.9979239
2 C	5.3651234	0.0000000	1.4016897 *	2.4416306 *
3 C	5.1571428	1.4016897 *	0.0000000	1.4319285 *
4 C	3.9979239	2.4416306 *	1.4319285 *	0.0000000
5 C	2.8058766 *	2.8381473 *	2.4721722 *	1.4074519 *
6 C	3.1297225	2.5313993 *	2.9228528 *	2.5080268 *
7 C	4.5401062	1.4443312 *	2.4801010 *	2.8455295 *
8 C	5.4402146	2.4861618 *	3.7803051	4.2890003
9 C	5.3026682	3.7791220	4.9560188	5.1789267
10 C	4.1657819	4.2930636	5.1853205	5.0065236
11 C	2.8957846 *	3.8355077	4.3836758	3.8924773
12 N	1.9405410 *	5.0488781	5.3190295	4.4863917
13 C	2.8602605 *	6.2326780	6.5816470	5.7541497
14 C	3.2587832	7.5512955	7.7634678	6.7869590
15 C	3.0066199	8.0330210	8.0419514	6.9269367
16 C	4.2765230	9.4255854	9.3878719	8.2262928
17 C	5.4355285	10.3338315	10.4108678	9.2986760
18 C	5.6044068	10.0076213	10.2394895	9.2334873
19 C	4.6917122	8.6952526	9.0059370	8.0812317
20 O	1.9510277 *	7.2596845	7.1010899	5.9294669
21 N	1.9764321 *	4.3410060	3.8140891	2.4741777 *
22 H	6.4260023	1.1051266 *	2.1799346 *	3.4513065
23 H	6.1038962	2.1871756 *	1.1042165 *	2.2009659 *
24 H	4.3235045	3.4394692	2.1947498 *	1.1077888 *
25 H	6.4885738	2.6830678 *	4.0826775	4.8919408
26 H	6.2762055	4.6689642	5.9305332	6.2526267
27 H	4.5269867	5.3929602	6.2685877	6.0082245
28 H	3.8779778	6.4062206	6.9358523	6.2685332
29 H	4.6135894	9.9253705	9.7667442	8.5495929
30 H	6.4148074	11.4116494	11.4528822	10.3096152
31 H	6.6698283	10.8808100	11.1744871	10.2054407
32 H	5.2753460	8.6502422	9.0966523	8.2925556
33 H	2.6579891 *	7.9448641	7.6888501	6.4869309

34 H	2.4985260 *	4.7742798	4.3305612	3.0670443
35 H	2.6227071 *	4.7369106	3.9162981	2.4848557 *

C C C C

1 CO	2.8058766 *	3.1297225	4.5401062	5.4402146
2 C	2.8381473 *	2.5313993 *	1.4443312 *	2.4861618 *
3 C	2.4721722 *	2.9228528 *	2.4801010 *	3.7803051
4 C	1.4074519 *	2.5080268 *	2.8455295 *	4.2890003
5 C	0.0000000	1.4576856 *	2.4751578 *	3.8144856
6 C	1.4576856 *	0.0000000	1.4672869 *	2.5268752 *
7 C	2.4751578 *	1.4672869 *	0.0000000	1.4441965 *
8 C	3.8144856	2.5268752 *	1.4441965 *	0.0000000
9 C	4.3635659	2.9119066 *	2.4781789 *	1.4018611 *
10 C	3.8854704	2.5035771 *	2.8500202 *	2.4453442 *
11 C	2.6239410 *	1.4658737 *	2.4972932 *	2.8593013 *
12 N	3.0876594	2.5269516 *	3.8339443	4.3072526
13 C	4.3472636	3.7324963	4.9356736	5.1612118
14 C	5.3981121	5.0236617	6.3097283	6.5965133
15 C	5.6263091	5.5511843	6.9264327	7.4104941
16 C	6.9639670	6.9531268	8.3316906	8.7976556
17 C	7.9765039	7.8125191	9.1439654	9.4525304
18 C	7.8538295	7.4855984	8.7282338	8.8712137
19 C	6.6817165	6.1933726	7.3874777	7.4897862
20 O	4.7509716	4.9280654	6.3228247	7.0197750
21 N	1.5088488 *	2.5917338 *	3.8857913	5.1089507
22 H	3.9429759	3.5195937	2.1966801 *	2.6814948 *
23 H	3.4659760	4.0268893	3.4870475	4.6721652
24 H	2.1820231 *	3.5067834	3.9528750	5.3960331
25 H	4.6719260	3.5170312	2.1975233 *	1.1050746 *
26 H	5.4677012	4.0160493	3.4837340	2.1842772 *
27 H	4.8020547	3.5050778	3.9514733	3.4315621
28 H	4.8909341	4.0437686	5.0330405	4.9936080
29 H	7.3808641	7.5307143	8.9270589	9.4966706
30 H	9.0109637	8.8957405	10.2362871	10.5509797
31 H	8.8173051	8.3793394	9.5668189	9.6076792
32 H	6.8938373	6.2323181	7.2914764	7.2226706
33 H	5.4250501	5.7268632	7.0959824	7.8402071
34 H	2.1113167 *	2.9526591 *	4.2383029	5.3626679
35 H	2.0887947 *	3.4245964	4.5633604	5.8889399

C C C N

1 CO	5.3026682	4.1657819	2.8957846 *	1.9405410 *
2 C	3.7791220	4.2930636	3.8355077	5.0488781
3 C	4.9560188	5.1853205	4.3836758	5.3190295

4 C	5.1789267	5.0065236	3.8924773	4.4863917
5 C	4.3635659	3.8854704	2.6239410 *	3.0876594
6 C	2.9119066 *	2.5035771 *	1.4658737 *	2.5269516 *
7 C	2.4781789 *	2.8500202 *	2.4972932 *	3.8339443
8 C	1.4018611 *	2.4453442 *	2.8593013 *	4.3072526
9 C	0.0000000	1.4301525 *	2.4824646 *	3.7966380
10 C	1.4301525 *	0.0000000	1.4145068 *	2.4722045 *
11 C	2.4824646 *	1.4145068 *	0.0000000	1.4540102 *
12 N	3.7966380	2.4722045 *	1.4540102 *	0.0000000
13 C	4.3534492	2.9303523 *	2.4473508 *	1.3317145 *
14 C	5.7696167	4.3402316	3.8369580	2.5071698 *
15 C	6.7379757	5.3262024	4.5926384	3.1519859
16 C	8.0740421	6.6559244	5.9900709	4.5531519
17 C	8.5745624	7.1542854	6.6944904	5.3119461
18 C	7.8759204	6.4899881	6.2362059	4.9857299
19 C	6.4951358	5.1138744	4.9012909	3.7415274
20 O	6.5922705	5.2762320	4.2893665	2.9413050 *
21 N	5.3846020	4.5618416	3.1528928	2.8932217 *
22 H	4.0808959	4.8943660	4.6931681	5.9981376
23 H	5.9322936	6.2593285	5.4875797	6.4002345
24 H	6.2659351	6.0063047	4.7998974	5.1664537
25 H	2.1807339 *	3.4537317	3.9642314	5.4111814
26 H	1.1042845 *	2.1977957 *	3.4741882	4.6682308
27 H	2.1815647 *	1.1042898 *	2.1884639 *	2.6939950 *
28 H	4.0016225	2.6641688 *	2.6616521 *	2.0967823 *
29 H	8.8667834	7.4714308	6.7047450	5.2715525
30 H	9.6626673	8.2462008	7.7940725	6.4042037
31 H	8.5348875	7.1982033	7.0830739	5.9176356
32 H	6.1311865	4.8423598	4.8759437	3.9683335
33 H	7.4595326	6.1761409	5.1890751	3.8929650
34 H	5.5386494	4.6646997	3.3162563	2.9833872 *
35 H	6.3016886	5.5554482	4.1520263	3.8829727

C C C C

1 CO	2.8602605 *	3.2587832	3.0066199	4.2765230
2 C	6.2326780	7.5512955	8.0330210	9.4255854
3 C	6.5816470	7.7634678	8.0419514	9.3878719
4 C	5.7541497	6.7869590	6.9269367	8.2262928
5 C	4.3472636	5.3981121	5.6263091	6.9639670
6 C	3.7324963	5.0236617	5.5511843	6.9531268
7 C	4.9356736	6.3097283	6.9264327	8.3316906
8 C	5.1612118	6.5965133	7.4104941	8.7976556
9 C	4.3534492	5.7696167	6.7379757	8.0740421
10 C	2.9303523 *	4.3402316	5.3262024	6.6559244
11 C	2.4473508 *	3.8369580	4.5926384	5.9900709

12 N	1.3317145 *	2.5071698 *	3.1519859	4.5531519
13 C	0.0000000	1.4671793 *	2.6073417 *	3.8855346
14 C	1.4671793 *	0.0000000	1.4378876 *	2.5009790 *
15 C	2.6073417 *	1.4378876 *	0.0000000	1.4065168 *
16 C	3.8855346	2.5009790 *	1.4065168 *	0.0000000
17 C	4.3446100	2.8824128 *	2.4413507 *	1.4283844 *
18 C	3.7930958	2.4978844 *	2.8250240 *	2.4726262 *
19 C	2.4691334 *	1.4426001 *	2.4454118 *	2.8452841 *
20 O	3.0499423	2.5032156 *	1.4659000 *	2.4598006 *
21 N	3.9755346	4.6904569	4.6786053	5.9115835
22 H	7.1295215	8.4911830	9.0343213	10.4326032
23 H	7.6693844	8.8235500	9.0413690	10.3633927
24 H	6.3997194	7.2786666	7.2481755	8.4606780
25 H	6.2476984	7.6846237	8.5059650	9.8898600
26 H	5.0150345	6.3701786	7.4257914	8.7025091
27 H	2.6529240 *	3.9105512	5.0264608	6.2516863
28 H	1.1084643 *	2.1768716 *	3.5334512	4.6744754
29 H	4.7975071	3.5035577	2.1947526 *	1.1068688 *
30 H	5.4495795	3.9876220	3.4398264	2.1916740 *
31 H	4.6565211	3.4934615	3.9292730	3.4747547
32 H	2.6390430 *	2.1970374 *	3.4501580	3.9511579
33 H	4.0179117	3.3306414	2.0467683 *	2.5108319 *
34 H	3.8276685	4.5237534	4.6724672	5.8675218
35 H	4.9367156	5.5065735	5.2922616	6.4095988

C C C O

1 CO	5.4355285	5.6044068	4.6917122	1.9510277 *
2 C	10.3338315	10.0076213	8.6952526	7.2596845
3 C	10.4108678	10.2394895	9.0059370	7.1010899
4 C	9.2986760	9.2334873	8.0812317	5.9294669
5 C	7.9765039	7.8538295	6.6817165	4.7509716
6 C	7.8125191	7.4855984	6.1933726	4.9280654
7 C	9.1439654	8.7282338	7.3874777	6.3228247
8 C	9.4525304	8.8712137	7.4897862	7.0197750
9 C	8.5745624	7.8759204	6.4951358	6.5922705
10 C	7.1542854	6.4899881	5.1138744	5.2762320
11 C	6.6944904	6.2362059	4.9012909	4.2893665
12 N	5.3119461	4.9857299	3.7415274	2.9413050 *
13 C	4.3446100	3.7930958	2.4691334 *	3.0499423
14 C	2.8824128 *	2.4978844 *	1.4426001 *	2.5032156 *
15 C	2.4413507 *	2.8250240 *	2.4454118 *	1.4659000 *
16 C	1.4283844 *	2.4726262 *	2.8452841 *	2.4598006 *
17 C	0.0000000	1.4231523 *	2.4555926 *	3.7708714
18 C	1.4231523 *	0.0000000	1.4159947 *	4.2907190
19 C	2.4555926 *	1.4159947 *	0.0000000	3.7950659

20	O	3.7708714	4.2907190	3.7950659	0.0000000
21	N	6.9820036	7.0200336	6.0037762	3.7533845
22	H	11.3053844	10.9215187	9.5819472	8.2944857
23	H	11.4250246	11.2964123	10.0808063	8.0350459
24	H	9.5988858	9.6584315	8.5988596	6.1532882
25	H	10.5345746	9.9271169	8.5413837	8.0946211
26	H	9.0764804	8.2735588	6.9168271	7.4142986
27	H	6.5761399	5.8000203	4.4535534	5.2453014
28	H	4.8529552	3.9961644	2.5810128 *	4.1434787
29	H	2.2003044 *	3.4735162	3.9521267	2.6867589 *
30	H	1.1052520 *	2.2010734 *	3.4610769	4.6496861
31	H	2.1979129 *	1.1042501 *	2.1875979 *	5.3949567
32	H	3.4570774	2.1860749 *	1.1058857 *	4.6920765
33	H	3.9312324	4.7318014	4.4876228	0.9920171 *
34	H	6.7968152	6.7227726	5.6982017	4.0149164
35	H	7.5623060	7.7426627	6.8300005	4.2205141

N H H H

1	CO	1.9764321 *	6.4260023	6.1038962	4.3235045
2	C	4.3410060	1.1051266 *	2.1871756 *	3.4394692
3	C	3.8140891	2.1799346 *	1.1042165 *	2.1947498 *
4	C	2.4741777 *	3.4513065	2.2009659 *	1.1077888 *
5	C	1.5088488 *	3.9429759	3.4659760	2.1820231 *
6	C	2.5917338 *	3.5195937	4.0268893	3.5067834
7	C	3.8857913	2.1966801 *	3.4870475	3.9528750
8	C	5.1089507	2.6814948 *	4.6721652	5.3960331
9	C	5.3846020	4.0808959	5.9322936	6.2659351
10	C	4.5618416	4.8943660	6.2593285	6.0063047
11	C	3.1528928	4.6931681	5.4875797	4.7998974
12	N	2.8932217 *	5.9981376	6.4002345	5.1664537
13	C	3.9755346	7.1295215	7.6693844	6.3997194
14	C	4.6904569	8.4911830	8.8235500	7.2786666
15	C	4.6786053	9.0343213	9.0413690	7.2481755
16	C	5.9115835	10.4326032	10.3633927	8.4606780
17	C	6.9820036	11.3053844	11.4250246	9.5988858
18	C	7.0200336	10.9215187	11.2964123	9.6584315
19	C	6.0037762	9.5819472	10.0808063	8.5988596
20	O	3.7533845	8.2944857	8.0350459	6.1532882
21	N	0.0000000	5.4450417	4.6740157	2.6513871 *
22	H	5.4450417	0.0000000	2.5309896 *	4.3605874
23	H	4.6740157	2.5309896 *	0.0000000	2.5194019 *
24	H	2.6513871 *	4.3605874	2.5194019 *	0.0000000
25	H	6.0548812	2.4026734 *	4.7836368	5.9769147
26	H	6.4682347	4.7789828	6.8527391	7.3470210
27	H	5.2554713	5.9688278	7.3485775	6.9648492

28 H	4.7291761	7.2016891	8.0342467	7.0088094
29 H	6.2434197	10.9544983	10.6858841	8.6700689
30 H	7.9593595	12.3908005	12.4518049	10.5578470
31 H	8.0198552	11.7605963	12.2414621	10.6555078
32 H	6.3920145	9.4633126	10.1858949	8.9019302
33 H	4.3752852	8.9803782	8.5603273	6.5951597
34 H	1.0439679 *	5.8506374	5.1865931	3.2271569
35 H	1.0392609 *	5.8199092	4.5835398	2.2094902 *

H H H H

1 CO	6.4885738	6.2762055	4.5269867	3.8779778
2 C	2.6830678 *	4.6689642	5.3929602	6.4062206
3 C	4.0826775	5.9305332	6.2685877	6.9358523
4 C	4.8919408	6.2526267	6.0082245	6.2685332
5 C	4.6719260	5.4677012	4.8020547	4.8909341
6 C	3.5170312	4.0160493	3.5050778	4.0437686
7 C	2.1975233 *	3.4837340	3.9514733	5.0330405
8 C	1.1050746 *	2.1842772 *	3.4315621	4.9936080
9 C	2.1807339 *	1.1042845 *	2.1815647 *	4.0016225
10 C	3.4537317	2.1977957 *	1.1042898 *	2.6641688 *
11 C	3.9642314	3.4741882	2.1884639 *	2.6616521 *
12 N	5.4111814	4.6682308	2.6939950 *	2.0967823 *
13 C	6.2476984	5.0150345	2.6529240 *	1.1084643 *
14 C	7.6846237	6.3701786	3.9105512	2.1768716 *
15 C	8.5059650	7.4257914	5.0264608	3.5334512
16 C	9.8898600	8.7025091	6.2516863	4.6744754
17 C	10.5345746	9.0764804	6.5761399	4.8529552
18 C	9.9271169	8.2735588	5.8000203	3.9961644
19 C	8.5413837	6.9168271	4.4535534	2.5810128 *
20 O	8.0946211	7.4142986	5.2453014	4.1434787
21 N	6.0548812	6.4682347	5.2554713	4.7291761
22 H	2.4026734 *	4.7789828	5.9688278	7.2016891
23 H	4.7836368	6.8527391	7.3485775	8.0342467
24 H	5.9769147	7.3470210	6.9648492	7.0088094
25 H	0.0000000	2.5273724 *	4.3483609	6.0242563
26 H	2.5273724 *	0.0000000	2.5006813 *	4.4931643
27 H	4.3483609	2.5006813 *	0.0000000	2.1601929 *
28 H	6.0242563	4.4931643	2.1601929 *	0.0000000
29 H	10.5827944	9.5427897	7.1426445	5.6721626
30 H	11.6312436	10.1412419	7.6413873	5.9327964
31 H	10.6346666	8.8297891	6.4213516	4.6537176
32 H	8.2243575	6.4295830	4.0864466	2.2635924 *
33 H	8.8937523	8.2781612	6.1410152	5.1006689
34 H	6.3225868	6.5878730	5.2925952	4.4632259
35 H	6.7604454	7.3979350	6.2733418	5.7352441

	H	H	H	H
1 CO	4.6135894	6.4148074	6.6698283	5.2753460
2 C	9.9253705	11.4116494	10.8808100	8.6502422
3 C	9.7667442	11.4528822	11.1744871	9.0966523
4 C	8.5495929	10.3096152	10.2054407	8.2925556
5 C	7.3808641	9.0109637	8.8173051	6.8938373
6 C	7.5307143	8.8957405	8.3793394	6.2323181
7 C	8.9270589	10.2362871	9.5668189	7.2914764
8 C	9.4966706	10.5509797	9.6076792	7.2226706
9 C	8.8667834	9.6626673	8.5348875	6.1311865
10 C	7.4714308	8.2462008	7.1982033	4.8423598
11 C	6.7047450	7.7940725	7.0830739	4.8759437
12 N	5.2715525	6.4042037	5.9176356	3.9683335
13 C	4.7975071	5.4495795	4.6565211	2.6390430 *
14 C	3.5035577	3.9876220	3.4934615	2.1970374 *
15 C	2.1947526 *	3.4398264	3.9292730	3.4501580
16 C	1.1068688 *	2.1916740 *	3.4747547	3.9511579
17 C	2.2003044 *	1.1052520 *	2.1979129 *	3.4570774
18 C	3.4735162	2.2010734 *	1.1042501 *	2.1860749 *
19 C	3.9521267	3.4610769	2.1875979 *	1.1058857 *
20 O	2.6867589 *	4.6496861	5.3949567	4.6920765
21 N	6.2434197	7.9593595	8.0198552	6.3920145
22 H	10.9544983	12.3908005	11.7605963	9.4633126
23 H	10.6858841	12.4518049	12.2414621	10.1858949
24 H	8.6700689	10.5578470	10.6555078	8.9019302
25 H	10.5827944	11.6312436	10.6346666	8.2243575
26 H	9.5427897	10.1412419	8.8297891	6.4295830
27 H	7.1426445	7.6413873	6.4213516	4.0864466
28 H	5.6721626	5.9327964	4.6537176	2.2635924 *
29 H	0.0000000	2.5196475 *	4.3869908	5.0580010
30 H	2.5196475 *	0.0000000	2.5417511 *	4.3749051
31 H	4.3869908	2.5417511 *	0.0000000	2.5149021 *
32 H	5.0580010	4.3749051	2.5149021 *	0.0000000
33 H	2.3103058 *	4.6324789	5.8177814	5.4663387
34 H	6.2958742	7.7736033	7.6588647	6.0086063
35 H	6.5866873	8.4745241	8.7616340	7.2940496

	H	H	H
1 CO	2.6579891 *	2.4985260 *	2.6227071 *
2 C	7.9448641	4.7742798	4.7369106
3 C	7.6888501	4.3305612	3.9162981
4 C	6.4869309	3.0670443	2.4848557 *
5 C	5.4250501	2.1113167 *	2.0887947 *

6 C	5.7268632	2.9526591 *	3.4245964
7 C	7.0959824	4.2383029	4.5633604
8 C	7.8402071	5.3626679	5.8889399
9 C	7.4595326	5.5386494	6.3016886
10 C	6.1761409	4.6646997	5.5554482
11 C	5.1890751	3.3162563	4.1520263
12 N	3.8929650	2.9833872 *	3.8829727
13 C	4.0179117	3.8276685	4.9367156
14 C	3.3306414	4.5237534	5.5065735
15 C	2.0467683 *	4.6724672	5.2922616
16 C	2.5108319 *	5.8675218	6.4095988
17 C	3.9312324	6.7968152	7.5623060
18 C	4.7318014	6.7227726	7.7426627
19 C	4.4876228	5.6982017	6.8300005
20 O	0.9920171 *	4.0149164	4.2205141
21 N	4.3752852	1.0439679 *	1.0392609 *
22 H	8.9803782	5.8506374	5.8199092
23 H	8.5603273	5.1865931	4.5835398
24 H	6.5951597	3.2271569	2.2094902 *
25 H	8.8937523	6.3225868	6.7604454
26 H	8.2781612	6.5878730	7.3979350
27 H	6.1410152	5.2925952	6.2733418
28 H	5.1006689	4.4632259	5.7352441
29 H	2.3103058 *	6.2958742	6.5866873
30 H	4.6324789	7.7736033	8.4745241
31 H	5.8177814	7.6588647	8.7616340
32 H	5.4663387	6.0086063	7.2940496
33 H	0.0000000	4.7210651	4.6558707
34 H	4.7210651	0.0000000	1.6672976 *
35 H	4.6558707	1.6672976 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.71 , TOTAL = 8966.3 SECONDS (149.4 MIN)

WALL CLOCK TIME: STEP = 0.70 , TOTAL = 8294.5 SECONDS (138.2 MIN)

CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.91 , TOTAL = 8967.2 SECONDS (149.5 MIN)

WALL CLOCK TIME: STEP = 0.91 , TOTAL = 8295.4 SECONDS (138.3 MIN)

CPU UTILIZATION: STEP = 99.74%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636962300	-284.636962300	0.003514823	0.000421962	198401273
11313496						
2	1	-284.636973801	-0.000011501	0.000638080	0.000031083	147586329
15586027						
3	2	-284.636973847	-0.000000046	0.000397746	0.000043330	129416241
17006214						
4	3	-284.636973947	-0.000000100	0.000125040	0.000011173	123369386
17437399						
5	4	-284.636973953	-0.000000006	0.000081216	0.000006657	117018179
17930311						
6	5	-284.636973993	-0.000000039	0.000066879	0.000005425	109029306
18455133						
7	6	-284.636974024	-0.000000031	0.000041488	0.000004740	106336507
18727634						
8	7	-284.636973980	0.000000044	0.000040445	0.000004846	101681631
19035483						
9	8	-284.636973981	-0.000000001	0.000102067	0.000004629	128194083
17176249						
10	9	-284.636973983	-0.000000003	0.000101649	0.000004393	156041070
15021382						
11	10	-284.636973987	-0.000000003	0.000127931	0.000003822	150905830
15487061						

-----DISABLING FDIFF OPTION-----

12	11	-284.636973958	0.000000029	0.000056991	0.000005227	198401394
11313477						
13	12	-284.636973959	-0.000000002	0.000063174	0.000003607	198401350
11313480						
14	13	-284.636973960	-0.000000001	0.000040762	0.000001844	198401303
11313481						
15	14	-284.636973961	0.000000000	0.000032378	0.000001603	198401308
11313482						
16	15	-284.636973961	0.000000000	0.000018173	0.000001164	198401317
11313481						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 51.9 SECONDS (3.2 SEC/ITER)

OF THE ABOVE TIME, DFT PART= 17.5 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369739608 AFTER 16 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6020754915
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998723299

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 55.03 , TOTAL = 9022.3 SECONDS (150.4 MIN)
WALL CLOCK TIME: STEP = 51.14 , TOTAL = 8346.5 SECONDS (139.1
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.60 , TOTAL = 9025.9 SECONDS (150.4 MIN)
WALL CLOCK TIME: STEP = 3.57 , TOTAL = 8350.1 SECONDS (139.2
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.81 , TOTAL = 9028.7 SECONDS (150.5 MIN)
WALL CLOCK TIME: STEP = 2.71 , TOTAL = 8352.8 SECONDS (139.2
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH=104 ENERGY= -284.6369740

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000280	0.0000230	-0.0000497
2 C	6.0	0.0000044	-0.0000423	0.0000522
3 C	6.0	0.0000006	0.0000095	0.0000139
4 C	6.0	-0.0000042	-0.0000083	-0.0000092
5 C	6.0	0.0000079	-0.0000022	0.0000719
6 C	6.0	0.0000127	0.0000097	0.0000388
7 C	6.0	0.0000300	0.0000020	0.0000192
8 C	6.0	0.0000474	0.0000033	-0.0000533
9 C	6.0	-0.0000092	0.0000087	-0.0000571
10 C	6.0	-0.0000280	-0.0000235	-0.0000132
11 C	6.0	-0.0000125	0.0000067	-0.0000556
12 N	7.0	-0.0000192	0.0000595	-0.0000709
13 C	6.0	0.0000117	0.0000165	-0.0000487
14 C	6.0	0.0000297	-0.0000039	0.0000370
15 C	6.0	0.0000228	-0.0000360	-0.0000105
16 C	6.0	-0.0000112	0.0000115	-0.0000206
17 C	6.0	-0.0000058	0.0000109	0.0000462
18 C	6.0	-0.0000069	-0.0000064	0.0000191
19 C	6.0	0.0000348	0.0000030	0.0000100
20 O	8.0	0.0001380	0.0001744	-0.0000279
21 N	7.0	0.0000107	0.0000098	0.0000369
22 H	1.0	0.0000149	0.0000455	-0.0000389
23 H	1.0	0.0000228	-0.0000445	-0.0000393
24 H	1.0	-0.0001108	-0.0000202	0.0000621
25 H	1.0	0.0000039	0.0000256	0.0000571
26 H	1.0	0.0000140	-0.0000250	0.0000781
27 H	1.0	-0.0000124	0.0000331	-0.0000204
28 H	1.0	-0.0000771	0.0000156	-0.0000484
29 H	1.0	-0.0001002	-0.0000057	0.0000078
30 H	1.0	-0.0000233	-0.0000671	0.0000346
31 H	1.0	-0.0000275	0.0000478	-0.0000066
32 H	1.0	0.0000557	-0.0000321	-0.0000092
33 H	1.0	-0.0000251	-0.0002385	-0.0000078
34 H	1.0	-0.0000565	0.0000105	0.0000364
35 H	1.0	0.0000396	0.0000290	-0.0000339

MAXIMUM GRADIENT = 0.0002385 RMS GRADIENT = 0.0000476

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0000018329

PREDICTED ENERGY CHANGE WAS -0.0000011431 RATIO= 1.603

GDIIS STEP HAS LENGTH = 0.016683

RADIUS OF STEP TAKEN= 0.01668 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 9028.7 SECONDS (150.5 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8352.8 SECONDS (139.2 MIN)
 CPU UTILIZATION: STEP = 82.30% , TOTAL = 100.00%

INSERCH= 105

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1605315389	-1.7149297448	0.8972858947
C	6.0	4.9806751705	0.6158931046	0.5523841021
C	6.0	5.1728740446	-0.7261158643	0.1963013428
C	6.0	4.0296396970	-1.5388065178	-0.0917133335
C	6.0	2.7257100850	-1.0171936632	0.0007821442
C	6.0	2.4660253245	0.3501568658	0.4341527300
C	6.0	3.6549294417	1.1752548382	0.6765670534
C	6.0	3.5182854950	2.5629553119	1.0524629494
C	6.0	2.2545544912	3.1464919668	1.2185178465
C	6.0	1.0825945743	2.3451740412	1.0457547027
C	6.0	1.1647120433	0.9899384378	0.6490267188
N	7.0	-0.0500304396	0.1919608974	0.6058546901
C	6.0	-1.2478598982	0.7122207006	0.3450100165
C	6.0	-2.5479103004	0.0406588226	0.4520155284
C	6.0	-2.8142798889	-1.2852357366	0.9404859903
C	6.0	-4.1113439983	-1.8185859817	1.0465148084
C	6.0	-5.2229996649	-1.0137311958	0.6507191284
C	6.0	-5.0138997518	0.3030051634	0.1528946692
C	6.0	-3.6981276851	0.8176764839	0.0592209216
O	8.0	-1.6908204036	-2.1337554551	1.3485684397
N	7.0	1.6114009391	-1.9408089911	-0.4258049529
H	1.0	5.8483205688	1.2719623717	0.7472114825
H	1.0	6.1872185175	-1.1538755884	0.1109661369
H	1.0	4.1836694088	-2.5838312540	-0.4254832828
H	1.0	4.4354633581	3.1560195256	1.2206863526
H	1.0	2.1549726756	4.2035944259	1.5216918307
H	1.0	0.1021620249	2.7958325042	1.2805003005
H	1.0	-1.2973769166	1.7642437670	-0.0004430766
H	1.0	-4.2802068207	-2.8439178757	1.4275310006
H	1.0	-6.2446630196	-1.4270689577	0.7325814512
H	1.0	-5.8725428486	0.9252005958	-0.1551402296
H	1.0	-3.5375198801	1.8445341232	-0.3185935190
H	1.0	-2.0062608734	-2.9461518432	1.8224264992

H 1.0 1.2378903130 -1.6512639954 -1.3567004260
H 1.0 2.0002096780 -2.8963962828 -0.5513489108

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3652099	5.1568120	3.9973912
2 C	5.3652099	0.0000000	1.4016859 *	2.4417331 *
3 C	5.1568120	1.4016859 *	0.0000000	1.4319229 *
4 C	3.9973912	2.4417331 *	1.4319229 *	0.0000000
5 C	2.8054760 *	2.8383278 *	2.4721581 *	1.4074331 *
6 C	3.1295969	2.5314143 *	2.9226642 *	2.5079090 *
7 C	4.5401212	1.4442675 *	2.4799237 *	2.8454862 *
8 C	5.4404864	2.4859030 *	3.7800351	4.2889477
9 C	5.3029749	3.7788092	4.9556641	5.1787697
10 C	4.1661356	4.2928847	5.1850534	5.0064172
11 C	2.8959149 *	3.8354692	4.3835106	3.8924359
12 N	1.9404897 *	5.0488193	5.3187715	4.4861861
13 C	2.8600060 *	6.2327307	6.5815462	5.7541162
14 C	3.2582225	7.5511964	7.7629791	6.7863478
15 C	3.0059950	8.0328226	8.0412097	6.9259634
16 C	4.2757379	9.4252674	9.3868556	8.2249289
17 C	5.4346005	10.3334566	10.4097747	9.2972171
18 C	5.6036523	10.0074482	10.2387174	9.2324270
19 C	4.6910232	8.6951449	9.0053738	8.0804815
20 O	1.9510446 *	7.2597059	7.1006669	5.9289155
21 N	1.9765153 *	4.3411506	3.8139987	2.4740861 *
22 H	6.4261179	1.1050761 *	2.1799189 *	3.4513500
23 H	6.1036085	2.1869334 *	1.1041536 *	2.2009991 *
24 H	4.3232333	3.4394300	2.1945953 *	1.1077925 *
25 H	6.4888964	2.6825596 *	4.0821703	4.8916743
26 H	6.2766716	4.6685922	5.9301292	6.2524092
27 H	4.5273874	5.3927896	6.2683114	6.0080901
28 H	3.8776362	6.4061115	6.9357586	6.2686185
29 H	4.6125840	9.9247221	9.7653341	8.5478049
30 H	6.4137749	11.4111517	11.4515975	10.3079214
31 H	6.6690236	10.8806527	11.1737009	10.2043409
32 H	5.2748204	8.6503068	9.0963905	8.2921874
33 H	2.6583420 *	7.9447119	7.6884863	6.4866515
34 H	2.4990417 *	4.7742061	4.3303361	3.0670350
35 H	2.6227508 *	4.7368320	3.9159797	2.4845324 *

C C C C

1 CO	2.8054760 *	3.1295969	4.5401212	5.4404864
2 C	2.8383278 *	2.5314143 *	1.4442675 *	2.4859030 *
3 C	2.4721581 *	2.9226642 *	2.4799237 *	3.7800351
4 C	1.4074331 *	2.5079090 *	2.8454862 *	4.2889477
5 C	0.0000000	1.4577015 *	2.4752705 *	3.8146658
6 C	1.4577015 *	0.0000000	1.4673256 *	2.5270607 *
7 C	2.4752705 *	1.4673256 *	0.0000000	1.4441890 *
8 C	3.8146658	2.5270607 *	1.4441890 *	0.0000000
9 C	4.3636161	2.9119476 *	2.4780106 *	1.4018221 *
10 C	3.8855261	2.5036036 *	2.8498977 *	2.4454169 *
11 C	2.6240265 *	1.4659153 *	2.4972552 *	2.8594494 *
12 N	3.0875400	2.5268645 *	3.8338747	4.3074299
13 C	4.3472549	3.7325568	4.9357547	5.1615744
14 C	5.3975675	5.0235106	6.3097506	6.5970636
15 C	5.6255114	5.5509013	6.9263509	7.4109714
16 C	6.9628367	6.9527131	8.3315633	8.7982490
17 C	7.9752377	7.8120546	9.1438478	9.4532614
18 C	7.8528736	7.4853596	8.7283247	8.8721352
19 C	6.6810071	6.1932165	7.3875860	7.4906039
20 O	4.7506820	4.9280161	6.3228298	7.0200822
21 N	1.5088826 *	2.5919943 *	3.8860117	5.1093422
22 H	3.9431064	3.5196097	2.1966583 *	2.6812133 *
23 H	3.4659577	4.0266415	3.4867235	4.6716648
24 H	2.1821322 *	3.5067879	3.9528229	5.3959682
25 H	4.6719515	3.5171276	2.1974366 *	1.1050971 *
26 H	5.4676810	4.0160274	3.4835251	2.1841461 *
27 H	4.8020674	3.5050654	3.9513496	3.4316370
28 H	4.8909738	4.0437250	5.0329503	4.9937116
29 H	7.3793906	7.5299776	8.9265942	9.4969172
30 H	9.0095017	8.8951494	10.2360714	10.5516720
31 H	8.8163009	8.3791205	9.5669740	9.6087566
32 H	6.8934415	6.2323627	7.2917492	7.2235943
33 H	5.4250177	5.7266307	7.0956369	7.8398800
34 H	2.1114952 *	2.9531604 *	4.2385686	5.3632000
35 H	2.0886843 *	3.4246613	4.5633560	5.8890820

C C C N

1 CO	5.3029749	4.1661356	2.8959149 *	1.9404897 *
2 C	3.7788092	4.2928847	3.8354692	5.0488193
3 C	4.9556641	5.1850534	4.3835106	5.3187715
4 C	5.1787697	5.0064172	3.8924359	4.4861861
5 C	4.3636161	3.8855261	2.6240265 *	3.0875400
6 C	2.9119476 *	2.5036036 *	1.4659153 *	2.5268645 *
7 C	2.4780106 *	2.8498977 *	2.4972552 *	3.8338747
8 C	1.4018221 *	2.4454169 *	2.8594494 *	4.3074299

9 C	0.0000000	1.4301914 *	2.4824987 *	3.7968041
10 C	1.4301914 *	0.0000000	1.4144963 *	2.4723831 *
11 C	2.4824987 *	1.4144963 *	0.0000000	1.4540396 *
12 N	3.7968041	2.4723831 *	1.4540396 *	0.0000000
13 C	4.3538028	2.9306310 *	2.4474592 *	1.3317303 *
14 C	5.7703894	4.3409541	3.8371226	2.5071822 *
15 C	6.7387383	5.3269679	4.5927925	3.1520094
16 C	8.0750386	6.6568683	5.9902065	4.5531031
17 C	8.5757605	7.1553348	6.6945915	5.3118092
18 C	7.8772709	6.4911398	6.2364467	4.9857299
19 C	6.4962894	5.1148610	4.9015054	3.7415160
20 O	6.5927164	5.2767733	4.2896256	2.9415594 *
21 N	5.3849861	4.5623212	3.1534227	2.8936799 *
22 H	4.0805815	4.8941859	4.6931191	5.9980772
23 H	5.9317517	6.2589427	5.4873508	6.3999582
24 H	6.2658462	6.0063549	4.8000526	5.1665167
25 H	2.1809308 *	3.4539543	3.9644062	5.4114061
26 H	1.1042176 *	2.1977801 *	3.4741539	4.6684044
27 H	2.1816501 *	1.1042855 *	2.1883841 *	2.6941523 *
28 H	4.0015863	2.6638833 *	2.6614360 *	2.0965552 *
29 H	8.8674575	7.4720858	6.7046003	5.2712526
30 H	9.6638653	8.2472176	7.7940840	6.4039668
31 H	8.5364385	7.1994729	7.0833489	5.9176350
32 H	6.1323675	4.8432989	4.8762288	3.9683983
33 H	7.4591931	6.1759515	5.1889058	3.8928956
34 H	5.5392976	4.6655572	3.3172649	2.9846006 *
35 H	6.3018742	5.5557913	4.1524156	3.8833690

C C C C

1 CO	2.8600060 *	3.2582225	3.0059950	4.2757379
2 C	6.2327307	7.5511964	8.0328226	9.4252674
3 C	6.5815462	7.7629791	8.0412097	9.3868556
4 C	5.7541162	6.7863478	6.9259634	8.2249289
5 C	4.3472549	5.3975675	5.6255114	6.9628367
6 C	3.7325568	5.0235106	5.5509013	6.9527131
7 C	4.9357547	6.3097506	6.9263509	8.3315633
8 C	5.1615744	6.5970636	7.4109714	8.7982490
9 C	4.3538028	5.7703894	6.7387383	8.0750386
10 C	2.9306310 *	4.3409541	5.3269679	6.6568683
11 C	2.4474592 *	3.8371226	4.5927925	5.9902065
12 N	1.3317303 *	2.5071822 *	3.1520094	4.5531031
13 C	0.0000000	1.4671662 *	2.6073158 *	3.8854385
14 C	1.4671662 *	0.0000000	1.4378987 *	2.5009089 *
15 C	2.6073158 *	1.4378987 *	0.0000000	1.4064423 *
16 C	3.8854385	2.5009089 *	1.4064423 *	0.0000000

17 C	4.3444337	2.8822430 *	2.4412314 *	1.4283640 *
18 C	3.7930755	2.4978797 *	2.8250906 *	2.4727137 *
19 C	2.4691311 *	1.4425824 *	2.4454151 *	2.8452376 *
20 O	3.0500695	2.5032954 *	1.4658370 *	2.4595737 *
21 N	3.9759395	4.6900590	4.6779459	5.9103700
22 H	7.1295760	8.4911685	9.0342274	10.4324489
23 H	7.6692557	8.8230212	9.0405936	10.3623106
24 H	6.3999320	7.2781947	7.2473110	8.4592923
25 H	6.2481297	7.6852999	8.5065879	9.8906497
26 H	5.0153305	6.3711340	7.4268787	8.7039747
27 H	2.6531377 *	3.9115537	5.0275602	6.2530984
28 H	1.1083963 *	2.1769928 *	3.5335064	4.6745268
29 H	4.7971972	3.5033219	2.1944577 *	1.1067942 *
30 H	5.4492948	3.9873453	3.4396031	2.1915496 *
31 H	4.6565226	3.4934559	3.9292999	3.4747893
32 H	2.6391374 *	2.1970734 *	3.4501908	3.9511067
33 H	4.0176636	3.3305327	2.0467917 *	2.5109398 *
34 H	3.8289467	4.5239742	4.6723790	5.8666641
35 H	4.9371583	5.5062172	5.2915706	6.4082706

C C C O

1 CO	5.4346005	5.6036523	4.6910232	1.9510446 *
2 C	10.3334566	10.0074482	8.6951449	7.2597059
3 C	10.4097747	10.2387174	9.0053738	7.1006669
4 C	9.2972171	9.2324270	8.0804815	5.9289155
5 C	7.9752377	7.8528736	6.6810071	4.7506820
6 C	7.8120546	7.4853596	6.1932165	4.9280161
7 C	9.1438478	8.7283247	7.3875860	6.3228298
8 C	9.4532614	8.8721352	7.4906039	7.0200822
9 C	8.5757605	7.8772709	6.4962894	6.5927164
10 C	7.1553348	6.4911398	5.1148610	5.2767733
11 C	6.6945915	6.2364467	4.9015054	4.2896256
12 N	5.3118092	4.9857299	3.7415160	2.9415594 *
13 C	4.3444337	3.7930755	2.4691311 *	3.0500695
14 C	2.8822430 *	2.4978797 *	1.4425824 *	2.5032954 *
15 C	2.4412314 *	2.8250906 *	2.4454151 *	1.4658370 *
16 C	1.4283640 *	2.4727137 *	2.8452376 *	2.4595737 *
17 C	0.0000000	1.4231467 *	2.4554345 *	3.7706416
18 C	1.4231467 *	0.0000000	1.4159511 *	4.2907219
19 C	2.4554345 *	1.4159511 *	0.0000000	3.7950823
20 O	3.7706416	4.2907219	3.7950823	0.0000000
21 N	6.9805021	7.0188464	6.0029648	3.7537042
22 H	11.3052128	10.9215347	9.5819821	8.2945278
23 H	11.4238370	11.2955438	10.0801669	8.0346326
24 H	9.5973355	9.6573094	8.5981346	6.1530040

25 H	10.5355395	9.9282593	8.5423740	8.0950248
26 H	9.0781912	8.2753208	6.9182400	7.4149915
27 H	6.5777463	5.8017041	4.4549777	5.2459753
28 H	4.8530064	3.9964075	2.5813085 *	4.1435526
29 H	2.2004268 *	3.4736332	3.9520073	2.6861660 *
30 H	1.1051450 *	2.2009024 *	3.4608003	4.6493363
31 H	2.1979018 *	1.1042104 *	2.1875999 *	5.3949193
32 H	3.4568902	2.1859346 *	1.1058821 *	4.6921760
33 H	3.9312283	4.7318336	4.4875061	0.9919839 *
34 H	6.7955339	6.7218245	5.6977868	4.0160458
35 H	7.5606976	7.7414378	6.8292152	4.2207831

N H H H

1 CO	1.9765153 *	6.4261179	6.1036085	4.3232333
2 C	4.3411506	1.1050761 *	2.1869334 *	3.4394300
3 C	3.8139987	2.1799189 *	1.1041536 *	2.1945953 *
4 C	2.4740861 *	3.4513500	2.2009991 *	1.1077925 *
5 C	1.5088826 *	3.9431064	3.4659577	2.1821322 *
6 C	2.5919943 *	3.5196097	4.0266415	3.5067879
7 C	3.8860117	2.1966583 *	3.4867235	3.9528229
8 C	5.1093422	2.6812133 *	4.6716648	5.3959682
9 C	5.3849861	4.0805815	5.9317517	6.2658462
10 C	4.5623212	4.8941859	6.2589427	6.0063549
11 C	3.1534227	4.6931191	5.4873508	4.8000526
12 N	2.8936799 *	5.9980772	6.3999582	5.1665167
13 C	3.9759395	7.1295760	7.6692557	6.3999320
14 C	4.6900590	8.4911685	8.8230212	7.2781947
15 C	4.6779459	9.0342274	9.0405936	7.2473110
16 C	5.9103700	10.4324489	10.3623106	8.4592923
17 C	6.9805021	11.3052128	11.4238370	9.5973355
18 C	7.0188464	10.9215347	11.2955438	9.6573094
19 C	6.0029648	9.5819821	10.0801669	8.5981346
20 O	3.7537042	8.2945278	8.0346326	6.1530040
21 N	0.0000000	5.4451222	4.6739163	2.6514228 *
22 H	5.4451222	0.0000000	2.5306817 *	4.3604382
23 H	4.6739163	2.5306817 *	0.0000000	2.5192777 *
24 H	2.6514228 *	4.3604382	2.5192777 *	0.0000000
25 H	6.0550742	2.4020856 *	4.7828152	5.9765510
26 H	6.4685321	4.7786091	6.8521266	7.3468530
27 H	5.2559540	5.9686611	7.3481914	6.9649023
28 H	4.7296234	7.2015499	8.0341148	7.0091572
29 H	6.2419149	10.9540117	10.6844082	8.6682471
30 H	7.9576082	12.3905301	12.4504104	10.5560092
31 H	8.0185214	11.7606599	12.2405561	10.6542853
32 H	6.3915336	9.4634972	10.1855544	8.9016071

33 H	4.3763839	8.9801461	8.5600500	6.5954235
34 H	1.0439889 *	5.8504500	5.1862597	3.2271445
35 H	1.0392693 *	5.8197449	4.5832393	2.2093066 *

H H H H

1 CO	6.4888964	6.2766716	4.5273874	3.8776362
2 C	2.6825596 *	4.6685922	5.3927896	6.4061115
3 C	4.0821703	5.9301292	6.2683114	6.9357586
4 C	4.8916743	6.2524092	6.0080901	6.2686185
5 C	4.6719515	5.4676810	4.8020674	4.8909738
6 C	3.5171276	4.0160274	3.5050654	4.0437250
7 C	2.1974366 *	3.4835251	3.9513496	5.0329503
8 C	1.1050971 *	2.1841461 *	3.4316370	4.9937116
9 C	2.1809308 *	1.1042176 *	2.1816501 *	4.0015863
10 C	3.4539543	2.1977801 *	1.1042855 *	2.6638833 *
11 C	3.9644062	3.4741539	2.1883841 *	2.6614360 *
12 N	5.4114061	4.6684044	2.6941523 *	2.0965552 *
13 C	6.2481297	5.0153305	2.6531377 *	1.1083963 *
14 C	7.6852999	6.3711340	3.9115537	2.1769928 *
15 C	8.5065879	7.4268787	5.0275602	3.5335064
16 C	9.8906497	8.7039747	6.2530984	4.6745268
17 C	10.5355395	9.0781912	6.5777463	4.8530064
18 C	9.9282593	8.2753208	5.8017041	3.9964075
19 C	8.5423740	6.9182400	4.4549777	2.5813085 *
20 O	8.0950248	7.4149915	5.2459753	4.1435526
21 N	6.0550742	6.4685321	5.2559540	4.7296234
22 H	2.4020856 *	4.7786091	5.9686611	7.2015499
23 H	4.7828152	6.8521266	7.3481914	8.0341148
24 H	5.9765510	7.3468530	6.9649023	7.0091572
25 H	0.0000000	2.5275789 *	4.3486564	6.0244215
26 H	2.5275789 *	0.0000000	2.5007996 *	4.4928882
27 H	4.3486564	2.5007996 *	0.0000000	2.1595603 *
28 H	6.0244215	4.4928882	2.1595603 *	0.0000000
29 H	10.5832386	9.5439945	7.1437776	5.6719959
30 H	11.6321987	10.1430245	7.6429903	5.9327432
31 H	10.6359975	8.8317969	6.4231944	4.6540378
32 H	8.2254385	6.4308854	4.0877077	2.2640465 *
33 H	8.8935031	8.2779936	6.1408074	5.1003134
34 H	6.3227661	6.5882888	5.2935219	4.4646061
35 H	6.7603481	7.3980617	6.2737329	5.7357772

H H H H

1 CO	4.6125840	6.4137749	6.6690236	5.2748204
2 C	9.9247221	11.4111517	10.8806527	8.6503068

3 C	9.7653341	11.4515975	11.1737009	9.0963905
4 C	8.5478049	10.3079214	10.2043409	8.2921874
5 C	7.3793906	9.0095017	8.8163009	6.8934415
6 C	7.5299776	8.8951494	8.3791205	6.2323627
7 C	8.9265942	10.2360714	9.5669740	7.2917492
8 C	9.4969172	10.5516720	9.6087566	7.2235943
9 C	8.8674575	9.6638653	8.5364385	6.1323675
10 C	7.4720858	8.2472176	7.1994729	4.8432989
11 C	6.7046003	7.7940840	7.0833489	4.8762288
12 N	5.2712526	6.4039668	5.9176350	3.9683983
13 C	4.7971972	5.4492948	4.6565226	2.6391374 *
14 C	3.5033219	3.9873453	3.4934559	2.1970734 *
15 C	2.1944577 *	3.4396031	3.9292999	3.4501908
16 C	1.1067942 *	2.1915496 *	3.4747893	3.9511067
17 C	2.2004268 *	1.1051450 *	2.1979018 *	3.4568902
18 C	3.4736332	2.2009024 *	1.1042104 *	2.1859346 *
19 C	3.9520073	3.4608003	2.1875999 *	1.1058821 *
20 O	2.6861660 *	4.6493363	5.3949193	4.6921760
21 N	6.2419149	7.9576082	8.0185214	6.3915336
22 H	10.9540117	12.3905301	11.7606599	9.4634972
23 H	10.6844082	12.4504104	12.2405561	10.1855544
24 H	8.6682471	10.5560092	10.6542853	8.9016071
25 H	10.5832386	11.6321987	10.6359975	8.2254385
26 H	9.5439945	10.1430245	8.8317969	6.4308854
27 H	7.1437776	7.6429903	6.4231944	4.0877077
28 H	5.6719959	5.9327432	4.6540378	2.2640465 *
29 H	0.0000000	2.5198222 *	4.3870988	5.0578767
30 H	2.5198222 *	0.0000000	2.5415931 *	4.3745834
31 H	4.3870988	2.5415931 *	0.0000000	2.5148009 *
32 H	5.0578767	4.3745834	2.5148009 *	0.0000000
33 H	2.3102434 *	4.6324322	5.8177553	5.4662046
34 H	6.2947410	7.7719989	7.6576874	6.0085616
35 H	6.5850096	8.4726221	8.7602407	7.2936304

H H H

1 CO	2.6583420 *	2.4990417 *	2.6227508 *
2 C	7.9447119	4.7742061	4.7368320
3 C	7.6884863	4.3303361	3.9159797
4 C	6.4866515	3.0670350	2.4845324 *
5 C	5.4250177	2.1114952 *	2.0886843 *
6 C	5.7266307	2.9531604 *	3.4246613
7 C	7.0956369	4.2385686	4.5633560
8 C	7.8398800	5.3632000	5.8890820
9 C	7.4591931	5.5392976	6.3018742
10 C	6.1759515	4.6655572	5.5557913

11 C	5.1889058	3.3172649	4.1524156
12 N	3.8928956	2.9846006 *	3.8833690
13 C	4.0176636	3.8289467	4.9371583
14 C	3.3305327	4.5239742	5.5062172
15 C	2.0467917 *	4.6723790	5.2915706
16 C	2.5109398 *	5.8666641	6.4082706
17 C	3.9312283	6.7955339	7.5606976
18 C	4.7318336	6.7218245	7.7414378
19 C	4.4875061	5.6977868	6.8292152
20 O	0.9919839 *	4.0160458	4.2207831
21 N	4.3763839	1.0439889 *	1.0392693 *
22 H	8.9801461	5.8504500	5.8197449
23 H	8.5600500	5.1862597	4.5832393
24 H	6.5954235	3.2271445	2.2093066 *
25 H	8.8935031	6.3227661	6.7603481
26 H	8.2779936	6.5882888	7.3980617
27 H	6.1408074	5.2935219	6.2737329
28 H	5.1003134	4.4646061	5.7357772
29 H	2.3102434 *	6.2947410	6.5850096
30 H	4.6324322	7.7719989	8.4726221
31 H	5.8177553	7.6576874	8.7602407
32 H	5.4662046	6.0085616	7.2936304
33 H	0.0000000	4.7231451	4.6571549
34 H	4.7231451	0.0000000	1.6673561 *
35 H	4.6571549	1.6673561 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.60 , TOTAL = 9029.3 SECONDS (150.5 MIN)

WALL CLOCK TIME: STEP = 0.60 , TOTAL = 8353.4 SECONDS (139.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.16 , TOTAL = 9030.4 SECONDS (150.5 MIN)

WALL CLOCK TIME: STEP = 1.16 , TOTAL = 8354.6 SECONDS (139.2 MIN)

CPU UTILIZATION: STEP = 99.64%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636969304	-284.636969304	0.002814866	0.000263576	198406372
11313213						
2	1	-284.636975078	-0.000005774	0.000608064	0.000020451	144818354
15815639						
3	2	-284.636975096	-0.000000019	0.000322438	0.000025374	127030394
17178880						
4	3	-284.636975151	-0.000000054	0.000128318	0.000015342	120074539
17682736						
5	4	-284.636975106	0.000000045	0.000076480	0.000024854	115677773
18052727						
6	5	-284.636975154	-0.000000048	0.000050910	0.000006724	108084098
18585212						
7	6	-284.636975172	-0.000000017	0.000040857	0.000006070	108342947
18572917						
8	7	-284.636975163	0.000000009	0.000073782	0.000005780	99749085
19220611						
9	8	-284.636975166	-0.000000003	0.000107091	0.000006004	131870823
16871483						
10	9	-284.636975169	-0.000000004	0.000148376	0.000005996	153054338
15295198						

-----DISABLING FDIFF OPTION-----

11	10	-284.636975192	-0.000000023	0.000108208	0.000005425	198406277
11313160						
12	11	-284.636975194	-0.000000002	0.000070524	0.000004586	198406376
11313157						
13	12	-284.636975196	-0.000000002	0.000050436	0.000002877	198406350
11313157						
14	13	-284.636975197	-0.000000001	0.000034336	0.000001719	198406398
11313160						
15	14	-284.636975197	0.000000000	0.000008393	0.000001464	198406416
11313162						
16	15	-284.636975197	0.000000000	0.000008692	0.000001219	198406398
11313162						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 52.6 SECONDS (3.3 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 17.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
TIME TO SOLVE SCF EQUATIONS= 1.6 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369751975 AFTER 16 ITERATIONS

DFT EXCHANGE + CORRELATION ENERGY IS -46.6022744436
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998738550

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 55.30 , TOTAL = 9085.7 SECONDS (151.4 MIN)
WALL CLOCK TIME: STEP = 51.03 , TOTAL = 8405.6 SECONDS (140.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.90 , TOTAL = 9089.6 SECONDS (151.5 MIN)
WALL CLOCK TIME: STEP = 3.88 , TOTAL = 8409.5 SECONDS (140.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.92 , TOTAL = 9092.6 SECONDS (151.5 MIN)
WALL CLOCK TIME: STEP = 2.74 , TOTAL = 8412.2 SECONDS (140.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH=105 ENERGY= -284.6369752

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000043	0.0000740	-0.0000464

2 C	6.0	0.0000472	0.0000595	-0.0000166
3 C	6.0	-0.0000136	-0.0000236	0.0000300
4 C	6.0	-0.0000694	-0.0000316	0.0000644
5 C	6.0	-0.0000033	-0.0000025	0.0000616
6 C	6.0	0.0000390	-0.0000392	0.0000304
7 C	6.0	0.0000212	0.0000040	0.0000233
8 C	6.0	0.0000732	0.0000261	0.0000319
9 C	6.0	0.0000159	-0.0000135	0.0000043
10 C	6.0	-0.0000348	0.0000002	-0.0000479
11 C	6.0	-0.0000307	0.0000474	-0.0000590
12 N	7.0	0.0000073	0.0000403	-0.0000687
13 C	6.0	-0.0000706	0.0000485	-0.0000044
14 C	6.0	0.0000168	-0.0000012	0.0000269
15 C	6.0	0.0000209	-0.0000667	-0.0000278
16 C	6.0	0.0000062	-0.0000347	-0.0000127
17 C	6.0	0.0000009	0.0000021	0.0000343
18 C	6.0	-0.0000348	0.0000676	0.0000217
19 C	6.0	0.0000242	-0.0000596	-0.0000119
20 O	8.0	0.0000687	0.0001068	-0.0000074
21 N	7.0	0.0000256	-0.0000035	-0.0000110
22 H	1.0	-0.0000086	0.0000230	-0.0000279
23 H	1.0	-0.0000072	0.0000014	-0.0000361
24 H	1.0	-0.0000887	-0.0000124	0.0000414
25 H	1.0	0.0000382	0.0000221	0.0000252
26 H	1.0	0.0000282	-0.0000574	0.0000199
27 H	1.0	-0.0000181	0.0000139	-0.0000164
28 H	1.0	-0.0000313	-0.0000249	-0.0000368
29 H	1.0	-0.0000568	0.0000371	0.0000042
30 H	1.0	0.0000448	-0.0000314	0.0000337
31 H	1.0	-0.0000094	0.0000299	-0.0000079
32 H	1.0	0.0000346	-0.0000291	0.0000034
33 H	1.0	-0.0000253	-0.00002034	-0.0000026
34 H	1.0	-0.0000632	0.0000043	0.0000096
35 H	1.0	0.0000571	0.0000267	-0.0000243

MAXIMUM GRADIENT = 0.0002034 RMS GRADIENT = 0.0000423
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000012367
 PREDICTED ENERGY CHANGE WAS -0.0000009542 RATIO= 1.296
 GDIIS STEP HAS LENGTH = 0.016223
 RADIUS OF STEP TAKEN= 0.01622 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:
 CPU TIME: STEP = 0.02 , TOTAL = 9092.6 SECONDS (151.5 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8412.3 SECONDS (140.2 MIN)

CPU UTILIZATION: STEP = 81.22%, TOTAL = 100.00%

INSERCH= 106

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1601645922	-1.7146682689	0.8973219878
C	6.0	4.9804803947	0.6156331449	0.5517050289
C	6.0	5.1723228326	-0.7264240764	0.1958843958
C	6.0	4.0289537796	-1.5389689073	-0.0919011174
C	6.0	2.7251172789	-1.0170520817	0.0004131835
C	6.0	2.4657915798	0.3502728688	0.4341367324
C	6.0	3.6548756117	1.1751095787	0.6764090412
C	6.0	3.5188061282	2.5627324898	1.0527205878
C	6.0	2.2553372060	3.1466775938	1.2190575592
C	6.0	1.0831899705	2.3456303446	1.0464325286
C	6.0	1.1647681622	0.9903149495	0.6497729756
N	7.0	-0.0501100334	0.1924482632	0.6069271911
C	6.0	-1.2479729363	0.7128014995	0.3464183197
C	6.0	-2.5479951496	0.0409059711	0.4526021578
C	6.0	-2.8142179285	-1.2849960565	0.9411885339
C	6.0	-4.1110204101	-1.8190220851	1.0462139944
C	6.0	-5.2226424303	-1.0148262368	0.6492317530
C	6.0	-5.0138085498	0.3019658980	0.1515379587
C	6.0	-3.6982911427	0.8174078822	0.0588624207
O	8.0	-1.6908417728	-2.1331426484	1.3501727821
N	7.0	1.6106002104	-1.9403354848	-0.4264475441
H	1.0	5.8483519283	1.2714130210	0.7463545851
H	1.0	6.1865837359	-1.1542107564	0.1105219856
H	1.0	4.1831256420	-2.5838616084	-0.4259097358
H	1.0	4.4363440013	3.1554009193	1.2203937543
H	1.0	2.1561143263	4.2040256463	1.5215957616
H	1.0	0.1029334975	2.7964398051	1.2813421284
H	1.0	-1.2974509938	1.7650109451	0.0015734917
H	1.0	-4.2791519479	-2.8444903494	1.4271852602
H	1.0	-6.2442183152	-1.4283791805	0.7302389476
H	1.0	-5.8725357355	0.9236405850	-0.1572387453
H	1.0	-3.5381075675	1.8442878866	-0.3189909743
H	1.0	-2.0061533241	-2.9440315297	1.8265708546
H	1.0	1.2374846230	-1.6505592091	-1.3574299803
H	1.0	1.9991697364	-2.8960458130	-0.5519808041

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C	
1	CO	0.0000000	5.3651841	5.1565853	3.9971193
2	C	5.3651841	0.0000000	1.4016167 *	2.4417088 *
3	C	5.1565853	1.4016167 *	0.0000000	1.4319017 *
4	C	3.9971193	2.4417088 *	1.4319017 *	0.0000000
5	C	2.8053691 *	2.8383528 *	2.4721425 *	1.4074476 *
6	C	3.1296067	2.5313827 *	2.9225591 *	2.5078729 *
7	C	4.5401127	1.4442275 *	2.4797944 *	2.8454274 *
8	C	5.4406598	2.4856999 *	3.7797932	4.2888651
9	C	5.3033900	3.7786176	4.9554621	5.1787654
10	C	4.1665615	4.2926121	5.1847814	5.0063399
11	C	2.8961083 *	3.8353179	4.3833437	3.8924178
12	N	1.9405252 *	5.0486607	5.3185607	4.4860816
13	C	2.8598873 *	6.2325930	6.5813546	5.7540029
14	C	3.2579051	7.5510315	7.7626032	6.7859226
15	C	3.0055771	8.0325221	8.0406663	6.9253719
16	C	4.2750532	9.4248327	9.3860158	8.2239234
17	C	5.4337776	10.3330356	10.4088425	9.2960226
18	C	5.6029461	10.0072140	10.2380088	9.2314600
19	C	4.6906401	8.6950953	9.0049977	8.0799477
20	O	1.9510047 *	7.2594668	7.1003005	5.9286323
21	N	1.9766272 *	4.3411808	3.8140197	2.4741565 *
22	H	6.4261145	1.1050505 *	2.1797674 *	3.4512503
23	H	6.1033511	2.1867042 *	1.1040894 *	2.2009955 *
24	H	4.3232690	3.4392255	2.1943594 *	1.1077597 *
25	H	6.4890415	2.6820979 *	4.0816479	4.8913385
26	H	6.2772980	4.6684358	5.9299544	6.2524304
27	H	4.5277857	5.3924718	6.2679739	6.0079282
28	H	3.8775219	6.4059454	6.9356311	6.2686209
29	H	4.6113755	9.9236944	9.7638457	8.5461471
30	H	6.4129555	11.4106845	11.4505759	10.3066100
31	H	6.6683015	10.8805068	11.1730171	10.2033430
32	H	5.2747325	8.6506673	9.0964419	8.2920693
33	H	2.6585279 *	7.9441517	7.6881364	6.4866982
34	H	2.4997270 *	4.7739336	4.3300997	3.0669718
35	H	2.6226077 *	4.7369003	3.9160518	2.4846236 *

	C	C	C	C	
1	CO	2.8053691 *	3.1296067	4.5401127	5.4406598
2	C	2.8383528 *	2.5313827 *	1.4442275 *	2.4856999 *
3	C	2.4721425 *	2.9225591 *	2.4797944 *	3.7797932
4	C	1.4074476 *	2.5078729 *	2.8454274 *	4.2888651
5	C	0.0000000	1.4577186 *	2.4752765 *	3.8147281

6 C	1.4577186 *	0.0000000	1.4673010 *	2.5271453 *
7 C	2.4752765 *	1.4673010 *	0.0000000	1.4441685 *
8 C	3.8147281	2.5271453 *	1.4441685 *	0.0000000
9 C	4.3637635	2.9120905 *	2.4779539 *	1.4017894 *
10 C	3.8855778	2.5035864 *	2.8496672 *	2.4452810 *
11 C	2.6240960 *	1.4658836 *	2.4970970 *	2.8594332 *
12 N	3.0874969	2.5267620 *	3.8337149	4.3074519
13 C	4.3471323	3.7324480	4.9356404	5.1617139
14 C	5.3971719	5.0233561	6.3096841	6.5974108
15 C	5.6250410	5.5506492	6.9261388	7.4111165
16 C	6.9620136	6.9523331	8.3313097	8.7985265
17 C	7.9741993	7.8116438	9.1436800	9.4538168
18 C	7.8519819	7.4850928	8.7283420	8.8729200
19 C	6.6804817	6.1931383	7.3877179	7.4913554
20 O	4.7506003	4.9278875	6.3225932	7.0199824
21 N	1.5089104 *	2.5920733 *	3.8860459	5.1094823
22 H	3.9431074	3.5196156	2.1967032 *	2.6810725 *
23 H	3.4659323	4.0264739	3.4864749	4.6712357
24 H	2.1822996 *	3.5068592	3.9527230	5.3958409
25 H	4.6718319	3.5171040	2.1973088 *	1.1051000 *
26 H	5.4678527	4.0162019	3.4835267	2.1841740 *
27 H	4.8020149	3.5049377	3.9510693	3.4314826
28 H	4.8909029	4.0435862	5.0327851	4.9937564
29 H	7.3780076	7.5290717	8.9257852	9.4966538
30 H	9.0083748	8.8946924	10.2358738	10.5522326
31 H	8.8153718	8.3789127	9.5671193	9.6097828
32 H	6.8932772	6.2326629	7.2922992	7.2248035
33 H	5.4252210	5.7262209	7.0948886	7.8389075
34 H	2.1114261 *	2.9532657 *	4.2384767	5.3633087
35 H	2.0887212 *	3.4247261	4.5633989	5.8891954

C C C N

1 CO	5.3033900	4.1665615	2.8961083 *	1.9405252 *
2 C	3.7786176	4.2926121	3.8353179	5.0486607
3 C	4.9554621	5.1847814	4.3833437	5.3185607
4 C	5.1787654	5.0063399	3.8924178	4.4860816
5 C	4.3637635	3.8855778	2.6240960 *	3.0874969
6 C	2.9120905 *	2.5035864 *	1.4658836 *	2.5267620 *
7 C	2.4779539 *	2.8496672 *	2.4970970 *	3.8337149
8 C	1.4017894 *	2.4452810 *	2.8594332 *	4.3074519
9 C	0.0000000	1.4301766 *	2.4826046 *	3.7970069
10 C	1.4301766 *	0.0000000	1.4145224 *	2.4725952 *
11 C	2.4826046 *	1.4145224 *	0.0000000	1.4540825 *
12 N	3.7970069	2.4725952 *	1.4540825 *	0.0000000
13 C	4.3541284	2.9309504 *	2.4475207 *	1.3317312 *

14 C	5.7710721	4.3416465	3.8372992	2.5072318 *
15 C	6.7392382	5.3275053	4.5928524	3.1519621
16 C	8.0758007	6.6576386	5.9902826	4.5530187
17 C	8.5768873	7.1563929	6.6947446	5.3117222
18 C	7.8786079	6.4923641	6.2367357	4.9857473
19 C	6.4974796	5.1159867	4.9018790	3.7416808
20 O	6.5928766	5.2770179	4.2896451	2.9415621 *
21 N	5.3852646	4.5625695	3.1536850	2.8938881 *
22 H	4.0804191	4.8939512	4.6930055	5.9979545
23 H	5.9313734	6.2585497	5.4871134	6.3997076
24 H	6.2658890	6.0064369	4.8002410	5.1667139
25 H	2.1810246 *	3.4539301	3.9643932	5.4114415
26 H	1.1042461 *	2.1978580 *	3.4743026	4.6687041
27 H	2.1816021 *	1.1042257 *	2.1882549 *	2.6942587 *
28 H	4.0016964	2.6638883 *	2.6613605 *	2.0964890 *
29 H	8.8677482	7.4724184	6.7042052	5.2707319
30 H	9.6650159	8.2482749	7.7942053	6.4038477
31 H	8.5380562	7.2009027	7.0837391	5.9177050
32 H	6.1339885	4.8448030	4.8769677	3.9688821
33 H	7.4582915	6.1752069	5.1883214	3.8924467
34 H	5.5396564	4.6660361	3.3178860	2.9855110 *
35 H	6.3021191	5.5559979	4.1526182	3.8834792

C C C C

1 CO	2.8598873 *	3.2579051	3.0055771	4.2750532
2 C	6.2325930	7.5510315	8.0325221	9.4248327
3 C	6.5813546	7.7626032	8.0406663	9.3860158
4 C	5.7540029	6.7859226	6.9253719	8.2239234
5 C	4.3471323	5.3971719	5.6250410	6.9620136
6 C	3.7324480	5.0233561	5.5506492	6.9523331
7 C	4.9356404	6.3096841	6.9261388	8.3313097
8 C	5.1617139	6.5974108	7.4111165	8.7985265
9 C	4.3541284	5.7710721	6.7392382	8.0758007
10 C	2.9309504 *	4.3416465	5.3275053	6.6576386
11 C	2.4475207 *	3.8372992	4.5928524	5.9902826
12 N	1.3317312 *	2.5072318 *	3.1519621	4.5530187
13 C	0.0000000	1.4672343 *	2.6073109 *	3.8854711
14 C	1.4672343 *	0.0000000	1.4379177 *	2.5009509 *
15 C	2.6073109 *	1.4379177 *	0.0000000	1.4063822 *
16 C	3.8854711	2.5009509 *	1.4063822 *	0.0000000
17 C	4.3444667	2.8821818 *	2.4410529 *	1.4282960 *
18 C	3.7931889	2.4978046 *	2.8249239 *	2.4726629 *
19 C	2.4693502 *	1.4426251 *	2.4454421 *	2.8453421 *
20 O	3.0500908	2.5033642 *	1.4658086 *	2.4593347 *
21 N	3.9759147	4.6895588	4.6774901	5.9093478

22 H	7.1295037	8.4911178	9.0340082	10.4321523
23 H	7.6690296	8.8225955	9.0399968	10.3613776
24 H	6.4001023	7.2779925	7.2469874	8.4584270
25 H	6.2483265	7.6857385	8.5068049	9.8910394
26 H	5.0157251	6.3720451	7.4276803	8.7051749
27 H	2.6534090 *	3.9124416	5.0282796	6.2542131
28 H	1.1083820 *	2.1771140 *	3.5335536	4.6746914
29 H	4.7969187	3.5031740	2.1941392 *	1.1067938 *
30 H	5.4492606	3.9872229	3.4394710	2.1915692 *
31 H	4.6566839	3.4933789	3.9291126	3.4746846
32 H	2.6396491 *	2.1972403 *	3.4502879	3.9511838
33 H	4.0172275	3.3303505	2.0467704 *	2.5109896 *
34 H	3.8296308	4.5240610	4.6726413	5.8662075
35 H	4.9370877	5.5055954	5.2909108	6.4069205

C C C O

1 CO	5.4337776	5.6029461	4.6906401	1.9510047 *
2 C	10.3330356	10.0072140	8.6950953	7.2594668
3 C	10.4088425	10.2380088	9.0049977	7.1003005
4 C	9.2960226	9.2314600	8.0799477	5.9286323
5 C	7.9741993	7.8519819	6.6804817	4.7506003
6 C	7.8116438	7.4850928	6.1931383	4.9278875
7 C	9.1436800	8.7283420	7.3877179	6.3225932
8 C	9.4538168	8.8729200	7.4913554	7.0199824
9 C	8.5768873	7.8786079	6.4974796	6.5928766
10 C	7.1563929	6.4923641	5.1159867	5.2770179
11 C	6.6947446	6.2367357	4.9018790	4.2896451
12 N	5.3117222	4.9857473	3.7416808	2.9415621 *
13 C	4.3444667	3.7931889	2.4693502 *	3.0500908
14 C	2.8821818 *	2.4978046 *	1.4426251 *	2.5033642 *
15 C	2.4410529 *	2.8249239 *	2.4454421 *	1.4658086 *
16 C	1.4282960 *	2.4726629 *	2.8453421 *	2.4593347 *
17 C	0.0000000	1.4231136 *	2.4554561 *	3.7703535
18 C	1.4231136 *	0.0000000	1.4159291 *	4.2905230
19 C	2.4554561 *	1.4159291 *	0.0000000	3.7951395
20 O	3.7703535	4.2905230	3.7951395	0.0000000
21 N	6.9790299	7.0174621	6.0020831	3.7540743
22 H	11.3050095	10.9215459	9.5821271	8.2942774
23 H	11.4227877	11.2947297	10.0797173	8.0342314
24 H	9.5961593	9.6563474	8.5976955	6.1531382
25 H	10.5362726	9.9292461	8.5432813	8.0949331
26 H	9.0798395	8.2771325	6.9197422	7.4154001
27 H	6.5792911	5.8034392	4.4564933	5.2462511
28 H	4.8532550	3.9967867	2.5817178 *	4.1435586
29 H	2.2006946 *	3.4737852	3.9521140	2.6853856 *

30 H	1.1050817 *	2.2006583 *	3.4606432	4.6491125
31 H	2.1978193 *	1.1041897 *	2.1875385 *	5.3946990
32 H	3.4568261	2.1858289 *	1.1058547 *	4.6923824
33 H	3.9311274	4.7316196	4.4873767	0.9919260 *
34 H	6.7944160	6.7207146	5.6972474	4.0173492
35 H	7.5588670	7.7397727	6.8281717	4.2209471

N H H H

1 CO	1.9766272 *	6.4261145	6.1033511	4.3232690
2 C	4.3411808	1.1050505 *	2.1867042 *	3.4392255
3 C	3.8140197	2.1797674 *	1.1040894 *	2.1943594 *
4 C	2.4741565 *	3.4512503	2.2009955 *	1.1077597 *
5 C	1.5089104 *	3.9431074	3.4659323	2.1822996 *
6 C	2.5920733 *	3.5196156	4.0264739	3.5068592
7 C	3.8860459	2.1967032 *	3.4864749	3.9527230
8 C	5.1094823	2.6810725 *	4.6712357	5.3958409
9 C	5.3852646	4.0804191	5.9313734	6.2658890
10 C	4.5625695	4.8939512	6.2585497	6.0064369
11 C	3.1536850	4.6930055	5.4871134	4.8002410
12 N	2.8938881 *	5.9979545	6.3997076	5.1667139
13 C	3.9759147	7.1295037	7.6690296	6.4001023
14 C	4.6895588	8.4911178	8.8225955	7.2779925
15 C	4.6774901	9.0340082	9.0399968	7.2469874
16 C	5.9093478	10.4321523	10.3613776	8.4584270
17 C	6.9790299	11.3050095	11.4227877	9.5961593
18 C	7.0174621	10.9215459	11.2947297	9.6563474
19 C	6.0020831	9.5821271	10.0797173	8.5976955
20 O	3.7540743	8.2942774	8.0342314	6.1531382
21 N	0.0000000	5.4451201	4.6739655	2.6517943 *
22 H	5.4451201	0.0000000	2.5302835 *	4.3600831
23 H	4.6739655	2.5302835 *	0.0000000	2.5190286 *
24 H	2.6517943 *	4.3600831	2.5190286 *	0.0000000
25 H	6.0550346	2.4016432 *	4.7820401	5.9760831
26 H	6.4688200	4.7784761	6.8517523	7.3469018
27 H	5.2561055	5.9683960	7.3477384	6.9649350
28 H	4.7296465	7.2014469	8.0339592	7.0094333
29 H	6.2404031	10.9531058	10.6828026	8.6667197
30 H	7.9560164	12.3902943	12.4492593	10.5546824
31 H	8.0169917	11.7608092	12.2397518	10.6532193
32 H	6.3909399	9.4640778	10.1855337	8.9015382
33 H	4.3777167	8.9794261	8.5597443	6.5962539
34 H	1.0439894 *	5.8501221	5.1860223	3.2273184
35 H	1.0392916 *	5.8197587	4.5833760	2.2097548 *

H H H H

1	CO	6.4890415	6.2772980	4.5277857	3.8775219
2	C	2.6820979 *	4.6684358	5.3924718	6.4059454
3	C	4.0816479	5.9299544	6.2679739	6.9356311
4	C	4.8913385	6.2524304	6.0079282	6.2686209
5	C	4.6718319	5.4678527	4.8020149	4.8909029
6	C	3.5171040	4.0162019	3.5049377	4.0435862
7	C	2.1973088 *	3.4835267	3.9510693	5.0327851
8	C	1.1051000 *	2.1841740 *	3.4314826	4.9937564
9	C	2.1810246 *	1.1042461 *	2.1816021 *	4.0016964
10	C	3.4539301	2.1978580 *	1.1042257 *	2.6638883 *
11	C	3.9643932	3.4743026	2.1882549 *	2.6613605 *
12	N	5.4114415	4.6687041	2.6942587 *	2.0964890 *
13	C	6.2483265	5.0157251	2.6534090 *	1.1083820 *
14	C	7.6857385	6.3720451	3.9124416	2.1771140 *
15	C	8.5068049	7.4276803	5.0282796	3.5335536
16	C	9.8910394	8.7051749	6.2542131	4.6746914
17	C	10.5362726	9.0798395	6.5792911	4.8532550
18	C	9.9292461	8.2771325	5.8034392	3.9967867
19	C	8.5432813	6.9197422	4.4564933	2.5817178 *
20	O	8.0949331	7.4154001	5.2462511	4.1435586
21	N	6.0550346	6.4688200	5.2561055	4.7296465
22	H	2.4016432 *	4.7784761	5.9683960	7.2014469
23	H	4.7820401	6.8517523	7.3477384	8.0339592
24	H	5.9760831	7.3469018	6.9649350	7.0094333
25	H	0.0000000	2.5278022 *	4.3486796	6.0245425
26	H	2.5278022 *	0.0000000	2.5009141 *	4.4929249
27	H	4.3486796	2.5009141 *	0.0000000	2.1593355 *
28	H	6.0245425	4.4929249	2.1593355 *	0.0000000
29	H	10.5830680	9.5447967	7.1445109	5.6718967
30	H	11.6329576	10.1447434	7.6445501	5.9328914
31	H	10.6372754	8.8339478	6.4251945	4.6545167
32	H	8.2268220	6.4327510	4.0896014	2.2648594 *
33	H	8.8924855	8.2772099	6.1399131	5.0997995
34	H	6.3225888	6.5885380	5.2939706	4.4653005
35	H	6.7602616	7.3983354	6.2738487	5.7358156

H H H H

1	CO	4.6113755	6.4129555	6.6683015	5.2747325
2	C	9.9236944	11.4106845	10.8805068	8.6506673
3	C	9.7638457	11.4505759	11.1730171	9.0964419
4	C	8.5461471	10.3066100	10.2033430	8.2920693
5	C	7.3780076	9.0083748	8.8153718	6.8932772
6	C	7.5290717	8.8946924	8.3789127	6.2326629
7	C	8.9257852	10.2358738	9.5671193	7.2922992

8 C	9.4966538	10.5522326	9.6097828	7.2248035
9 C	8.8677482	9.6650159	8.5380562	6.1339885
10 C	7.4724184	8.2482749	7.2009027	4.8448030
11 C	6.7042052	7.7942053	7.0837391	4.8769677
12 N	5.2707319	6.4038477	5.9177050	3.9688821
13 C	4.7969187	5.4492606	4.6566839	2.6396491 *
14 C	3.5031740	3.9872229	3.4933789	2.1972403 *
15 C	2.1941392 *	3.4394710	3.9291126	3.4502879
16 C	1.1067938 *	2.1915692 *	3.4746846	3.9511838
17 C	2.2006946 *	1.1050817 *	2.1978193 *	3.4568261
18 C	3.4737852	2.2006583 *	1.1041897 *	2.1858289 *
19 C	3.9521140	3.4606432	2.1875385 *	1.1058547 *
20 O	2.6853856 *	4.6491125	5.3946990	4.6923824
21 N	6.2404031	7.9560164	8.0169917	6.3909399
22 H	10.9531058	12.3902943	11.7608092	9.4640778
23 H	10.6828026	12.4492593	12.2397518	10.1855337
24 H	8.6667197	10.5546824	10.6532193	8.9015382
25 H	10.5830680	11.6329576	10.6372754	8.2268220
26 H	9.5447967	10.1447434	8.8339478	6.4327510
27 H	7.1445109	7.6445501	6.4251945	4.0896014
28 H	5.6718967	5.9328914	4.6545167	2.2648594 *
29 H	0.0000000	2.5204347 *	4.3872636	5.0579561
30 H	2.5204347 *	0.0000000	2.5412126 *	4.3742735
31 H	4.3872636	2.5412126 *	0.0000000	2.5146193 *
32 H	5.0579561	4.3742735	2.5146193 *	0.0000000
33 H	2.3099654 *	4.6325307	5.8174996	5.4661067
34 H	6.2938726	7.7706888	7.6563276	6.0082104
35 H	6.5830904	8.4706304	8.7584001	7.2929067

H H H

1 CO	2.6585279 *	2.4997270 *	2.6226077 *
2 C	7.9441517	4.7739336	4.7369003
3 C	7.6881364	4.3300997	3.9160518
4 C	6.4866982	3.0669718	2.4846236 *
5 C	5.4252210	2.1114261 *	2.0887212 *
6 C	5.7262209	2.9532657 *	3.4247261
7 C	7.0948886	4.2384767	4.5633989
8 C	7.8389075	5.3633087	5.8891954
9 C	7.4582915	5.5396564	6.3021191
10 C	6.1752069	4.6660361	5.5559979
11 C	5.1883214	3.3178860	4.1526182
12 N	3.8924467	2.9855110 *	3.8834792
13 C	4.0172275	3.8296308	4.9370877
14 C	3.3303505	4.5240610	5.5055954
15 C	2.0467704 *	4.6726413	5.2909108

16 C	2.5109896 *	5.8662075	6.4069205
17 C	3.9311274	6.7944160	7.5588670
18 C	4.7316196	6.7207146	7.7397727
19 C	4.4873767	5.6972474	6.8281717
20 O	0.9919260 *	4.0173492	4.2209471
21 N	4.3777167	1.0439894 *	1.0392916 *
22 H	8.9794261	5.8501221	5.8197587
23 H	8.5597443	5.1860223	4.5833760
24 H	6.5962539	3.2273184	2.2097548 *
25 H	8.8924855	6.3225888	6.7602616
26 H	8.2772099	6.5885380	7.3983354
27 H	6.1399131	5.2939706	6.2738487
28 H	5.0997995	4.4653005	5.7358156
29 H	2.3099654 *	6.2938726	6.5830904
30 H	4.6325307	7.7706888	8.4706304
31 H	5.8174996	7.6563276	8.7584001
32 H	5.4661067	6.0082104	7.2929067
33 H	0.0000000	4.7256872	4.6585860
34 H	4.7256872	0.0000000	1.6673780 *
35 H	4.6585860	1.6673780 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.77 , TOTAL = 9093.4 SECONDS (151.6 MIN)
WALL CLOCK TIME: STEP = 0.79 , TOTAL = 8413.0 SECONDS (140.2 MIN)
CPU UTILIZATION: STEP = 97.86% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.95 , TOTAL = 9094.3 SECONDS (151.6 MIN)
WALL CLOCK TIME: STEP = 0.94 , TOTAL = 8414.0 SECONDS (140.2 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0 -284.636971338 -284.636971338 0.002202837 0.000222427 198412116
11312847

2 1	-284.636976164	-0.000004825	0.000545285	0.000018503	144158166
15877862					
3 2	-284.636976172	-0.000000009	0.000311738	0.000037470	126565592
17213285					
4 3	-284.636976245	-0.000000072	0.000149908	0.000013759	120098992
17695935					
5 4	-284.636976195	0.000000050	0.000064462	0.000022780	115348239
18080433					
6 5	-284.636976232	-0.000000037	0.000052212	0.000005612	107453896
18633235					
7 6	-284.636976246	-0.000000015	0.000043748	0.000006059	107675403
18629196					
8 7	-284.636976274	-0.000000028	0.000071531	0.000005944	100061124
19186760					
9 8	-284.636976275	-0.000000001	0.000110405	0.000006064	132641254
16798172					
10 9	-284.636976278	-0.000000003	0.000130981	0.000005905	154768139
15131001					

-----DISABLING FDIFF OPTION-----

11 10	-284.636976251	0.000000027	0.000111765	0.000005147	198410846
11312898					
12 11	-284.636976252	-0.000000002	0.000057521	0.000004511	198410764
11312906					
13 12	-284.636976254	-0.000000001	0.000042386	0.000002357	198410588
11312915					
14 13	-284.636976254	-0.000000001	0.000037689	0.000001418	198410746
11312909					
15 14	-284.636976255	0.000000000	0.000018900	0.000001042	198410810
11312904					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 48.0 SECONDS (3.2 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 16.4 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
 TIME TO SOLVE SCF EQUATIONS= 2.8 SECONDS (0.2 SEC/ITER)

FINAL ENERGY IS -284.6369762546 AFTER 15 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6024359864
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998743946

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 51.80 , TOTAL = 9146.1 SECONDS (152.4 MIN)
WALL CLOCK TIME: STEP = 47.83 , TOTAL = 8461.8 SECONDS (141.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.94 , TOTAL = 9150.0 SECONDS (152.5 MIN)
WALL CLOCK TIME: STEP = 3.93 , TOTAL = 8465.8 SECONDS (141.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.88 , TOTAL = 9152.9 SECONDS (152.5 MIN)
WALL CLOCK TIME: STEP = 2.73 , TOTAL = 8468.5 SECONDS (141.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH=106 ENERGY= -284.6369763

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000311	0.0000769	-0.0000181
2 C	6.0	0.0000501	0.0000690	-0.0000665
3 C	6.0	-0.0000128	-0.0000143	0.0000420
4 C	6.0	-0.0000808	-0.0000597	0.0001144
5 C	6.0	-0.0000160	0.0000238	0.0000249
6 C	6.0	0.0000284	-0.0000413	0.0000008
7 C	6.0	-0.0000088	0.0000020	0.0000145
8 C	6.0	0.0000527	0.0000093	0.0000887

9 C	6.0	0.0000222	-0.0000503	0.0000464
10 C	6.0	0.0000000	0.0000530	-0.0000647
11 C	6.0	-0.0000217	0.0000501	-0.0000387
12 N	7.0	0.0000165	0.0000055	-0.0000485
13 C	6.0	-0.0000563	0.0000629	0.0000103
14 C	6.0	0.0000017	-0.0000243	0.0000043
15 C	6.0	-0.0000061	-0.0000942	0.0000037
16 C	6.0	-0.0000128	-0.0000092	-0.0000030
17 C	6.0	0.0000400	-0.0000130	0.0000016
18 C	6.0	-0.0000355	0.0000540	0.0000361
19 C	6.0	-0.0000177	-0.0000174	-0.0000281
20 O	8.0	0.0000088	0.0000255	-0.0000175
21 N	7.0	0.0000096	0.0000103	-0.0000381
22 H	1.0	-0.0000109	-0.0000014	-0.0000249
23 H	1.0	-0.0000397	0.0000361	-0.0000265
24 H	1.0	-0.0000548	0.0000173	0.0000371
25 H	1.0	0.0000517	0.0000130	0.0000033
26 H	1.0	0.0000328	-0.0000265	-0.0000105
27 H	1.0	0.0000171	-0.0000121	-0.0000265
28 H	1.0	-0.0000133	-0.0000318	-0.0000281
29 H	1.0	-0.0000028	0.0000272	0.0000067
30 H	1.0	0.0000763	0.0000077	0.0000304
31 H	1.0	0.0000029	0.0000222	-0.0000030
32 H	1.0	0.0000084	-0.0000447	0.0000031
33 H	1.0	-0.0000183	-0.0001437	-0.0000026
34 H	1.0	-0.0000351	0.0000090	-0.0000083
35 H	1.0	0.0000552	0.0000091	-0.0000148

MAXIMUM GRADIENT = 0.0001437 RMS GRADIENT = 0.0000390
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000010572
 PREDICTED ENERGY CHANGE WAS -0.0000007650 RATIO= 1.382
 GDIIS STEP HAS LENGTH = 0.016991
 RADIUS OF STEP TAKEN= 0.01699 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 9152.9 SECONDS (152.5 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8468.5 SECONDS (141.1 MIN)
 CPU UTILIZATION: STEP = 80.72% , TOTAL = 100.00%

INSERCH= 107

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM CHARGE X Y Z

CO	27.0	0.1598779962	-1.7147700454	0.8970079654
C	6.0	4.9802539137	0.6152383681	0.5515109167
C	6.0	5.1719627276	-0.7266910784	0.1953620331
C	6.0	4.0285524395	-1.5389737148	-0.0927437143
C	6.0	2.7247116127	-1.0169647466	-0.0002800315
C	6.0	2.4656031101	0.3503315863	0.4339232576
C	6.0	3.6547965816	1.1749138356	0.6762968298
C	6.0	3.5190892438	2.5624851733	1.0529527957
C	6.0	2.2559186773	3.1469102286	1.2197110087
C	6.0	1.0837014196	2.3458383533	1.0473737374
C	6.0	1.1648365969	0.9905027706	0.6504497935
N	7.0	-0.0501821795	0.1927842849	0.6078268096
C	6.0	-1.2479709595	0.7132314865	0.3472856242
C	6.0	-2.5480474302	0.0412692994	0.4529107145
C	6.0	-2.8141812734	-1.2844221215	0.9419814827
C	6.0	-4.1107004636	-1.8192682966	1.0463912580
C	6.0	-5.2224771177	-1.0158390147	0.6481659370
C	6.0	-5.0137033449	0.3008046869	0.1500321762
C	6.0	-3.6984350668	0.8171315926	0.0581977547
O	8.0	-1.6908043057	-2.1322652263	1.3518645219
N	7.0	1.6099047735	-1.9398434358	-0.4273401108
H	1.0	5.8483399692	1.2707436181	0.7460842971
H	1.0	6.1861991129	-1.1546159871	0.1103039730
H	1.0	4.1829768108	-2.5838395355	-0.4267849986
H	1.0	4.4369040080	3.1546324345	1.2205675254
H	1.0	2.1569724911	4.2043974626	1.5220432261
H	1.0	0.1035529684	2.7968323366	1.2822570228
H	1.0	-1.2974195307	1.7656511216	0.0029974311
H	1.0	-4.2780089907	-2.8448829710	1.4275155733
H	1.0	-6.2440784401	-1.4295237734	0.7283023571
H	1.0	-5.8726244602	0.9219205922	-0.1593757518
H	1.0	-3.5388587214	1.8440064072	-0.3200919221
H	1.0	-2.0059999034	-2.9411658842	1.8315577754
H	1.0	1.2373596850	-1.6497203517	-1.3584755984
H	1.0	1.9979750499	-2.8957344562	-0.5528946703

 INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3651031	5.1565105	3.9971433
2 C	5.3651031	0.0000000	1.4015595 *	2.4416039 *
3 C	5.1565105	1.4015595 *	0.0000000	1.4318502 *
4 C	3.9971433	2.4416039 *	1.4318502 *	0.0000000

5 C	2.8054286 *	2.8383149 *	2.4721595 *	1.4074956 *
6 C	3.1297700	2.5312983 *	2.9225454 *	2.5079201 *
7 C	4.5402029	1.4441763 *	2.4797566 *	2.8454002 *
8 C	5.4409127	2.4856018 *	3.7797001	4.2888388
9 C	5.3040983	3.7786051	4.9555414	5.1790227
10 C	4.1670853	4.2923161	5.1846159	5.0063740
11 C	2.8964174 *	3.8351039	4.3832544	3.8924872
12 N	1.9407510 *	5.0484578	5.3184922	4.4861856
13 C	2.8599694 *	6.2323427	6.5811858	5.7539337
14 C	3.2578761	7.5507936	7.7623870	6.7857625
15 C	3.0053703	8.0320855	8.0403358	6.9252045
16 C	4.2744679	9.4242867	9.3854042	8.2233589
17 C	5.4332471	10.3327381	10.4083148	9.2953841
18 C	5.6023618	10.0069593	10.2374604	9.2307158
19 C	4.6904912	8.6950423	9.0047854	8.0796257
20 O	1.9509540 *	7.2589503	7.1000499	5.9287376
21 N	1.9766470 *	4.3411802	3.8141517	2.4743702 *
22 H	6.4260929	1.1050427 *	2.1795703 *	3.4510535
23 H	6.1032141	2.1866302 *	1.1040969 *	2.2009994 *
24 H	4.3235441	3.4390134	2.1941195 *	1.1077793 *
25 H	6.4891234	2.6816764 *	4.0811800	4.8909586
26 H	6.2781844	4.6685023	5.9300829	6.2527323
27 H	4.5283712	5.3921753	6.2678015	6.0079499
28 H	3.8776671	6.4057396	6.9355375	6.2686274
29 H	4.6101447	9.9224622	9.7625255	8.5449137
30 H	6.4125256	11.4104314	11.4500653	10.3059711
31 H	6.6677710	10.8804588	11.1725854	10.2026342
32 H	5.2751185	8.6512914	9.0968450	8.2922828
33 H	2.6586570 *	7.9431904	7.6879245	6.4872877
34 H	2.5004808 *	4.7736091	4.3298378	3.0667734
35 H	2.6221166 *	4.7371541	3.9164825	2.4851123 *

C C C C

1 CO	2.8054286 *	3.1297700	4.5402029	5.4409127
2 C	2.8383149 *	2.5312983 *	1.4441763 *	2.4856018 *
3 C	2.4721595 *	2.9225454 *	2.4797566 *	3.7797001
4 C	1.4074956 *	2.5079201 *	2.8454002 *	4.2888388
5 C	0.0000000	1.4577959 *	2.4753073 *	3.8148128
6 C	1.4577959 *	0.0000000	1.4672634 *	2.5271830 *
7 C	2.4753073 *	1.4672634 *	0.0000000	1.4441746 *
8 C	3.8148128	2.5271830 *	1.4441746 *	0.0000000
9 C	4.3641723	2.9124358 *	2.4780896 *	1.4017706 *
10 C	3.8857351	2.5036016 *	2.8494372 *	2.4450114 *
11 C	2.6242304 *	1.4658432 *	2.4969133 *	2.8593081 *
12 N	3.0876078	2.5267052 *	3.8335537	4.3073563

13 C	4.3470206	3.7322694	4.9354360	5.1616440
14 C	5.3969648	5.0232033	6.3095424	6.5974789
15 C	5.6248311	5.5503753	6.9257921	7.4108924
16 C	6.9614704	6.9519817	8.3309688	8.7984940
17 C	7.9735997	7.8114595	9.1436414	9.4542709
18 C	7.8512532	7.4848562	8.7283396	8.8735006
19 C	6.6801304	6.1930960	7.3878326	7.4918925
20 O	4.7506811	4.9276390	6.3221257	7.0194744
21 N	1.5089333 *	2.5920833 *	3.8860404	5.1095220
22 H	3.9430602	3.5195897	2.1967445 *	2.6810769 *
23 H	3.4659879	4.0264663	3.4864102	4.6710709
24 H	2.1825537 *	3.5070716	3.9527194	5.3958344
25 H	4.6716480	3.5169503	2.1970909 *	1.1050416 *
26 H	5.4683104	4.0166008	3.4837530	2.1843269 *
27 H	4.8021268	3.5048990	3.9508402	3.4312370
28 H	4.8908589	4.0434102	5.0325686	4.9936067
29 H	7.3768544	7.5281423	8.9248249	9.4960344
30 H	9.0077873	8.8945543	10.2358940	10.5527710
31 H	8.8146909	8.3788279	9.5673458	9.6106961
32 H	6.8934570	6.2332307	7.2930893	7.2260704
33 H	5.4256623	5.7256066	7.0937548	7.8372834
34 H	2.1112296 *	2.9532158 *	4.2382612	5.3632035
35 H	2.0888525 *	3.4248256	4.5635673	5.8893714

C C C N

1 CO	5.3040983	4.1670853	2.8964174 *	1.9407510 *
2 C	3.7786051	4.2923161	3.8351039	5.0484578
3 C	4.9555414	5.1846159	4.3832544	5.3184922
4 C	5.1790227	5.0063740	3.8924872	4.4861856
5 C	4.3641723	3.8857351	2.6242304 *	3.0876078
6 C	2.9124358 *	2.5036016 *	1.4658432 *	2.5267052 *
7 C	2.4780896 *	2.8494372 *	2.4969133 *	3.8335537
8 C	1.4017706 *	2.4450114 *	2.8593081 *	4.3073563
9 C	0.0000000	1.4302131 *	2.4828636 *	3.7972837
10 C	1.4302131 *	0.0000000	1.4145904 *	2.4727586 *
11 C	2.4828636 *	1.4145904 *	0.0000000	1.4541121 *
12 N	3.7972837	2.4727586 *	1.4541121 *	0.0000000
13 C	4.3544415	2.9312497 *	2.4475351 *	1.3317075 *
14 C	5.7715751	4.3421221	3.8373915	2.5072468 *
15 C	6.7394179	5.3276062	4.5926961	3.1517438
16 C	8.0763115	6.6580722	5.9902316	4.5528566
17 C	8.5779688	7.1573829	6.6950123	5.3117824
18 C	7.8798435	6.4935144	6.2370231	4.9857584
19 C	6.4985622	5.1170541	4.9022680	3.7418780
20 O	6.5927066	5.2767422	4.2893295	2.9412732 *

21 N	5.3856452	4.5627557	3.1538303	2.8940560 *
22 H	4.0804184	4.8937087	4.6928546	5.9978058
23 H	5.9313587	6.2583355	5.4870186	6.3996459
24 H	6.2662585	6.0066943	4.8005758	5.1671749
25 H	2.1809992 *	3.4537098	3.9642044	5.4112788
26 H	1.1042981 *	2.1980591 *	3.4746407	4.6690860
27 H	2.1815464 *	1.1041996 *	2.1882253 *	2.6943565 *
28 H	4.0018097	2.6640338 *	2.6613445 *	2.0965042 *
29 H	8.8677494	7.4723513	6.7036246	5.2700884
30 H	9.6661875	8.2493347	7.7945245	6.4039635
31 H	8.5396530	7.2023785	7.0842345	5.9178606
32 H	6.1357963	4.8466339	4.8780292	3.9696891
33 H	7.4567404	6.1736223	5.1872188	3.8915786
34 H	5.5400518	4.6664988	3.3184061	2.9864582 *
35 H	6.3025567	5.5561534	4.1527096	3.8834483

C C C C

1 CO	2.8599694 *	3.2578761	3.0053703	4.2744679
2 C	6.2323427	7.5507936	8.0320855	9.4242867
3 C	6.5811858	7.7623870	8.0403358	9.3854042
4 C	5.7539337	6.7857625	6.9252045	8.2233589
5 C	4.3470206	5.3969648	5.6248311	6.9614704
6 C	3.7322694	5.0232033	5.5503753	6.9519817
7 C	4.9354360	6.3095424	6.9257921	8.3309688
8 C	5.1616440	6.5974789	7.4108924	8.7984940
9 C	4.3544415	5.7715751	6.7394179	8.0763115
10 C	2.9312497 *	4.3421221	5.3276062	6.6580722
11 C	2.4475351 *	3.8373915	4.5926961	5.9902316
12 N	1.3317075 *	2.5072468 *	3.1517438	4.5528566
13 C	0.0000000	1.4672725 *	2.6071628 *	3.8855532
14 C	1.4672725 *	0.0000000	1.4378718 *	2.5011405 *
15 C	2.6071628 *	1.4378718 *	0.0000000	1.4063868 *
16 C	3.8855532	2.5011405 *	1.4063868 *	0.0000000
17 C	4.3447570	2.8823908 *	2.4409738 *	1.4283310 *
18 C	3.7933818	2.4977096 *	2.8245398 *	2.4725661 *
19 C	2.4696440 *	1.4426200 *	2.4453029 *	2.8455392 *
20 O	3.0499396	2.5034448 *	1.4658847 *	2.4591011 *
21 N	3.9757144	4.6891594	4.6773022	5.9086163
22 H	7.1293400	8.4909881	9.0336328	10.4317230
23 H	7.6688917	8.8223910	9.0396562	10.3607028
24 H	6.4003950	7.2781693	7.2472221	8.4581263
25 H	6.2482688	7.6858229	8.5065300	9.8909842
26 H	5.0161674	6.3727461	7.4280537	8.7060047
27 H	2.6537108 *	3.9130458	5.0284787	6.2549140
28 H	1.1084072 *	2.1771506 *	3.5334408	4.6749190

29 H	4.7966870	3.5032123	2.1939856 *	1.1068574 *
30 H	5.4495563	3.9874451	3.4396087	2.1918903 *
31 H	4.6570030	3.4933156	3.9287416	3.4745312
32 H	2.6404945 *	2.1975216 *	3.4503698	3.9514378
33 H	4.0165024	3.3300755	2.0467787 *	2.5109570 *
34 H	3.8301477	4.5243644	4.6733853	5.8663343
35 H	4.9367120	5.5049029	5.2903526	6.4056546

C C C O

1 CO	5.4332471	5.6023618	4.6904912	1.9509540 *
2 C	10.3327381	10.0069593	8.6950423	7.2589503
3 C	10.4083148	10.2374604	9.0047854	7.1000499
4 C	9.2953841	9.2307158	8.0796257	5.9287376
5 C	7.9735997	7.8512532	6.6801304	4.7506811
6 C	7.8114595	7.4848562	6.1930960	4.9276390
7 C	9.1436414	8.7283396	7.3878326	6.3221257
8 C	9.4542709	8.8735006	7.4918925	7.0194744
9 C	8.5779688	7.8798435	6.4985622	6.5927066
10 C	7.1573829	6.4935144	5.1170541	5.2767422
11 C	6.6950123	6.2370231	4.9022680	4.2893295
12 N	5.3117824	4.9857584	3.7418780	2.9412732 *
13 C	4.3447570	3.7933818	2.4696440 *	3.0499396
14 C	2.8823908 *	2.4977096 *	1.4426200 *	2.5034448 *
15 C	2.4409738 *	2.8245398 *	2.4453029 *	1.4658847 *
16 C	1.4283310 *	2.4725661 *	2.8455392 *	2.4591011 *
17 C	0.0000000	1.4231213 *	2.4557174 *	3.7701873
18 C	1.4231213 *	0.0000000	1.4159653 *	4.2902084
19 C	2.4557174 *	1.4159653 *	0.0000000	3.7951412
20 O	3.7701873	4.2902084	3.7951412	0.0000000
21 N	6.9779610	7.0161277	6.0012607	3.7546339
22 H	11.3049122	10.9215404	9.5822683	8.2937407
23 H	11.4221910	11.2941420	10.0795087	8.0339563
24 H	9.5956609	9.6557142	8.5975849	6.1537645
25 H	10.5367983	9.9299727	8.5439309	8.0942779
26 H	9.0813439	8.2788310	6.9211423	7.4153652
27 H	6.5806634	5.8050322	4.4578750	5.2460048
28 H	4.8537621	3.9972690	2.5821719 *	4.1434220
29 H	2.2010924 *	3.4739834	3.9523775	2.6846183 *
30 H	1.1050910 *	2.2005126 *	3.4607515	4.6491914
31 H	2.1976641 *	1.1042028 *	2.1875599 *	5.3943969
32 H	3.4569944	2.1857847 *	1.1059112 *	4.6927049
33 H	3.9310336	4.7311924	4.4870862	0.9918539 *
34 H	6.7939611	6.7198164	5.6968756	4.0190717
35 H	7.5572140	7.7379327	6.8269976	4.2211475

	N	H	H	H
1 CO	1.9766470 *	6.4260929	6.1032141	4.3235441
2 C	4.3411802	1.1050427 *	2.1866302 *	3.4390134
3 C	3.8141517	2.1795703 *	1.1040969 *	2.1941195 *
4 C	2.4743702 *	3.4510535	2.2009994 *	1.1077793 *
5 C	1.5089333 *	3.9430602	3.4659879	2.1825537 *
6 C	2.5920833 *	3.5195897	4.0264663	3.5070716
7 C	3.8860404	2.1967445 *	3.4864102	3.9527194
8 C	5.1095220	2.6810769 *	4.6710709	5.3958344
9 C	5.3856452	4.0804184	5.9313587	6.2662585
10 C	4.5627557	4.8937087	6.2583355	6.0066943
11 C	3.1538303	4.6928546	5.4870186	4.8005758
12 N	2.8940560 *	5.9978058	6.3996459	5.1671749
13 C	3.9757144	7.1293400	7.6688917	6.4003950
14 C	4.6891594	8.4909881	8.8223910	7.2781693
15 C	4.6773022	9.0336328	9.0396562	7.2472221
16 C	5.9086163	10.4317230	10.3607028	8.4581263
17 C	6.9779610	11.3049122	11.4221910	9.5956609
18 C	7.0161277	10.9215404	11.2941420	9.6557142
19 C	6.0012607	9.5822683	10.0795087	8.5975849
20 O	3.7546339	8.2937407	8.0339563	6.1537645
21 N	0.0000000	5.4451012	4.6741965	2.6524387 *
22 H	5.4451012	0.0000000	2.5299673 *	4.3596867
23 H	4.6741965	2.5299673 *	0.0000000	2.5187386 *
24 H	2.6524387 *	4.3596867	2.5187386 *	0.0000000
25 H	6.0548500	2.4013169 *	4.7814580	5.9756431
26 H	6.4692407	4.7785595	6.8517662	7.3472979
27 H	5.2562264	5.9681660	7.3475167	6.9652102
28 H	4.7295259	7.2013187	8.0339295	7.0098164
29 H	6.2391598	10.9519712	10.6813716	8.6657288
30 H	7.9549348	12.3902519	12.4486664	10.5541533
31 H	8.0155937	11.7610604	12.2392793	10.6525574
32 H	6.3905232	9.4649280	10.1859573	8.9019069
33 H	4.3795014	8.9782565	8.5595911	6.5978199
34 H	1.0440185 *	5.8497369	5.1858898	3.2275821
35 H	1.0392738 *	5.8199825	4.5839445	2.2107498 *

	H	H	H	H
1 CO	6.4891234	6.2781844	4.5283712	3.8776671
2 C	2.6816764 *	4.6685023	5.3921753	6.4057396
3 C	4.0811800	5.9300829	6.2678015	6.9355375
4 C	4.8909586	6.2527323	6.0079499	6.2686274
5 C	4.6716480	5.4683104	4.8021268	4.8908589
6 C	3.5169503	4.0166008	3.5048990	4.0434102

7 C	2.1970909 *	3.4837530	3.9508402	5.0325686
8 C	1.1050416 *	2.1843269 *	3.4312370	4.9936067
9 C	2.1809992 *	1.1042981 *	2.1815464 *	4.0018097
10 C	3.4537098	2.1980591 *	1.1041996 *	2.6640338 *
11 C	3.9642044	3.4746407	2.1882253 *	2.6613445 *
12 N	5.4112788	4.6690860	2.6943565 *	2.0965042 *
13 C	6.2482688	5.0161674	2.6537108 *	1.1084072 *
14 C	7.6858229	6.3727461	3.9130458	2.1771506 *
15 C	8.5065300	7.4280537	5.0284787	3.5334408
16 C	9.8909842	8.7060047	6.2549140	4.6749190
17 C	10.5367983	9.0813439	6.5806634	4.8537621
18 C	9.9299727	8.2788310	5.8050322	3.9972690
19 C	8.5439309	6.9211423	4.4578750	2.5821719 *
20 O	8.0942779	7.4153652	5.2460048	4.1434220
21 N	6.0548500	6.4692407	5.2562264	4.7295259
22 H	2.4013169 *	4.7785595	5.9681660	7.2013187
23 H	4.7814580	6.8517662	7.3475167	8.0339295
24 H	5.9756431	7.3472979	6.9652102	7.0098164
25 H	0.0000000	2.5280391 *	4.3485351	6.0244678
26 H	2.5280391 *	0.0000000	2.5010535 *	4.4930845
27 H	4.3485351	2.5010535 *	0.0000000	2.1592970 *
28 H	6.0244678	4.4930845	2.1592970 *	0.0000000
29 H	10.5823779	9.5451703	7.1447979	5.6718771
30 H	11.6335807	10.1463663	7.6460039	5.9333502
31 H	10.6384032	8.8360767	6.4271530	4.6551849
32 H	8.2282540	6.4348583	4.0917676	2.2659603 *
33 H	8.8906174	8.2755794	6.1381242	5.0990044
34 H	6.3222111	6.5889128	5.2944138	4.4658120
35 H	6.7602132	7.3988189	6.2739089	5.7356043

H H H H

1 CO	4.6101447	6.4125256	6.6677710	5.2751185
2 C	9.9224622	11.4104314	10.8804588	8.6512914
3 C	9.7625255	11.4500653	11.1725854	9.0968450
4 C	8.5449137	10.3059711	10.2026342	8.2922828
5 C	7.3768544	9.0077873	8.8146909	6.8934570
6 C	7.5281423	8.8945543	8.3788279	6.2332307
7 C	8.9248249	10.2358940	9.5673458	7.2930893
8 C	9.4960344	10.5527710	9.6106961	7.2260704
9 C	8.8677494	9.6661875	8.5396530	6.1357963
10 C	7.4723513	8.2493347	7.2023785	4.8466339
11 C	6.7036246	7.7945245	7.0842345	4.8780292
12 N	5.2700884	6.4039635	5.9178606	3.9696891
13 C	4.7966870	5.4495563	4.6570030	2.6404945 *
14 C	3.5032123	3.9874451	3.4933156	2.1975216 *

15 C	2.1939856 *	3.4396087	3.9287416	3.4503698
16 C	1.1068574 *	2.1918903 *	3.4745312	3.9514378
17 C	2.2010924 *	1.1050910 *	2.1976641 *	3.4569944
18 C	3.4739834	2.2005126 *	1.1042028 *	2.1857847 *
19 C	3.9523775	3.4607515	2.1875599 *	1.1059112 *
20 O	2.6846183 *	4.6491914	5.3943969	4.6927049
21 N	6.2391598	7.9549348	8.0155937	6.3905232
22 H	10.9519712	12.3902519	11.7610604	9.4649280
23 H	10.6813716	12.4486664	12.2392793	10.1859573
24 H	8.6657288	10.5541533	10.6525574	8.9019069
25 H	10.5823779	11.6335807	10.6384032	8.2282540
26 H	9.5451703	10.1463663	8.8360767	6.4348583
27 H	7.1447979	7.6460039	6.4271530	4.0917676
28 H	5.6718771	5.9333502	4.6551849	2.2659603 *
29 H	0.0000000	2.5214222 *	4.3874630	5.0582763
30 H	2.5214222 *	0.0000000	2.5407166 *	4.3741678
31 H	4.3874630	2.5407166 *	0.0000000	2.5144650 *
32 H	5.0582763	4.3741678	2.5144650 *	0.0000000
33 H	2.3096636 *	4.6328764	5.8170473	5.4659973
34 H	6.2936041	7.7701380	7.6552630	6.0080471
35 H	6.5812298	8.4689247	8.7564653	7.2921786

H H H

1 CO	2.6586570 *	2.5004808 *	2.6221166 *
2 C	7.9431904	4.7736091	4.7371541
3 C	7.6879245	4.3298378	3.9164825
4 C	6.4872877	3.0667734	2.4851123 *
5 C	5.4256623	2.1112296 *	2.0888525 *
6 C	5.7256066	2.9532158 *	3.4248256
7 C	7.0937548	4.2382612	4.5635673
8 C	7.8372834	5.3632035	5.8893714
9 C	7.4567404	5.5400518	6.3025567
10 C	6.1736223	4.6664988	5.5561534
11 C	5.1872188	3.3184061	4.1527096
12 N	3.8915786	2.9864582 *	3.8834483
13 C	4.0165024	3.8301477	4.9367120
14 C	3.3300755	4.5243644	5.5049029
15 C	2.0467787 *	4.6733853	5.2903526
16 C	2.5109570 *	5.8663343	6.4056546
17 C	3.9310336	6.7939611	7.5572140
18 C	4.7311924	6.7198164	7.7379327
19 C	4.4870862	5.6968756	6.8269976
20 O	0.9918539 *	4.0190717	4.2211475
21 N	4.3795014	1.0440185 *	1.0392738 *
22 H	8.9782565	5.8497369	5.8199825

23 H	8.5595911	5.1858898	4.5839445
24 H	6.5978199	3.2275821	2.2107498 *
25 H	8.8906174	6.3222111	6.7602132
26 H	8.2755794	6.5889128	7.3988189
27 H	6.1381242	5.2944138	6.2739089
28 H	5.0990044	4.4658120	5.7356043
29 H	2.3096636 *	6.2936041	6.5812298
30 H	4.6328764	7.7701380	8.4689247
31 H	5.8170473	7.6552630	8.7564653
32 H	5.4659973	6.0080471	7.2921786
33 H	0.0000000	4.7290090	4.6604177
34 H	4.7290090	0.0000000	1.6673474 *
35 H	4.6604177	1.6673474 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.81 , TOTAL = 9153.8 SECONDS (152.6 MIN)
 WALL CLOCK TIME: STEP = 0.81 , TOTAL = 8469.3 SECONDS (141.2 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.14 , TOTAL = 9154.9 SECONDS (152.6 MIN)
 WALL CLOCK TIME: STEP = 1.15 , TOTAL = 8470.5 SECONDS (141.2 MIN)

CPU UTILIZATION: STEP = 99.50%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
 INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636971876	-284.636971876	0.002104708	0.000206666	198412806
11312849					
2 1	-284.636977165	-0.000005289	0.000821296	0.000022229	145070198
15811137					
3 2	-284.636977156	0.000000009	0.000484991	0.000037879	127955125
17125738					
4 3	-284.636977254	-0.000000097	0.000153977	0.000012288	121580833
17604519					

5 4	-284.636977227	0.000000027	0.000154223	0.000019561	116718374
17965459					
6 5	-284.636977265	-0.000000039	0.000065842	0.000006027	109064522
18496489					
7 6	-284.636977285	-0.000000020	0.000046714	0.000007517	108352563
18597226					
8 7	-284.636977301	-0.000000017	0.000057144	0.000006094	101173700
19109483					
9 8	-284.636977307	-0.000000006	0.000069117	0.000006120	130755094
16970185					
10 9	-284.636977310	-0.000000002	0.000111925	0.000005894	150781897
15460394					

-----DISABLING FDIFF OPTION-----

11 10	-284.636977272	0.000000038	0.000082378	0.000004895	198412150
11312936					
12 11	-284.636977273	-0.000000001	0.000059295	0.000003953	198412472
11312933					
13 12	-284.636977274	-0.000000001	0.000037213	0.000003049	198412162
11312943					
14 13	-284.636977275	-0.000000001	0.000022760	0.000001603	198412288
11312934					
15 14	-284.636977275	0.000000000	0.000007940	0.000001330	198412273
11312935					

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 48.1 SECONDS (3.2 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 16.3 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.4
 TIME TO SOLVE SCF EQUATIONS= 2.2 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369772750 AFTER 15 ITERATIONS
 DFT EXCHANGE + CORRELATION ENERGY IS -46.6023473214
 INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998740923

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
 PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 51.27 , TOTAL = 9206.2 SECONDS (153.4 MIN)
WALL CLOCK TIME: STEP = 47.47 , TOTAL = 8517.9 SECONDS (142.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.80 , TOTAL = 9210.0 SECONDS (153.5 MIN)
WALL CLOCK TIME: STEP = 3.78 , TOTAL = 8521.7 SECONDS (142.0 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.86 , TOTAL = 9212.8 SECONDS (153.5 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 8524.4 SECONDS (142.1 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH=107 ENERGY= -284.6369773

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000193	0.0000142	0.0000047
2 C	6.0	0.0000063	0.0000261	-0.0000345
3 C	6.0	-0.0000305	-0.0000015	0.0000191
4 C	6.0	-0.0000459	-0.0000106	0.0001076
5 C	6.0	-0.0000332	-0.0000008	-0.0000074
6 C	6.0	0.0000053	0.0000067	-0.0000424
7 C	6.0	0.0000002	-0.0000197	-0.0000002
8 C	6.0	0.0000205	0.0000134	0.0000844
9 C	6.0	0.0000422	0.0000204	0.0000809
10 C	6.0	0.0000357	0.0000579	-0.0000279
11 C	6.0	-0.0000118	0.0000024	-0.0000322
12 N	7.0	0.0000031	0.0000137	-0.0000036
13 C	6.0	-0.0000349	0.0000102	-0.0000133
14 C	6.0	-0.0000078	-0.0000278	-0.0000097

15 C	6.0	-0.0000152	0.0000017	-0.0000065
16 C	6.0	0.0000173	-0.0000116	0.0000260
17 C	6.0	-0.0000038	-0.0000132	-0.0000013
18 C	6.0	0.0000000	0.0000126	0.0000032
19 C	6.0	0.0000101	-0.0000125	0.0000060
20 O	8.0	-0.0000436	-0.0000822	-0.0000261
21 N	7.0	-0.0000106	0.0000082	-0.0000174
22 H	1.0	-0.0000019	-0.0000179	-0.0000466
23 H	1.0	-0.0000308	0.0000355	-0.0000073
24 H	1.0	-0.0000086	0.0000088	0.0000492
25 H	1.0	0.0000249	-0.0000235	0.0000008
26 H	1.0	0.0000317	0.0000196	-0.0000169
27 H	1.0	0.0000404	-0.0000090	-0.0000508
28 H	1.0	-0.0000138	-0.0000165	-0.0000135
29 H	1.0	0.0000351	-0.0000235	0.0000171
30 H	1.0	0.0000548	0.0000338	0.0000146
31 H	1.0	-0.0000121	0.0000199	0.0000149
32 H	1.0	-0.0000190	-0.0000090	-0.0000215
33 H	1.0	-0.0000063	-0.0000688	-0.0000025
34 H	1.0	0.0000043	0.0000263	-0.0000469
35 H	1.0	0.0000172	0.0000167	0.0000000

MAXIMUM GRADIENT = 0.0001076 RMS GRADIENT = 0.0000293
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000010203
 PREDICTED ENERGY CHANGE WAS -0.0000007172 RATIO= 1.423
 GDIIS STEP HAS LENGTH = 0.007180
 RADIUS OF STEP TAKEN= 0.00718 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 9212.8 SECONDS (153.5 MIN)
 WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8524.4 SECONDS (142.1
 MIN)
 CPU UTILIZATION: STEP = 81.40% , TOTAL = 100.00%

INSERCH= 108

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1597843228	-1.7149578259	0.8968593356
C	6.0	4.9801884837	0.6150788934	0.5515050444
C	6.0	5.1719818042	-0.7267551556	0.1951231104
C	6.0	4.0285825225	-1.5389034528	-0.0933955066
C	6.0	2.7246980735	-1.0169532988	-0.0005372132

C	6.0	2.4655554833	0.3503115496	0.4339313699
C	6.0	3.6547529369	1.1748671397	0.6761457164
C	6.0	3.5191376219	2.5624514181	1.0526442695
C	6.0	2.2560513215	3.1470082995	1.2197015967
C	6.0	1.0838512645	2.3457871210	1.0479496927
C	6.0	1.1649129882	0.9904928367	0.6508995955
N	7.0	-0.0501755105	0.1928093591	0.6083117175
C	6.0	-1.2478877136	0.7133631664	0.3477588514
C	6.0	-2.5480675125	0.0414464356	0.4530467420
C	6.0	-2.8142159552	-1.2842069852	0.9421976983
C	6.0	-4.1106661021	-1.8193845762	1.0462526133
C	6.0	-5.2225436915	-1.0162152735	0.6477061740
C	6.0	-5.0136773880	0.3003482360	0.1494372020
C	6.0	-3.6985036640	0.8170577705	0.0579773675
O	8.0	-1.6907849781	-2.1318122871	1.3525179415
N	7.0	1.6097024645	-1.9396988105	-0.4275731320
H	1.0	5.8483130403	1.2705855303	0.7460487890
H	1.0	6.1862130110	-1.1548076714	0.1104224481
H	1.0	4.1831008450	-2.5838189532	-0.4272804921
H	1.0	4.4370722818	3.1543939131	1.2203435785
H	1.0	2.1572342846	4.2045370339	1.5221606549
H	1.0	0.1037559388	2.7969249572	1.2829056747
H	1.0	-1.2973700953	1.7659425489	0.0038289894
H	1.0	-4.2777156268	-2.8450591643	1.4273428397
H	1.0	-6.2442669313	-1.4299352899	0.7274842495
H	1.0	-5.8726593541	0.9212560143	-0.1601257043
H	1.0	-3.5391122442	1.8439569083	-0.3203942319
H	1.0	-2.0060889401	-2.9397672841	1.8336078071
H	1.0	1.2374142975	-1.6495128490	-1.3587781919
H	1.0	1.9974297207	-2.8957252541	-0.5531395973

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3651316	5.1566561	3.9973991
2 C	5.3651316	0.0000000	1.4015389 *	2.4415345 *
3 C	5.1566561	1.4015389 *	0.0000000	1.4318484 *
4 C	3.9973991	2.4415345 *	1.4318484 *	0.0000000
5 C	2.8055861 *	2.8382242 *	2.4721844 *	1.4075402 *
6 C	3.1298915	2.5312654 *	2.9226436 *	2.5080392 *
7 C	4.5403313	1.4441875 *	2.4798253 *	2.8454337 *
8 C	5.4411169	2.4855723 *	3.7796979	4.2888289
9 C	5.3044582	3.7786342	4.9556488	5.1791756
10 C	4.1672986	4.2922316	5.1846543	5.0064890

11 C	2.8965916 *	3.8349892	4.3832948	3.8926115
12 N	1.9408551 *	5.0483760	5.3185760	4.4863671
13 C	2.8600340 *	6.2321830	6.5811825	5.7539952
14 C	3.2579729	7.5507209	7.7624622	6.7858994
15 C	3.0053751	8.0319778	8.0404122	6.9254036
16 C	4.2743386	9.4241724	9.3854042	8.2234321
17 C	5.4332102	10.3327692	10.4083994	9.2954704
18 C	5.6022142	10.0069011	10.2374158	9.2306164
19 C	4.6905450	8.6950597	9.0048698	8.0796861
20 O	1.9508970 *	7.2587134	7.1000927	5.9290278
21 N	1.9765861 *	4.3411587	3.8142912	2.4745287 *
22 H	6.4261631	1.1050685 *	2.1795212 *	3.4509874
23 H	6.1032855	2.1866750 *	1.1041142 *	2.2010090 *
24 H	4.3238110	3.4389413	2.1940733 *	1.1077922 *
25 H	6.4892542	2.6814998 *	4.0809909	4.8907887
26 H	6.2786326	4.6685600	5.9302086	6.2529253
27 H	4.5287147	5.3921233	6.2678949	6.0081509
28 H	3.8778176	6.4056364	6.9356073	6.2687504
29 H	4.6097665	9.9221185	9.7622927	8.5447807
30 H	6.4126280	11.4105850	11.4502666	10.3061707
31 H	6.6676246	10.8804627	11.1725664	10.2025207
32 H	5.2753593	8.6515221	9.0971137	8.2924831
33 H	2.6586957 *	7.9428453	7.6880917	6.4879134
34 H	2.5006939 *	4.7734596	4.3297705	3.0666020
35 H	2.6217645 *	4.7373870	3.9169005	2.4855405 *

C C C C

1 CO	2.8055861 *	3.1298915	4.5403313	5.4411169
2 C	2.8382242 *	2.5312654 *	1.4441875 *	2.4855723 *
3 C	2.4721844 *	2.9226436 *	2.4798253 *	3.7796979
4 C	1.4075402 *	2.5080392 *	2.8454337 *	4.2888289
5 C	0.0000000	1.4578515 *	2.4752735 *	3.8147691
6 C	1.4578515 *	0.0000000	1.4672254 *	2.5271335 *
7 C	2.4752735 *	1.4672254 *	0.0000000	1.4441374 *
8 C	3.8147691	2.5271335 *	1.4441374 *	0.0000000
9 C	4.3643085	2.9125315 *	2.4781364 *	1.4017853 *
10 C	3.8858366	2.5036070 *	2.8493556 *	2.4449100 *
11 C	2.6243360 *	1.4658029 *	2.4967848 *	2.8591653 *
12 N	3.0877413	2.5266812 *	3.8334754	4.3072765
13 C	4.3470384	3.7321432	4.9352517	5.1614457
14 C	5.3970367	5.0231642	6.3094689	6.5974208
15 C	5.6249215	5.5503128	6.9257049	7.4108263
16 C	6.9614559	6.9519212	8.3309216	8.7985472
17 C	7.9736360	7.8115276	9.1437436	9.4545133
18 C	7.8511292	7.4848085	8.7283383	8.8736591

19 C	6.6801603	6.1931267	7.3878645	7.4920029
20 O	4.7508062	4.9274645	6.3218972	7.0192115
21 N	1.5089845 *	2.5920690 *	3.8859938	5.1094366
22 H	3.9429932	3.5195696	2.1967600 *	2.6810402 *
23 H	3.4660354	4.0265785	3.4865051	4.6710907
24 H	2.1826856 *	3.5072453	3.9527740	5.3958431
25 H	4.6715001	3.5168453	2.1969754 *	1.1050443 *
26 H	5.4685085	4.0167598	3.4838489	2.1844156 *
27 H	4.8023151	3.5049639	3.9507985	3.4311558
28 H	4.8909673	4.0433412	5.0323854	4.9933142
29 H	7.3766259	7.5278792	8.9245819	9.4959197
30 H	9.0079355	8.8947433	10.2361236	10.5531488
31 H	8.8145719	8.3788250	9.5674058	9.6109408
32 H	6.8936518	6.2334596	7.2933168	7.2263656
33 H	5.4260158	5.7253224	7.0933113	7.8366092
34 H	2.1111521 *	2.9532077 *	4.2381085	5.3630087
35 H	2.0890363 *	3.4249388	4.5637249	5.8894677

C C C N

1 CO	5.3044582	4.1672986	2.8965916 *	1.9408551 *
2 C	3.7786342	4.2922316	3.8349892	5.0483760
3 C	4.9556488	5.1846543	4.3832948	5.3185760
4 C	5.1791756	5.0064890	3.8926115	4.4863671
5 C	4.3643085	3.8858366	2.6243360 *	3.0877413
6 C	2.9125315 *	2.5036070 *	1.4658029 *	2.5266812 *
7 C	2.4781364 *	2.8493556 *	2.4967848 *	3.8334754
8 C	1.4017853 *	2.4449100 *	2.8591653 *	4.3072765
9 C	0.0000000	1.4302122 *	2.4828769 *	3.7973374
10 C	1.4302122 *	0.0000000	1.4145821 *	2.4727741 *
11 C	2.4828769 *	1.4145821 *	0.0000000	1.4541502 *
12 N	3.7973374	2.4727741 *	1.4541502 *	0.0000000
13 C	4.3543658	2.9312253 *	2.4475094 *	1.3316826 *
14 C	5.7716403	4.3422033	3.8374548	2.5072859 *
15 C	6.7394575	5.3275669	4.5926660	3.1516625
16 C	8.0765236	6.6582031	5.9902796	4.5528343
17 C	8.5784027	7.1577840	6.6952588	5.3119380
18 C	7.8802218	6.4939203	6.2372064	4.9858280
19 C	6.4988459	5.1174190	4.9024951	3.7420385
20 O	6.5925036	5.2763875	4.2890638	2.9409706 *
21 N	5.3857098	4.5627926	3.1538808	2.8941049 *
22 H	4.0803987	4.8935977	4.6927328	5.9977279
23 H	5.9314662	6.2583717	5.4870651	6.3997271
24 H	6.2664544	6.0068851	4.8007952	5.1674699
25 H	2.1810336 *	3.4536438	3.9640586	5.4111883
26 H	1.1043610 *	2.1981761 *	3.4747486	4.6692330

27 H	2.1814969 *	1.1042267 *	2.1883060 *	2.6944740 *
28 H	4.0015613	2.6639487 *	2.6613644 *	2.0965786 *
29 H	8.8678125	7.4722971	6.7034715	5.2698722
30 H	9.6667523	8.2498542	7.7948884	6.4042385
31 H	8.5401308	7.2029005	7.0844887	5.9179767
32 H	6.1362659	4.8472663	4.8784901	3.9700708
33 H	7.4559746	6.1726878	5.1866171	3.8910133
34 H	5.5401078	4.6667272	3.3186882	2.9868849 *
35 H	6.3027359	5.5562185	4.1527684	3.8833880

C C C C

1 CO	2.8600340 *	3.2579729	3.0053751	4.2743386
2 C	6.2321830	7.5507209	8.0319778	9.4241724
3 C	6.5811825	7.7624622	8.0404122	9.3854042
4 C	5.7539952	6.7858994	6.9254036	8.2234321
5 C	4.3470384	5.3970367	5.6249215	6.9614559
6 C	3.7321432	5.0231642	5.5503128	6.9519212
7 C	4.9352517	6.3094689	6.9257049	8.3309216
8 C	5.1614457	6.5974208	7.4108263	8.7985472
9 C	4.3543658	5.7716403	6.7394575	8.0765236
10 C	2.9312253 *	4.3422033	5.3275669	6.6582031
11 C	2.4475094 *	3.8374548	4.5926660	5.9902796
12 N	1.3316826 *	2.5072859 *	3.1516625	4.5528343
13 C	0.0000000	1.4673190 *	2.6071111 *	3.8856408
14 C	1.4673190 *	0.0000000	1.4378667 *	2.5012596 *
15 C	2.6071111 *	1.4378667 *	0.0000000	1.4064229 *
16 C	3.8856408	2.5012596 *	1.4064229 *	0.0000000
17 C	4.3450317	2.8825966 *	2.4410218 *	1.4283529 *
18 C	3.7935583	2.4976871 *	2.8243433 *	2.4724430 *
19 C	2.4698673 *	1.4426213 *	2.4452247 *	2.8455920 *
20 O	3.0497085	2.5034047 *	1.4659108 *	2.4591125 *
21 N	3.9756382	4.6890808	4.6772851	5.9084054
22 H	7.1291792	8.4909269	9.0335402	10.4316491
23 H	7.6689142	8.8224754	9.0397077	10.3606544
24 H	6.4006041	7.2784354	7.2475447	8.4582640
25 H	6.2481041	7.6857898	8.5064519	9.8910369
26 H	5.0162108	6.3729266	7.4281886	8.7063595
27 H	2.6538029 *	3.9132461	5.0285465	6.2552115
28 H	1.1084492 *	2.1771374 *	3.5333793	4.6750243
29 H	4.7966372	3.5032628	2.1939591 *	1.1068621 *
30 H	5.4499289	3.9877525	3.4398529	2.1921534 *
31 H	4.6572179	3.4932730	3.9285188	3.4743459
32 H	2.6409053 *	2.1975952 *	3.4503655	3.9515147
33 H	4.0159654	3.3297635	2.0465975 *	2.5108625 *
34 H	3.8304279	4.5245912	4.6737187	5.8664294

35 H	4.9365193	5.5046284	5.2900812	6.4051073
	C	C	C	O
1 CO	5.4332102	5.6022142	4.6905450	1.9508970 *
2 C	10.3327692	10.0069011	8.6950597	7.2587134
3 C	10.4083994	10.2374158	9.0048698	7.1000927
4 C	9.2954704	9.2306164	8.0796861	5.9290278
5 C	7.9736360	7.8511292	6.6801603	4.7508062
6 C	7.8115276	7.4848085	6.1931267	4.9274645
7 C	9.1437436	8.7283383	7.3878645	6.3218972
8 C	9.4545133	8.8736591	7.4920029	7.0192115
9 C	8.5784027	7.8802218	6.4988459	6.5925036
10 C	7.1577840	6.4939203	5.1174190	5.2763875
11 C	6.6952588	6.2372064	4.9024951	4.2890638
12 N	5.3119380	4.9858280	3.7420385	2.9409706 *
13 C	4.3450317	3.7935583	2.4698673 *	3.0497085
14 C	2.8825966 *	2.4976871 *	1.4426213 *	2.5034047 *
15 C	2.4410218 *	2.8243433 *	2.4452247 *	1.4659108 *
16 C	1.4283529 *	2.4724430 *	2.8455920 *	2.4591125 *
17 C	0.0000000	1.4231081 *	2.4558844 *	3.7702302
18 C	1.4231081 *	0.0000000	1.4159928 *	4.2900375
19 C	2.4558844 *	1.4159928 *	0.0000000	3.7950763
20 O	3.7702302	4.2900375	3.7950763	0.0000000
21 N	6.9777242	7.0156904	6.0010431	3.7548434
22 H	11.3049988	10.9215448	9.5823191	8.2934983
23 H	11.4222419	11.2940934	10.0796145	8.0339552
24 H	9.5957869	9.6556591	8.5977397	6.1542284
25 H	10.5370810	9.9302108	8.5441109	8.0939533
26 H	9.0819628	8.2794344	6.9215977	7.4152110
27 H	6.5812601	5.8056671	4.4584192	5.2457291
28 H	4.8540671	3.9975128	2.5823936 *	4.1432149
29 H	2.2011823 *	3.4739416	3.9524358	2.6844981 *
30 H	1.1051910 *	2.2005386 *	3.4609432	4.6494619
31 H	2.1975072 *	1.1041765 *	2.1875510 *	5.3941997
32 H	3.4571296	2.1858206 *	1.1059351 *	4.6927273
33 H	3.9309027	4.7307893	4.4867433	0.9917940 *
34 H	6.7939755	6.7195847	5.6968810	4.0197127
35 H	7.5566265	7.7371909	6.8265569	4.2211398
	N	H	H	H
1 CO	1.9765861 *	6.4261631	6.1032855	4.3238110
2 C	4.3411587	1.1050685 *	2.1866750 *	3.4389413
3 C	3.8142912	2.1795212 *	1.1041142 *	2.1940733 *
4 C	2.4745287 *	3.4509874	2.2010090 *	1.1077922 *

5 C	1.5089845 *	3.9429932	3.4660354	2.1826856 *
6 C	2.5920690 *	3.5195696	4.0265785	3.5072453
7 C	3.8859938	2.1967600 *	3.4865051	3.9527740
8 C	5.1094366	2.6810402 *	4.6710907	5.3958431
9 C	5.3857098	4.0803987	5.9314662	6.2664544
10 C	4.5627926	4.8935977	6.2583717	6.0068851
11 C	3.1538808	4.6927328	5.4870651	4.8007952
12 N	2.8941049 *	5.9977279	6.3997271	5.1674699
13 C	3.9756382	7.1291792	7.6689142	6.4006041
14 C	4.6890808	8.4909269	8.8224754	7.2784354
15 C	4.6772851	9.0335402	9.0397077	7.2475447
16 C	5.9084054	10.4316491	10.3606544	8.4582640
17 C	6.9777242	11.3049988	11.4222419	9.5957869
18 C	7.0156904	10.9215448	11.2940934	9.6556591
19 C	6.0010431	9.5823191	10.0796145	8.5977397
20 O	3.7548434	8.2934983	8.0339552	6.1542284
21 N	0.0000000	5.4451018	4.6743922	2.6527853 *
22 H	5.4451018	0.0000000	2.5299663 *	4.3595948
23 H	4.6743922	2.5299663 *	0.0000000	2.5186616 *
24 H	2.6527853 *	4.3595948	2.5186616 *	0.0000000
25 H	6.0547032	2.4011018 *	4.7812798	5.9754710
26 H	6.4693807	4.7785441	6.8518793	7.3475325
27 H	5.2563502	5.9680703	7.3475977	6.9655005
28 H	4.7295831	7.2011844	8.0340625	7.0101243
29 H	6.2387565	10.9516734	10.6810595	8.6656384
30 H	7.9548005	12.3904660	12.4488269	10.5543796
31 H	8.0151313	11.7611384	12.2392663	10.6524756
32 H	6.3904484	9.4651893	10.1862723	8.9022019
33 H	4.3802995	8.9778330	8.5597465	6.5988170
34 H	1.0440063 *	5.8495862	5.1859322	3.2276439
35 H	1.0392718 *	5.8202524	4.5844317	2.2113987 *

H H H H

1 CO	6.4892542	6.2786326	4.5287147	3.8778176
2 C	2.6814998 *	4.6685600	5.3921233	6.4056364
3 C	4.0809909	5.9302086	6.2678949	6.9356073
4 C	4.8907887	6.2529253	6.0081509	6.2687504
5 C	4.6715001	5.4685085	4.8023151	4.8909673
6 C	3.5168453	4.0167598	3.5049639	4.0433412
7 C	2.1969754 *	3.4838489	3.9507985	5.0323854
8 C	1.1050443 *	2.1844156 *	3.4311558	4.9933142
9 C	2.1810336 *	1.1043610 *	2.1814969 *	4.0015613
10 C	3.4536438	2.1981761 *	1.1042267 *	2.6639487 *
11 C	3.9640586	3.4747486	2.1883060 *	2.6613644 *
12 N	5.4111883	4.6692330	2.6944740 *	2.0965786 *

13 C	6.2481041	5.0162108	2.6538029 *	1.1084492 *
14 C	7.6857898	6.3729266	3.9132461	2.1771374 *
15 C	8.5064519	7.4281886	5.0285465	3.5333793
16 C	9.8910369	8.7063595	6.2552115	4.6750243
17 C	10.5370810	9.0819628	6.5812601	4.8540671
18 C	9.9302108	8.2794344	5.8056671	3.9975128
19 C	8.5441109	6.9215977	4.4584192	2.5823936 *
20 O	8.0939533	7.4152110	5.2457291	4.1432149
21 N	6.0547032	6.4693807	5.2563502	4.7295831
22 H	2.4011018 *	4.7785441	5.9680703	7.2011844
23 H	4.7812798	6.8518793	7.3475977	8.0340625
24 H	5.9754710	7.3475325	6.9655005	7.0101243
25 H	0.0000000	2.5281526 *	4.3484858	6.0242455
26 H	2.5281526 *	0.0000000	2.5010774 *	4.4929239
27 H	4.3484858	2.5010774 *	0.0000000	2.1591934 *
28 H	6.0242455	4.4929239	2.1591934 *	0.0000000
29 H	10.5822405	9.5453851	7.1449381	5.6718769
30 H	11.6340015	10.1471184	7.6467140	5.9337257
31 H	10.6387578	8.8368101	6.4279089	4.6554966
32 H	8.2286474	6.4355039	4.0925795	2.2664101 *
33 H	8.8898380	8.2747413	6.1371293	5.0984388
34 H	6.3219618	6.5890650	5.2947601	4.4662250
35 H	6.7602545	7.3990630	6.2740202	5.7355964

H H H H

1 CO	4.6097665	6.4126280	6.6676246	5.2753593
2 C	9.9221185	11.4105850	10.8804627	8.6515221
3 C	9.7622927	11.4502666	11.1725664	9.0971137
4 C	8.5447807	10.3061707	10.2025207	8.2924831
5 C	7.3766259	9.0079355	8.8145719	6.8936518
6 C	7.5278792	8.8947433	8.3788250	6.2334596
7 C	8.9245819	10.2361236	9.5674058	7.2933168
8 C	9.4959197	10.5531488	9.6109408	7.2263656
9 C	8.8678125	9.6667523	8.5401308	6.1362659
10 C	7.4722971	8.2498542	7.2029005	4.8472663
11 C	6.7034715	7.7948884	7.0844887	4.8784901
12 N	5.2698722	6.4042385	5.9179767	3.9700708
13 C	4.7966372	5.4499289	4.6572179	2.6409053 *
14 C	3.5032628	3.9877525	3.4932730	2.1975952 *
15 C	2.1939591 *	3.4398529	3.9285188	3.4503655
16 C	1.1068621 *	2.1921534 *	3.4743459	3.9515147
17 C	2.2011823 *	1.1051910 *	2.1975072 *	3.4571296
18 C	3.4739416	2.2005386 *	1.1041765 *	2.1858206 *
19 C	3.9524358	3.4609432	2.1875510 *	1.1059351 *
20 O	2.6844981 *	4.6494619	5.3941997	4.6927273

21 N	6.2387565	7.9548005	8.0151313	6.3904484
22 H	10.9516734	12.3904660	11.7611384	9.4651893
23 H	10.6810595	12.4488269	12.2392663	10.1862723
24 H	8.6656384	10.5543796	10.6524756	8.9022019
25 H	10.5822405	11.6340015	10.6387578	8.2286474
26 H	9.5453851	10.1471184	8.8368101	6.4355039
27 H	7.1449381	7.6467140	6.4279089	4.0925795
28 H	5.6718769	5.9337257	4.6554966	2.2664101 *
29 H	0.0000000	2.5218449 *	4.3873719	5.0583586
30 H	2.5218449 *	0.0000000	2.5404811 *	4.3742749
31 H	4.3873719	2.5404811 *	0.0000000	2.5144592 *
32 H	5.0583586	4.3742749	2.5144592 *	0.0000000
33 H	2.3096122 *	4.6330610	5.8166005	5.4657024
34 H	6.2935252	7.7702162	7.6549832	6.0081426
35 H	6.5804504	8.4684179	8.7556900	7.2919171

H H H

1 CO	2.6586957 *	2.5006939 *	2.6217645 *
2 C	7.9428453	4.7734596	4.7373870
3 C	7.6880917	4.3297705	3.9169005
4 C	6.4879134	3.0666020	2.4855405 *
5 C	5.4260158	2.1111521 *	2.0890363 *
6 C	5.7253224	2.9532077 *	3.4249388
7 C	7.0933113	4.2381085	4.5637249
8 C	7.8366092	5.3630087	5.8894677
9 C	7.4559746	5.5401078	6.3027359
10 C	6.1726878	4.6667272	5.5562185
11 C	5.1866171	3.3186882	4.1527684
12 N	3.8910133	2.9868849 *	3.8833880
13 C	4.0159654	3.8304279	4.9365193
14 C	3.3297635	4.5245912	5.5046284
15 C	2.0465975 *	4.6737187	5.2900812
16 C	2.5108625 *	5.8664294	6.4051073
17 C	3.9309027	6.7939755	7.5566265
18 C	4.7307893	6.7195847	7.7371909
19 C	4.4867433	5.6968810	6.8265569
20 O	0.9917940 *	4.0197127	4.2211398
21 N	4.3802995	1.0440063 *	1.0392718 *
22 H	8.9778330	5.8495862	5.8202524
23 H	8.5597465	5.1859322	4.5844317
24 H	6.5988170	3.2276439	2.2113987 *
25 H	8.8898380	6.3219618	6.7602545
26 H	8.2747413	6.5890650	7.3990630
27 H	6.1371293	5.2947601	6.2740202
28 H	5.0984388	4.4662250	5.7355964

29 H	2.3096122 *	6.2935252	6.5804504
30 H	4.6330610	7.7702162	8.4684179
31 H	5.8166005	7.6549832	8.7556900
32 H	5.4657024	6.0081426	7.2919171
33 H	0.0000000	4.7303698	4.6611870
34 H	4.7303698	0.0000000	1.6672499 *
35 H	4.6611870	1.6672499 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.80 , TOTAL = 9213.6 SECONDS (153.6 MIN)
WALL CLOCK TIME: STEP = 0.81 , TOTAL = 8525.2 SECONDS (142.1 MIN)

CPU UTILIZATION: STEP = 99.13%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.11 , TOTAL = 9214.8 SECONDS (153.6 MIN)
WALL CLOCK TIME: STEP = 1.09 , TOTAL = 8526.3 SECONDS (142.1 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1 0	-284.636976517	-284.636976517	0.001374643	0.000110332	198408936
11313123					
2 1	-284.636977739	-0.000001222	0.000199230	0.000009859	138983343
16281915					
3 2	-284.636977734	0.000000005	0.000098650	0.000017466	119225384
17779071					
4 3	-284.636977761	-0.000000027	0.000065397	0.000004816	112558652
18229056					
5 4	-284.636977734	0.000000027	0.000040618	0.000007095	107055690
18682544					
6 5	-284.636977730	0.000000004	0.000021827	0.000002863	96302954
19405215					
7 6	-284.636977726	0.000000004	0.000017545	0.000003386	125430969
17342818					

8 7 -284.636977722 0.000000005 0.000015363 0.000001841 117185216
17926607

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 25.1 SECONDS (3.1 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 8.8 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 4.1, LAST ITERATION= 3.0
TIME TO SOLVE SCF EQUATIONS= 0.6 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369777216 AFTER 8 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6022321174
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998738534

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 26.95 , TOTAL = 9241.7 SECONDS (154.0 MIN)
WALL CLOCK TIME: STEP = 25.23 , TOTAL = 8551.6 SECONDS (142.5
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.61 , TOTAL = 9245.3 SECONDS (154.1 MIN)
WALL CLOCK TIME: STEP = 3.59 , TOTAL = 8555.2 SECONDS (142.6
MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.87 , TOTAL = 9248.2 SECONDS (154.1 MIN)

WALL CLOCK TIME: STEP = 2.72 , TOTAL = 8557.9 SECONDS (142.6 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

NSERCH=108 ENERGY= -284.6369777

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	-0.0000044	-0.0000254	0.0000040
2 C	6.0	-0.0000369	-0.0000263	0.0000023
3 C	6.0	-0.0000222	0.0000151	0.0000093
4 C	6.0	-0.0000015	0.0000106	0.0000436
5 C	6.0	-0.0000313	-0.0000035	0.0000006
6 C	6.0	-0.0000243	0.0000481	-0.0000337
7 C	6.0	-0.0000114	0.0000020	-0.0000007
8 C	6.0	-0.0000025	-0.0000165	0.0000304
9 C	6.0	0.0000273	0.0000255	0.0000503
10 C	6.0	0.0000572	0.0000079	0.0000078
11 C	6.0	0.0000338	0.0000233	-0.0000244
12 N	7.0	-0.0000144	0.0000111	0.0000164
13 C	6.0	0.0000243	-0.0000327	-0.0000189
14 C	6.0	-0.0000041	-0.0000073	-0.0000179
15 C	6.0	-0.0000095	0.0000010	0.0000028
16 C	6.0	0.0000091	-0.0000134	0.0000222
17 C	6.0	-0.0000009	0.0000150	0.0000080
18 C	6.0	0.0000109	-0.0000266	-0.0000147
19 C	6.0	0.0000024	-0.0000041	0.0000161
20 O	8.0	-0.0000290	-0.0001177	-0.0000230
21 N	7.0	-0.0000418	0.0000241	-0.0000104
22 H	1.0	0.0000126	-0.0000087	-0.0000606
23 H	1.0	-0.0000216	0.0000207	0.0000086
24 H	1.0	0.0000101	-0.0000045	0.0000686
25 H	1.0	0.0000299	-0.0000372	0.0000194
26 H	1.0	0.0000309	0.0000612	0.0000042
27 H	1.0	0.0000294	0.0000171	-0.0000591
28 H	1.0	-0.0000274	0.0000114	-0.0000121
29 H	1.0	0.0000432	-0.0000271	0.0000146
30 H	1.0	-0.0000169	0.0000219	0.0000111
31 H	1.0	-0.0000044	0.0000012	0.0000319
32 H	1.0	-0.0000196	0.0000061	-0.0000290
33 H	1.0	-0.0000131	-0.0000054	-0.0000193
34 H	1.0	0.0000296	0.0000204	-0.0000462
35 H	1.0	-0.0000134	0.0000125	-0.0000018

MAXIMUM GRADIENT = 0.0001177 RMS GRADIENT = 0.0000272
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0000004466
PREDICTED ENERGY CHANGE WAS -0.0000003560 RATIO= 1.255
GDIIS STEP HAS LENGTH = 0.005823
RADIUS OF STEP TAKEN= 0.00582 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.04 , TOTAL = 9248.2 SECONDS (154.1 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8557.9 SECONDS (142.6
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

INSERCH= 109

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1597344856	-1.7150969614	0.8965958199
C	6.0	4.9801961154	0.6149859956	0.5515483325
C	6.0	5.1720838432	-0.7267972443	0.1949320861
C	6.0	4.0287048610	-1.5388485310	-0.0940375550
C	6.0	2.7248069000	-1.0169822958	-0.0007468920
C	6.0	2.4655572882	0.3501773268	0.4340653799
C	6.0	3.6547244792	1.1748090333	0.6760822168
C	6.0	3.5190933881	2.5624317539	1.0523629772
C	6.0	2.2559897155	3.1469540830	1.2195867723
C	6.0	1.0837805772	2.3456396362	1.0483645146
C	6.0	1.1649096391	0.9903504922	0.6512858788
N	7.0	-0.0501824827	0.1927628280	0.6085150776
C	6.0	-1.2478317401	0.7134668077	0.3480384335
C	6.0	-2.5480726526	0.0415917047	0.4530635015
C	6.0	-2.8142446266	-1.2839936395	0.9422668905
C	6.0	-4.1106611407	-1.8194055193	1.0461637566
C	6.0	-5.2225979858	-1.0164538635	0.6473784168
C	6.0	-5.0136593159	0.3000660095	0.1490055145
C	6.0	-3.6985406856	0.8170174187	0.0577473766
O	8.0	-1.6907162982	-2.1312273503	1.3531045130
N	7.0	1.6097165074	-1.9396892015	-0.4277599234
H	1.0	5.8482360586	1.2705574859	0.7462812437
H	1.0	6.1863106901	-1.1549683668	0.1104977935
H	1.0	4.1832531555	-2.5837795173	-0.4279019394
H	1.0	4.4370386891	3.1543321377	1.2201533416
H	1.0	2.1572451706	4.2044213211	1.5223213270

H	1.0	0.1037365872	2.7968868289	1.2835294814
H	1.0	-1.2972329662	1.7661067395	0.0043718563
H	1.0	-4.2776524110	-2.8450322361	1.4274363794
H	1.0	-6.2443756660	-1.4302176901	0.7270133494
H	1.0	-5.8726715265	0.9208026170	-0.1608345156
H	1.0	-3.5392423727	1.8439896958	-0.3204348637
H	1.0	-2.0060811329	-2.9384874843	1.8352504215
H	1.0	1.2374846571	-1.6494377689	-1.3589605697
H	1.0	1.9971571952	-2.8958272454	-0.5533993935

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3651836	5.1568124	3.9976680
2 C	5.3651836	0.0000000	1.4015628 *	2.4415405 *
3 C	5.1568124	1.4015628 *	0.0000000	1.4318681 *
4 C	3.9976680	2.4415405 *	1.4318681 *	0.0000000
5 C	2.8057413 *	2.8381563 *	2.4721776 *	1.4075501 *
6 C	3.1298740	2.5312713 *	2.9227290 *	2.5081351 *
7 C	4.5403896	1.4442249 *	2.4799176 *	2.8455023 *
8 C	5.4412138	2.4855948 *	3.7797609	4.2888737
9 C	5.3045405	3.7786821	4.9557514	5.1792735
10 C	4.1673105	4.2923237	5.1848278	5.0066865
11 C	2.8965497 *	3.8350042	4.3834119	3.8927725
12 N	1.9408721 *	5.0483885	5.3187129	4.4865778
13 C	2.8600839 *	6.2321301	6.5812703	5.7541458
14 C	3.2580509	7.5507159	7.7625943	6.7860971
15 C	3.0054097	8.0319419	8.0405485	6.9256650
16 C	4.2742870	9.4241494	9.3855071	8.2236276
17 C	5.4332048	10.3328499	10.4085551	9.2956548
18 C	5.6021225	10.0069157	10.2374763	9.2306569
19 C	4.6905818	8.6951210	9.0050077	8.0798185
20 O	1.9508287 *	7.2584608	7.1001277	5.9293264
21 N	1.9765646 *	4.3411453	3.8143562	2.4745805 *
22 H	6.4261790	1.1050739 *	2.1795857 *	3.4510276
23 H	6.1033855	2.1867731 *	1.1041358 *	2.2010138 *
24 H	4.3240729	3.4389739	2.1941038 *	1.1078048 *
25 H	6.4893267	2.6814793 *	4.0809968	4.8907851
26 H	6.2787163	4.6685649	5.9302724	6.2530094
27 H	4.5288907	5.3922486	6.2681367	6.0084664
28 H	3.8778341	6.4055130	6.9356286	6.2688139
29 H	4.6096581	9.9220293	9.7623512	8.5449734
30 H	6.4126860	11.4107256	11.4504785	10.3064111
31 H	6.6675369	10.8805215	11.1726352	10.2025291

32 H	5.2754802	8.6516841	9.0973487	8.2926881
33 H	2.6586677 *	7.9424892	7.6881903	6.4884346
34 H	2.5006781 *	4.7734210	4.3297712	3.0664589
35 H	2.6215897 *	4.7376408	3.9172504	2.4858782 *

C C C C

1 CO	2.8057413 *	3.1298740	4.5403896	5.4412138
2 C	2.8381563 *	2.5312713 *	1.4442249 *	2.4855948 *
3 C	2.4721776 *	2.9227290 *	2.4799176 *	3.7797609
4 C	1.4075501 *	2.5081351 *	2.8455023 *	4.2888737
5 C	0.0000000	1.4578743 *	2.4752361 *	3.8147262
6 C	1.4578743 *	0.0000000	1.4672110 *	2.5271130 *
7 C	2.4752361 *	1.4672110 *	0.0000000	1.4441190 *
8 C	3.8147262	2.5271130 *	1.4441190 *	0.0000000
9 C	4.3643293	2.9125457 *	2.4781469 *	1.4018063 *
10 C	3.8859784	2.5037053 *	2.8494194 *	2.4449465 *
11 C	2.6244640 *	1.4658413 *	2.4967615 *	2.8591054 *
12 N	3.0879199	2.5266893 *	3.8334470	4.3072105
13 C	4.3471787	3.7321090	4.9351299	5.1612324
14 C	5.3972013	5.0231535	6.3094066	6.5972948
15 C	5.6250922	5.5502335	6.9256138	7.4106869
16 C	6.9615751	6.9518633	8.3308760	8.7985050
17 C	7.9737890	7.8115885	9.1438127	9.4546075
18 C	7.8511720	7.4848147	8.7283368	8.8736814
19 C	6.6802972	6.1931946	7.3878861	7.4919939
20 O	4.7509263	4.9271302	6.3215483	7.0187604
21 N	1.5090244 *	2.5920446 *	3.8859522	5.1093617
22 H	3.9429303	3.5195304	2.1967223 *	2.6809571 *
23 H	3.4660387	4.0266817	3.4866427	4.6712120
24 H	2.1827461 *	3.5073593	3.9528612	5.3959043
25 H	4.6714237	3.5168107	2.1969389 *	1.1050445 *
26 H	5.4685390	4.0167841	3.4838363	2.1844041 *
27 H	4.8026007	3.5051639	3.9509041	3.4311906
28 H	4.8910546	4.0432763	5.0321676	4.9929369
29 H	7.3767141	7.5277505	8.9244753	9.4958197
30 H	9.0081427	8.8948613	10.2362562	10.5533137
31 H	8.8146057	8.3788769	9.5674565	9.6110375
32 H	6.8938867	6.2336478	7.2934223	7.2263986
33 H	5.4262667	5.7248743	7.0927850	7.8358521
34 H	2.1111304 *	2.9532296 *	4.2380205	5.3628411
35 H	2.0892480 *	3.4250593	4.5639056	5.8895971

C C C N

1 CO	5.3045405	4.1673105	2.8965497 *	1.9408721 *
------	-----------	-----------	-------------	-------------

2 C	3.7786821	4.2923237	3.8350042	5.0483885
3 C	4.9557514	5.1848278	4.3834119	5.3187129
4 C	5.1792735	5.0066865	3.8927725	4.4865778
5 C	4.3643293	3.8859784	2.6244640 *	3.0879199
6 C	2.9125457 *	2.5037053 *	1.4658413 *	2.5266893 *
7 C	2.4781469 *	2.8494194 *	2.4967615 *	3.8334470
8 C	1.4018063 *	2.4449465 *	2.8591054 *	4.3072105
9 C	0.0000000	1.4302084 *	2.4828131 *	3.7972470
10 C	1.4302084 *	0.0000000	1.4145890 *	2.4726945 *
11 C	2.4828131 *	1.4145890 *	0.0000000	1.4541060 *
12 N	3.7972470	2.4726945 *	1.4541060 *	0.0000000
13 C	4.3541040	2.9310170 *	2.4474363 *	1.3316698 *
14 C	5.7714685	4.3420477	3.8374044	2.5072840 *
15 C	6.7392492	5.3272971	4.5924917	3.1515456
16 C	8.0764501	6.6580651	5.9901840	4.5527843
17 C	8.5785000	7.1578539	6.6953366	5.3120239
18 C	7.8802737	6.4939966	6.2372664	4.9858565
19 C	6.4988390	5.1174803	4.9025995	3.7421326
20 O	6.5919280	5.2757025	4.2885192	2.9405263 *
21 N	5.3856625	4.5628495	3.1539381	2.8942153 *
22 H	4.0803328	4.8935766	4.6926630	5.9976631
23 H	5.9316134	6.2585672	5.4871954	6.3998631
24 H	6.2665677	6.0071013	4.8009842	5.1677195
25 H	2.1810615 *	3.4536698	3.9639949	5.4111134
26 H	1.1043712 *	2.1981880 *	3.4747207	4.6691736
27 H	2.1814741 *	1.1042703 *	2.1884684 *	2.6945867 *
28 H	4.0011096	2.6636450 *	2.6612857 *	2.0965531 *
29 H	8.8676705	7.4720635	6.7032867	5.2697564
30 H	9.6669200	8.2499842	7.7950237	6.4043842
31 H	8.5402838	7.2030930	7.0846260	5.9180503
32 H	6.1362935	4.8474329	4.8787280	3.9702691
33 H	7.4549909	6.1715828	5.1858194	3.8903917
34 H	5.5400030	4.6668493	3.3188612	2.9870973 *
35 H	6.3028311	5.5563369	4.1528641	3.8834307

C C C C

1 CO	2.8600839 *	3.2580509	3.0054097	4.2742870
2 C	6.2321301	7.5507159	8.0319419	9.4241494
3 C	6.5812703	7.7625943	8.0405485	9.3855071
4 C	5.7541458	6.7860971	6.9256650	8.2236276
5 C	4.3471787	5.3972013	5.6250922	6.9615751
6 C	3.7321090	5.0231535	5.5502335	6.9518633
7 C	4.9351299	6.3094066	6.9256138	8.3308760
8 C	5.1612324	6.5972948	7.4106869	8.7985050
9 C	4.3541040	5.7714685	6.7392492	8.0764501

10	C	2.9310170 *	4.3420477	5.3272971	6.6580651
11	C	2.4474363 *	3.8374044	4.5924917	5.9901840
12	N	1.3316698 *	2.5072840 *	3.1515456	4.5527843
13	C	0.0000000	1.4673353 *	2.6070299 *	3.8856934
14	C	1.4673353 *	0.0000000	1.4378261 *	2.5013519 *
15	C	2.6070299 *	1.4378261 *	0.0000000	1.4064694 *
16	C	3.8856934	2.5013519 *	1.4064694 *	0.0000000
17	C	4.3452269	2.8827599 *	2.4410454 *	1.4283433 *
18	C	3.7936752	2.4976745 *	2.8241695 *	2.4723386 *
19	C	2.4700134 *	1.4426145 *	2.4451179 *	2.8456170 *
20	O	3.0493589	2.5032532 *	1.4659156 *	2.4591825 *
21	N	3.9757618	4.6891934	4.6774290	5.9084380
22	H	7.1290340	8.4908382	9.0334220	10.4315595
23	H	7.6690253	8.8226164	9.0398276	10.3607228
24	H	6.4008281	7.2786964	7.2478811	8.4584958
25	H	6.2478924	7.6856594	8.5062957	9.8909813
26	H	5.0159997	6.3727921	7.4279790	8.7063118
27	H	2.6537746 *	3.9132362	5.0283854	6.2552095
28	H	1.1084214 *	2.1771257 *	3.5332823	4.6751050
29	H	4.7966476	3.5033479	2.1940358 *	1.1068717 *
30	H	5.4501795	3.9879728	3.4399876	2.1922732 *
31	H	4.6573687	3.4932564	3.9283501	3.4742288
32	H	2.6411174 *	2.1975795 *	3.4502634	3.9515283
33	H	4.0154093	3.3294245	2.0464354 *	2.5108284 *
34	H	3.8306607	4.5247603	4.6739392	5.8665301
35	H	4.9365521	5.5045901	5.2900485	6.4048990

C C C O

1	CO	5.4332048	5.6021225	4.6905818	1.9508287 *
2	C	10.3328499	10.0069157	8.6951210	7.2584608
3	C	10.4085551	10.2374763	9.0050077	7.1001277
4	C	9.2956548	9.2306569	8.0798185	5.9293264
5	C	7.9737890	7.8511720	6.6802972	4.7509263
6	C	7.8115885	7.4848147	6.1931946	4.9271302
7	C	9.1438127	8.7283368	7.3878861	6.3215483
8	C	9.4546075	8.8736814	7.4919939	7.0187604
9	C	8.5785000	7.8802737	6.4988390	6.5919280
10	C	7.1578539	6.4939966	5.1174803	5.2757025
11	C	6.6953366	6.2372664	4.9025995	4.2885192
12	N	5.3120239	4.9858565	3.7421326	2.9405263 *
13	C	4.3452269	3.7936752	2.4700134 *	3.0493589
14	C	2.8827599 *	2.4976745 *	1.4426145 *	2.5032532 *
15	C	2.4410454 *	2.8241695 *	2.4451179 *	1.4659156 *
16	C	1.4283433 *	2.4723386 *	2.8456170 *	2.4591825 *
17	C	0.0000000	1.4231147 *	2.4560196 *	3.7702729

18 C	1.4231147 *	0.0000000	1.4160169 *	4.2898709
19 C	2.4560196 *	1.4160169 *	0.0000000	3.7949250
20 O	3.7702729	4.2898709	3.7949250	0.0000000
21 N	6.9777365	7.0155733	6.0010618	3.7551327
22 H	11.3050241	10.9215092	9.5823131	8.2931404
23 H	11.4223738	11.2941549	10.0797717	8.0339721
24 H	9.5959769	9.6557023	8.5979038	6.1546978
25 H	10.5371774	9.9302510	8.5441137	8.0934663
26 H	9.0821334	8.2796049	6.9216840	7.4145725
27 H	6.5814964	5.8059452	4.4586699	5.2451131
28 H	4.8543374	3.9977518	2.5826146 *	4.1428398
29 H	2.2011614 *	3.4738645	3.9524709	2.6846380 *
30 H	1.1052474 *	2.2005993 *	3.4611065	4.6496471
31 H	2.1974454 *	1.1041815 *	2.1875544 *	5.3940382
32 H	3.4572368	2.1858591 *	1.1059249 *	4.6925615
33 H	3.9308057	4.7304521	4.4863965	0.9917603 *
34 H	6.7940218	6.7194738	5.6969122	4.0201715
35 H	7.5563732	7.7368375	6.8263966	4.2213483

N H H H

1 CO	1.9765646 *	6.4261790	6.1033855	4.3240729
2 C	4.3411453	1.1050739 *	2.1867731 *	3.4389739
3 C	3.8143562	2.1795857 *	1.1041358 *	2.1941038 *
4 C	2.4745805 *	3.4510276	2.2010138 *	1.1078048 *
5 C	1.5090244 *	3.9429303	3.4660387	2.1827461 *
6 C	2.5920446 *	3.5195304	4.0266817	3.5073593
7 C	3.8859522	2.1967223 *	3.4866427	3.9528612
8 C	5.1093617	2.6809571 *	4.6712120	5.3959043
9 C	5.3856625	4.0803328	5.9316134	6.2665677
10 C	4.5628495	4.8935766	6.2585672	6.0071013
11 C	3.1539381	4.6926630	5.4871954	4.8009842
12 N	2.8942153 *	5.9976631	6.3998631	5.1677195
13 C	3.9757618	7.1290340	7.6690253	6.4008281
14 C	4.6891934	8.4908382	8.8226164	7.2786964
15 C	4.6774290	9.0334220	9.0398276	7.2478811
16 C	5.9084380	10.4315595	10.3607228	8.4584958
17 C	6.9777365	11.3050241	11.4223738	9.5959769
18 C	7.0155733	10.9215092	11.2941549	9.6557023
19 C	6.0010618	9.5823131	10.0797717	8.5979038
20 O	3.7551327	8.2931404	8.0339721	6.1546978
21 N	0.0000000	5.4450991	4.6744756	2.6529122 *
22 H	5.4450991	0.0000000	2.5301563 *	4.3596775
23 H	4.6744756	2.5301563 *	0.0000000	2.5186534 *
24 H	2.6529122 *	4.3596775	2.5186534 *	0.0000000
25 H	6.0546199	2.4009664 *	4.7813553	5.9754848

26 H	6.4693662	4.7784107	6.8519831	7.3476357
27 H	5.2565806	5.9680475	7.3478480	6.9658469
28 H	4.7296952	7.2009531	8.0341377	7.0102852
29 H	6.2387909	10.9515144	10.6810658	8.6658789
30 H	7.9548618	12.3905535	12.4490087	10.5546188
31 H	8.0149731	11.7611590	12.2393422	10.6524665
32 H	6.3905807	9.4652765	10.1865517	8.9024506
33 H	4.3809595	8.9773165	8.5598479	6.5996618
34 H	1.0440005 *	5.8495678	5.1860088	3.2276023
35 H	1.0392764 *	5.8205446	4.5847962	2.2118180 *

H H H H

1 CO	6.4893267	6.2787163	4.5288907	3.8778341
2 C	2.6814793 *	4.6685649	5.3922486	6.4055130
3 C	4.0809968	5.9302724	6.2681367	6.9356286
4 C	4.8907851	6.2530094	6.0084664	6.2688139
5 C	4.6714237	5.4685390	4.8026007	4.8910546
6 C	3.5168107	4.0167841	3.5051639	4.0432763
7 C	2.1969389 *	3.4838363	3.9509041	5.0321676
8 C	1.1050445 *	2.1844041 *	3.4311906	4.9929369
9 C	2.1810615 *	1.1043712 *	2.1814741 *	4.0011096
10 C	3.4536698	2.1981880 *	1.1042703 *	2.6636450 *
11 C	3.9639949	3.4747207	2.1884684 *	2.6612857 *
12 N	5.4111134	4.6691736	2.6945867 *	2.0965531 *
13 C	6.2478924	5.0159997	2.6537746 *	1.1084214 *
14 C	7.6856594	6.3727921	3.9132362	2.1771257 *
15 C	8.5062957	7.4279790	5.0283854	3.5332823
16 C	9.8909813	8.7063118	6.2552095	4.6751050
17 C	10.5371774	9.0821334	6.5814964	4.8543374
18 C	9.9302510	8.2796049	5.8059452	3.9977518
19 C	8.5441137	6.9216840	4.4586699	2.5826146 *
20 O	8.0934663	7.4145725	5.2451131	4.1428398
21 N	6.0546199	6.4693662	5.2565806	4.7296952
22 H	2.4009664 *	4.7784107	5.9680475	7.2009531
23 H	4.7813553	6.8519831	7.3478480	8.0341377
24 H	5.9754848	7.3476357	6.9658469	7.0102852
25 H	0.0000000	2.5281320 *	4.3484814	6.0238829
26 H	2.5281320 *	0.0000000	2.5010143 *	4.4925458
27 H	4.3484814	2.5010143 *	0.0000000	2.1590432 *
28 H	6.0238829	4.4925458	2.1590432 *	0.0000000
29 H	10.5821161	9.5452452	7.1448254	5.6719146
30 H	11.6341694	10.1473595	7.6470028	5.9340476
31 H	10.6388865	8.8371221	6.4283227	4.6557996
32 H	8.2286979	6.4356319	4.0929220	2.2667535 *
33 H	8.8890150	8.2735939	6.1359796	5.0978220

34 H	6.3218019	6.5890372	5.2950865	4.4664766
35 H	6.7603949	7.3991739	6.2742603	5.7356555

H H H H

1 CO	4.6096581	6.4126860	6.6675369	5.2754802
2 C	9.9220293	11.4107256	10.8805215	8.6516841
3 C	9.7623512	11.4504785	11.1726352	9.0973487
4 C	8.5449734	10.3064111	10.2025291	8.2926881
5 C	7.3767141	9.0081427	8.8146057	6.8938867
6 C	7.5277505	8.8948613	8.3788769	6.2336478
7 C	8.9244753	10.2362562	9.5674565	7.2934223
8 C	9.4958197	10.5533137	9.6110375	7.2263986
9 C	8.8676705	9.6669200	8.5402838	6.1362935
10 C	7.4720635	8.2499842	7.2030930	4.8474329
11 C	6.7032867	7.7950237	7.0846260	4.8787280
12 N	5.2697564	6.4043842	5.9180503	3.9702691
13 C	4.7966476	5.4501795	4.6573687	2.6411174 *
14 C	3.5033479	3.9879728	3.4932564	2.1975795 *
15 C	2.1940358 *	3.4399876	3.9283501	3.4502634
16 C	1.1068717 *	2.1922732 *	3.4742288	3.9515283
17 C	2.2011614 *	1.1052474 *	2.1974454 *	3.4572368
18 C	3.4738645	2.2005993 *	1.1041815 *	2.1858591 *
19 C	3.9524709	3.4611065	2.1875544 *	1.1059249 *
20 O	2.6846380 *	4.6496471	5.3940382	4.6925615
21 N	6.2387909	7.9548618	8.0149731	6.3905807
22 H	10.9515144	12.3905535	11.7611590	9.4652765
23 H	10.6810658	12.4490087	12.2393422	10.1865517
24 H	8.6658789	10.5546188	10.6524665	8.9024506
25 H	10.5821161	11.6341694	10.6388865	8.2286979
26 H	9.5452452	10.1473595	8.8371221	6.4356319
27 H	7.1448254	7.6470028	6.4283227	4.0929220
28 H	5.6719146	5.9340476	4.6557996	2.2667535 *
29 H	0.0000000	2.5219621 *	4.3872774	5.0583821
30 H	2.5219621 *	0.0000000	2.5404201 *	4.3743946
31 H	4.3872774	2.5404201 *	0.0000000	2.5144857 *
32 H	5.0583821	4.3743946	2.5144857 *	0.0000000
33 H	2.3097797 *	4.6331639	5.8162700	5.4653134
34 H	6.2936628	7.7703011	7.6548000	6.0083019
35 H	6.5802375	8.4681953	8.7552827	7.2919035

H H H

1 CO	2.6586677 *	2.5006781 *	2.6215897 *
2 C	7.9424892	4.7734210	4.7376408
3 C	7.6881903	4.3297712	3.9172504

4 C	6.4884346	3.0664589	2.4858782 *
5 C	5.4262667	2.1111304 *	2.0892480 *
6 C	5.7248743	2.9532296 *	3.4250593
7 C	7.0927850	4.2380205	4.5639056
8 C	7.8358521	5.3628411	5.8895971
9 C	7.4549909	5.5400030	6.3028311
10 C	6.1715828	4.6668493	5.5563369
11 C	5.1858194	3.3188612	4.1528641
12 N	3.8903917	2.9870973 *	3.8834307
13 C	4.0154093	3.8306607	4.9365521
14 C	3.3294245	4.5247603	5.5045901
15 C	2.0464354 *	4.6739392	5.2900485
16 C	2.5108284 *	5.8665301	6.4048990
17 C	3.9308057	6.7940218	7.5563732
18 C	4.7304521	6.7194738	7.7368375
19 C	4.4863965	5.6969122	6.8263966
20 O	0.9917603 *	4.0201715	4.2213483
21 N	4.3809595	1.0440005 *	1.0392764 *
22 H	8.9773165	5.8495678	5.8205446
23 H	8.5598479	5.1860088	4.5847962
24 H	6.5996618	3.2276023	2.2118180 *
25 H	8.8890150	6.3218019	6.7603949
26 H	8.2735939	6.5890372	7.3991739
27 H	6.1359796	5.2950865	6.2742603
28 H	5.0978220	4.4664766	5.7356555
29 H	2.3097797 *	6.2936628	6.5802375
30 H	4.6331639	7.7703011	8.4681953
31 H	5.8162700	7.6548000	8.7552827
32 H	5.4653134	6.0083019	7.2919035
33 H	0.0000000	4.7313161	4.6619079
34 H	4.7313161	0.0000000	1.6671886 *
35 H	4.6619079	1.6671886 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.82 , TOTAL = 9249.0 SECONDS (154.2 MIN)
WALL CLOCK TIME: STEP = 0.82 , TOTAL = 8558.7 SECONDS (142.6 MIN)
CPU UTILIZATION: STEP = 99.48% , TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.09 , TOTAL = 9250.1 SECONDS (154.2 MIN)

WALL CLOCK TIME: STEP = 1.08 , TOTAL = 8559.8 SECONDS (142.7 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS
ITER EX TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
INTEGRALS SKIPPED

-----START SECOND ORDER SCF-----

1	0	-284.636977318	-284.636977318	0.001849010	0.000097211	198406038
11313283						
2	1	-284.636978190	-0.000000872	0.000143958	0.000007047	137026776
16430027						
3	2	-284.636978185	0.000000005	0.000101450	0.000017062	117830164
17902105						
4	3	-284.636978179	0.000000006	0.000078345	0.000006517	111490732
18339217						
5	4	-284.636978137	0.000000041	0.000036590	0.000010141	107381116
18664944						
6	5	-284.636978135	0.000000002	0.000033472	0.000002271	97899764
19314324						
7	6	-284.636978144	-0.000000008	0.000025249	0.000002750	100197609
19157690						
8	7	-284.636978137	0.000000007	0.000022968	0.000002088	90634516
19845725						
9	8	-284.636978142	-0.000000006	0.000023328	0.000002076	125386701
17335989						
10	9	-284.636978142	0.000000000	0.000041351	0.000002011	146091578
15760972						

-----DISABLING FDIFF OPTION-----

11	10	-284.636978202	-0.000000061	0.000063270	0.000001664	198405243
11313375						
12	11	-284.636978203	0.000000000	0.000051511	0.000001820	198405181
11313373						
13	12	-284.636978203	0.000000000	0.000016393	0.000001423	198405239
11313363						
14	13	-284.636978203	0.000000000	0.000043960	0.000000585	198405251
11313361						
15	14	-284.636978203	0.000000000	0.000014319	0.000000489	198405220
11313366						
16	15	-284.636978203	0.000000000	0.000004008	0.000000406	198405184
11313372						

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 51.7 SECONDS (3.2 SEC/ITER)
OF THE ABOVE TIME, DFT PART= 17.4 SECONDS (1.1 SEC/ITER)
FOCK TIME ON FIRST ITERATION= 3.9, LAST ITERATION= 3.3
TIME TO SOLVE SCF EQUATIONS= 1.7 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369782029 AFTER 16 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6021450076
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998736496

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 54.98 , TOTAL = 9305.1 SECONDS (155.1 MIN)
WALL CLOCK TIME: STEP = 50.86 , TOTAL = 8610.7 SECONDS (143.5
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 3.77 , TOTAL = 9308.9 SECONDS (155.1 MIN)
WALL CLOCK TIME: STEP = 3.75 , TOTAL = 8614.4 SECONDS (143.6
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:
CPU TIME: STEP = 2.93 , TOTAL = 9311.8 SECONDS (155.2 MIN)
WALL CLOCK TIME: STEP = 2.73 , TOTAL = 8617.2 SECONDS (143.6
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH=109 ENERGY= -284.6369782

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 CO	27.0	0.0000007	-0.0000384	-0.0000041
2 C	6.0	-0.0000324	-0.0000321	0.0000198
3 C	6.0	-0.0000135	0.0000041	0.0000062
4 C	6.0	0.0000009	0.0000129	-0.0000229
5 C	6.0	-0.0000039	0.0000191	0.0000123
6 C	6.0	-0.0000257	0.0000297	-0.0000073
7 C	6.0	-0.0000360	0.0000283	0.0000023
8 C	6.0	0.0000063	-0.0000157	-0.0000104
9 C	6.0	0.0000076	0.0000266	0.0000031
10 C	6.0	0.0000397	-0.0000204	0.0000275
11 C	6.0	0.0000372	0.0000268	-0.0000037
12 N	7.0	-0.0000126	0.0000254	0.0000139
13 C	6.0	0.0000552	-0.0000232	-0.0000216
14 C	6.0	0.0000114	-0.0000100	-0.0000129
15 C	6.0	-0.0000016	0.0000150	-0.0000130
16 C	6.0	-0.0000137	-0.0000081	0.0000070
17 C	6.0	-0.0000026	0.0000085	0.0000215
18 C	6.0	0.0000273	-0.0000511	0.0000003
19 C	6.0	0.0000081	0.0000031	-0.0000020
20 O	8.0	-0.0000056	-0.0001049	-0.0000219
21 N	7.0	-0.0000326	0.0000302	-0.0000028
22 H	1.0	0.0000082	0.0000016	-0.0000609
23 H	1.0	-0.0000117	0.0000022	0.0000187
24 H	1.0	0.0000172	-0.0000193	0.0000824
25 H	1.0	0.0000323	-0.0000459	0.0000357
26 H	1.0	0.0000331	0.0000620	0.0000246
27 H	1.0	0.0000075	0.0000470	-0.0000540
28 H	1.0	-0.0000263	-0.0000049	-0.0000034
29 H	1.0	0.0000329	-0.0000297	0.0000193
30 H	1.0	-0.0000566	0.0000112	0.0000130
31 H	1.0	-0.0000094	-0.0000056	0.0000274
32 H	1.0	-0.0000160	0.0000041	-0.0000127
33 H	1.0	-0.0000221	0.0000354	-0.0000309
34 H	1.0	0.0000358	0.0000153	-0.0000411
35 H	1.0	-0.0000387	0.0000008	-0.0000090

MAXIMUM GRADIENT = 0.0001049 RMS GRADIENT = 0.0000278
 HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0000004813
 PREDICTED ENERGY CHANGE WAS -0.0000003381 RATIO= 1.424

GDIIS STEP HAS LENGTH = 0.012781
RADIUS OF STEP TAKEN= 0.01278 CURRENT TRUST RADIUS= 0.05000

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.02 , TOTAL = 9311.8 SECONDS (155.2 MIN)
WALL CLOCK TIME: STEP = 0.02 , TOTAL = 8617.2 SECONDS (143.6 MIN)
CPU UTILIZATION: STEP = 80.90%, TOTAL = 100.00%

INSERCH= 110

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.1596841167	-1.7149970402	0.8965027875
C	6.0	4.9802664340	0.6147131425	0.5514391919
C	6.0	5.1720179545	-0.7270268484	0.1945093316
C	6.0	4.0285658312	-1.5388511176	-0.0949443459
C	6.0	2.7247000188	-1.0169757205	-0.0011884160
C	6.0	2.4655475047	0.3500358959	0.4343569907
C	6.0	3.6548401040	1.1746264956	0.6760492592
C	6.0	3.5192207504	2.5623322217	1.0521038981
C	6.0	2.2560889860	3.1467777057	1.2195661789
C	6.0	1.0837167190	2.3455690774	1.0490688395
C	6.0	1.1648482648	0.9902371361	0.6520488852
N	7.0	-0.0502444270	0.1928296652	0.6090908051
C	6.0	-1.2478565740	0.7137795684	0.3488309044
C	6.0	-2.5481174225	0.0418376775	0.4533403641
C	6.0	-2.8141765919	-1.2836339390	0.9428062009
C	6.0	-4.1104392170	-1.8195134178	1.0461031031
C	6.0	-5.2224205206	-1.0170765947	0.6464188720
C	6.0	-5.0135767940	0.2993782607	0.1478461451
C	6.0	-3.6985671901	0.8167742798	0.0571646770
O	8.0	-1.6905150214	-2.1299251671	1.3549050955
N	7.0	1.6094051906	-1.9394348597	-0.4282212923
H	1.0	5.8482429134	1.2701927713	0.7466759637
H	1.0	6.1861656807	-1.1554552093	0.1102377535
H	1.0	4.1829886945	-2.5836701215	-0.4292190095
H	1.0	4.4370962430	3.1544067599	1.2197836069
H	1.0	2.1574786564	4.2041423534	1.5225517350
H	1.0	0.1038675619	2.7969373819	1.2849518078
H	1.0	-1.2969452572	1.7664902362	0.0053840987
H	1.0	-4.2774911814	-2.8449681230	1.4277509449
H	1.0	-6.2441024528	-1.4311592802	0.7257222330
H	1.0	-5.8725682992	0.9196532662	-0.1628324871

H	1.0	-3.5393915532	1.8438028245	-0.3209303276
H	1.0	-2.0057500184	-2.9363198441	1.8385518795
H	1.0	1.2368885182	-1.6487737587	-1.3591819991
H	1.0	1.9965293778	-2.8956306780	-0.5543566756

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C	
1	CO	0.0000000	5.3651312	5.1567791	3.9977794
2	C	5.3651312	0.0000000	1.4015826 *	2.4415947 *
3	C	5.1567791	1.4015826 *	0.0000000	1.4318955 *
4	C	3.9977794	2.4415947 *	1.4318955 *	0.0000000
5	C	2.8057779 *	2.8382011 *	2.4721919 *	1.4075547 *
6	C	3.1296878	2.5313185 *	2.9227681 *	2.5082026 *
7	C	4.5403347	1.4442249 *	2.4799183 *	2.8455338 *
8	C	5.4411620	2.4856669 *	3.7798267	4.2889226
9	C	5.3043508	3.7787415	4.9557790	5.1792596
10	C	4.1671705	4.2926213	5.1851060	5.0069574
11	C	2.8962743 *	3.8351736	4.3835770	3.8929635
12	N	1.9407417 *	5.0484997	5.3188380	4.4867669
13	C	2.8600824 *	6.2322051	6.5813773	5.7542953
14	C	3.2580746	7.5507863	7.7626436	6.7861591
15	C	3.0053395	8.0318262	8.0404641	6.9256903
16	C	4.2740212	9.4239631	9.3852411	8.2233913
17	C	5.4329260	10.3327915	10.4082997	9.2953008
18	C	5.6018589	10.0069589	10.2372860	9.2302967
19	C	4.6904645	8.6952452	9.0049690	8.0796468
20	O	1.9507780 *	7.2579558	7.0999296	5.9295293
21	N	1.9766025 *	4.3412109	3.8144379	2.4746473 *
22	H	6.4260024	1.1050584 *	2.1796914 *	3.4511269
23	H	6.1032598	2.1868580 *	1.1041504 *	2.2009837 *
24	H	4.3242469	3.4390402	2.1941605 *	1.1078054 *
25	H	6.4893650	2.6817460 *	4.0812773	4.8910200
26	H	6.2784816	4.6685322	5.9302254	6.2529381
27	H	4.5289690	5.3925327	6.2684557	6.0088628
28	H	3.8777075	6.4053223	6.9354799	6.2686853
29	H	4.6095102	9.9218644	9.7621608	8.5448889
30	H	6.4123484	11.4106277	11.4501439	10.3059597
31	H	6.6672065	10.8805880	11.1723827	10.2020248
32	H	5.2754489	8.6519514	9.0974446	8.2926109
33	H	2.6586069 *	7.9417202	7.6879259	6.4887822
34	H	2.5005737 *	4.7735442	4.3299905	3.0665684
35	H	2.6216196 *	4.7379305	3.9175720	2.4861783 *

	C	C	C	C
1 CO	2.8057779 *	3.1296878	4.5403347	5.4411620
2 C	2.8382011 *	2.5313185 *	1.4442249 *	2.4856669 *
3 C	2.4721919 *	2.9227681 *	2.4799183 *	3.7798267
4 C	1.4075547 *	2.5082026 *	2.8455338 *	4.2889226
5 C	0.0000000	1.4579371 *	2.4752640 *	3.8147258
6 C	1.4579371 *	0.0000000	1.4672361 *	2.5270721 *
7 C	2.4752640 *	1.4672361 *	0.0000000	1.4441388 *
8 C	3.8147258	2.5270721 *	1.4441388 *	0.0000000
9 C	4.3642503	2.9124201 *	2.4781638 *	1.4018281 *
10 C	3.8862030	2.5038929 *	2.8497238 *	2.4451330 *
11 C	2.6246447 *	1.4659693 *	2.4969251 *	2.8591252 *
12 N	3.0881040	2.5267479 *	3.8335440	4.3071899
13 C	4.3473248	3.7321568	4.9351683	5.1610819
14 C	5.3972480	5.0231646	6.3094764	6.5972724
15 C	5.6250677	5.5500346	6.9254878	7.4104874
16 C	6.9613228	6.9516026	8.3307489	8.7984270
17 C	7.9734635	7.8114544	9.1438611	9.4547893
18 C	7.8508552	7.4847816	8.7284884	8.8739662
19 C	6.6801501	6.1932567	7.3880766	7.4922186
20 O	4.7509757	4.9265070	6.3208962	7.0178569
21 N	1.5090297 *	2.5920450 *	3.8859485	5.1092725
22 H	3.9429635	3.5194971	2.1966194 *	2.6809056 *
23 H	3.4660261	4.0267302	3.4866936	4.6713649
24 H	2.1827385 *	3.5074205	3.9528916	5.3959471
25 H	4.6715635	3.5168729	2.1970666 *	1.1050630 *
26 H	5.4684182	4.0166168	3.4837658	2.1843084 *
27 H	4.8030045	3.5054772	3.9512101	3.4313110
28 H	4.8909464	4.0431068	5.0319253	4.9924385
29 H	7.3765917	7.5275131	8.9243530	9.4957214
30 H	9.0077392	8.8946924	10.2362909	10.5535292
31 H	8.8141751	8.3788588	9.5676666	9.6114601
32 H	6.8938474	6.2338665	7.2937463	7.2267223
33 H	5.4263877	5.7240195	7.0917962	7.8344736
34 H	2.1111368 *	2.9532398 *	4.2379529	5.3625324
35 H	2.0893951 *	3.4251838	4.5640866	5.8897083

	C	C	C	N
1 CO	5.3043508	4.1671705	2.8962743 *	1.9407417 *
2 C	3.7787415	4.2926213	3.8351736	5.0484997
3 C	4.9557790	5.1851060	4.3835770	5.3188380
4 C	5.1792596	5.0069574	3.8929635	4.4867669
5 C	4.3642503	3.8862030	2.6246447 *	3.0881040
6 C	2.9124201 *	2.5038929 *	1.4659693 *	2.5267479 *

7 C	2.4781638 *	2.8497238 *	2.4969251 *	3.8335440
8 C	1.4018281 *	2.4451330 *	2.8591252 *	4.3071899
9 C	0.0000000	1.4301963 *	2.4826497 *	3.7970598
10 C	1.4301963 *	0.0000000	1.4146137 *	2.4725969 *
11 C	2.4826497 *	1.4146137 *	0.0000000	1.4540132 *
12 N	3.7970598	2.4725969 *	1.4540132 *	0.0000000
13 C	4.3537678	2.9307515 *	2.4473485 *	1.3316902 *
14 C	5.7713217	4.3419224	3.8373247	2.5072747 *
15 C	6.7388973	5.3269108	4.5921311	3.1512905
16 C	8.0763122	6.6578658	5.9898777	4.5525472
17 C	8.5787111	7.1579941	6.6952627	5.3119368
18 C	7.8806287	6.4943119	6.2373426	4.9858567
19 C	6.4990787	5.1177463	4.9027326	3.7422170
20 O	6.5907202	5.2744617	4.2874840	2.9397137 *
21 N	5.3854398	4.5628931	3.1539804	2.8943057 *
22 H	4.0802899	4.8937292	4.6927087	5.9976490
23 H	5.9317215	6.2588785	5.4873658	6.3999639
24 H	6.2665355	6.0073472	4.8011587	5.1679107
25 H	2.1810206 *	3.4537684	3.9640333	5.4111099
26 H	1.1043298 *	2.1980549 *	3.4745182	4.6689487
27 H	2.1814492 *	1.1043000 *	2.1887010 *	2.6947942 *
28 H	4.0004355	2.6631113 *	2.6610471 *	2.0964571 *
29 H	8.8674703	7.4717887	6.7029525	5.2695384
30 H	9.6671942	8.2501614	7.7949432	6.4042814
31 H	8.5408535	7.2035992	7.0847897	5.9180735
32 H	6.1366496	4.8478652	4.8790506	3.9704911
33 H	7.4532202	6.1698005	5.1844317	3.8893641
34 H	5.5394969	4.6666807	3.3188278	2.9870240 *
35 H	6.3027671	5.5564715	4.1529600	3.8834882

C C C C

1 CO	2.8600824 *	3.2580746	3.0053395	4.2740212
2 C	6.2322051	7.5507863	8.0318262	9.4239631
3 C	6.5813773	7.7626436	8.0404641	9.3852411
4 C	5.7542953	6.7861591	6.9256903	8.2233913
5 C	4.3473248	5.3972480	5.6250677	6.9613228
6 C	3.7321568	5.0231646	5.5500346	6.9516026
7 C	4.9351683	6.3094764	6.9254878	8.3307489
8 C	5.1610819	6.5972724	7.4104874	8.7984270
9 C	4.3537678	5.7713217	6.7388973	8.0763122
10 C	2.9307515 *	4.3419224	5.3269108	6.6578658
11 C	2.4473485 *	3.8373247	4.5921311	5.9898777
12 N	1.3316902 *	2.5072747 *	3.1512905	4.5525472
13 C	0.0000000	1.4673467 *	2.6068805 *	3.8856327
14 C	1.4673467 *	0.0000000	1.4377897 *	2.5013686 *

15 C	2.6068805 *	1.4377897 *	0.0000000	1.4064615 *
16 C	3.8856327	2.5013686 *	1.4064615 *	0.0000000
17 C	4.3452940	2.8827896 *	2.4410115 *	1.4283399 *
18 C	3.7937807	2.4976276 *	2.8240486 *	2.4722914 *
19 C	2.4701538 *	1.4425729 *	2.4450404 *	2.8456371 *
20 O	3.0487355	2.5029692 *	1.4658273 *	2.4592168 *
21 N	3.9758397	4.6890922	4.6773782	5.9080144
22 H	7.1289904	8.4908050	9.0331617	10.4312651
23 H	7.6691363	8.8226374	9.0396770	10.3603518
24 H	6.4009856	7.2787356	7.2479562	8.4582183
25 H	6.2477122	7.6856185	8.5061084	9.8909256
26 H	5.0156317	6.3726468	7.4275938	8.7062177
27 H	2.6538702 *	3.9134609	5.0282311	6.2553216
28 H	1.1084066 *	2.1772742 *	3.5332717	4.6752825
29 H	4.7966071	3.5034065	2.1941343 *	1.1068508 *
30 H	5.4502553	3.9880092	3.4399536	2.1922549 *
31 H	4.6574824	3.4931652	3.9281893	3.4741414
32 H	2.6413378 *	2.1975436 *	3.4501924	3.9515518
33 H	4.0145855	3.3290232	2.0462855 *	2.5109656 *
34 H	3.8305254	4.5243424	4.6737143	5.8658727
35 H	4.9365606	5.5043608	5.2898887	6.4042615

C C C O

1 CO	5.4329260	5.6018589	4.6904645	1.9507780 *
2 C	10.3327915	10.0069589	8.6952452	7.2579558
3 C	10.4082997	10.2372860	9.0049690	7.0999296
4 C	9.2953008	9.2302967	8.0796468	5.9295293
5 C	7.9734635	7.8508552	6.6801501	4.7509757
6 C	7.8114544	7.4847816	6.1932567	4.9265070
7 C	9.1438611	8.7284884	7.3880766	6.3208962
8 C	9.4547893	8.8739662	7.4922186	7.0178569
9 C	8.5787111	7.8806287	6.4990787	6.5907202
10 C	7.1579941	6.4943119	5.1177463	5.2744617
11 C	6.6952627	6.2373426	4.9027326	4.2874840
12 N	5.3119368	4.9858567	3.7422170	2.9397137 *
13 C	4.3452940	3.7937807	2.4701538 *	3.0487355
14 C	2.8827896 *	2.4976276 *	1.4425729 *	2.5029692 *
15 C	2.4410115 *	2.8240486 *	2.4450404 *	1.4658273 *
16 C	1.4283399 *	2.4722914 *	2.8456371 *	2.4592168 *
17 C	0.0000000	1.4231106 *	2.4560860 *	3.7702442
18 C	1.4231106 *	0.0000000	1.4160410 *	4.2896674
19 C	2.4560860 *	1.4160410 *	0.0000000	3.7946596
20 O	3.7702442	4.2896674	3.7946596	0.0000000
21 N	6.9770652	7.0148434	6.0005716	3.7557023
22 H	11.3049211	10.9215478	9.5824108	8.2923830

23 H	11.4220172	11.2939004	10.0797048	8.0337343
24 H	9.5954643	9.6551431	8.5975877	6.1552440
25 H	10.5373756	9.9305316	8.5443097	8.0925918
26 H	9.0824913	8.2801591	6.9220586	7.4132026
27 H	6.5820796	5.8068104	4.4594862	5.2439181
28 H	4.8547426	3.9982575	2.5831046 *	4.1422406
29 H	2.2010358 *	3.4737433	3.9524698	2.6849653 *
30 H	1.1052545 *	2.2006577 *	3.4612027	4.6496563
31 H	2.1973854 *	1.1041416 *	2.1875246 *	5.3937951
32 H	3.4573085	2.1859142 *	1.1059296 *	4.6922578
33 H	3.9308580	4.7302484	4.4860546	0.9917458 *
34 H	6.7929485	6.7182399	5.6959361	4.0208789
35 H	7.5553997	7.7358102	6.8256893	4.2220708

N H H H

1 CO	1.9766025 *	6.4260024	6.1032598	4.3242469
2 C	4.3412109	1.1050584 *	2.1868580 *	3.4390402
3 C	3.8144379	2.1796914 *	1.1041504 *	2.1941605 *
4 C	2.4746473 *	3.4511269	2.2009837 *	1.1078054 *
5 C	1.5090297 *	3.9429635	3.4660261	2.1827385 *
6 C	2.5920450 *	3.5194971	4.0267302	3.5074205
7 C	3.8859485	2.1966194 *	3.4866936	3.9528916
8 C	5.1092725	2.6809056 *	4.6713649	5.3959471
9 C	5.3854398	4.0802899	5.9317215	6.2665355
10 C	4.5628931	4.8937292	6.2588785	6.0073472
11 C	3.1539804	4.6927087	5.4873658	4.8011587
12 N	2.8943057 *	5.9976490	6.3999639	5.1679107
13 C	3.9758397	7.1289904	7.6691363	6.4009856
14 C	4.6890922	8.4908050	8.8226374	7.2787356
15 C	4.6773782	9.0331617	9.0396770	7.2479562
16 C	5.9080144	10.4312651	10.3603518	8.4582183
17 C	6.9770652	11.3049211	11.4220172	9.5954643
18 C	7.0148434	10.9215478	11.2939004	9.6551431
19 C	6.0005716	9.5824108	10.0797048	8.5975877
20 O	3.7557023	8.2923830	8.0337343	6.1552440
21 N	0.0000000	5.4451665	4.6745373	2.6529930 *
22 H	5.4451665	0.0000000	2.5304177 *	4.3598234
23 H	4.6745373	2.5304177 *	0.0000000	2.5186364 *
24 H	2.6529930 *	4.3598234	2.5186364 *	0.0000000
25 H	6.0546659	2.4011306 *	4.7817618	5.9757264
26 H	6.4691144	4.7782616	6.8520242	7.3475505
27 H	5.2568838	5.9681269	7.3481774	6.9662435
28 H	4.7295631	7.2006624	8.0340344	7.0101677
29 H	6.2386034	10.9512056	10.6807495	8.6658141
30 H	7.9540878	12.3904220	12.4485501	10.5539756

31 H	8.0140342	11.7612711	12.2390240	10.6516883
32 H	6.3901883	9.4655424	10.1866539	8.9022132
33 H	4.3819388	8.9761989	8.5595579	6.6005783
34 H	1.0440021 *	5.8497515	5.1863187	3.2277498
35 H	1.0392717 *	5.8208649	4.5850789	2.2121445 *

H H H H

1 CO	6.4893650	6.2784816	4.5289690	3.8777075
2 C	2.6817460 *	4.6685322	5.3925327	6.4053223
3 C	4.0812773	5.9302254	6.2684557	6.9354799
4 C	4.8910200	6.2529381	6.0088628	6.2686853
5 C	4.6715635	5.4684182	4.8030045	4.8909464
6 C	3.5168729	4.0166168	3.5054772	4.0431068
7 C	2.1970666 *	3.4837658	3.9512101	5.0319253
8 C	1.1050630 *	2.1843084 *	3.4313110	4.9924385
9 C	2.1810206 *	1.1043298 *	2.1814492 *	4.0004355
10 C	3.4537684	2.1980549 *	1.1043000 *	2.6631113 *
11 C	3.9640333	3.4745182	2.1887010 *	2.6610471 *
12 N	5.4111099	4.6689487	2.6947942 *	2.0964571 *
13 C	6.2477122	5.0156317	2.6538702 *	1.1084066 *
14 C	7.6856185	6.3726468	3.9134609	2.1772742 *
15 C	8.5061084	7.4275938	5.0282311	3.5332717
16 C	9.8909256	8.7062177	6.2553216	4.6752825
17 C	10.5373756	9.0824913	6.5820796	4.8547426
18 C	9.9305316	8.2801591	5.8068104	3.9982575
19 C	8.5443097	6.9220586	4.4594862	2.5831046 *
20 O	8.0925918	7.4132026	5.2439181	4.1422406
21 N	6.0546659	6.4691144	5.2568838	4.7295631
22 H	2.4011306 *	4.7782616	5.9681269	7.2006624
23 H	4.7817618	6.8520242	7.3481774	8.0340344
24 H	5.9757264	7.3475505	6.9662435	7.0101677
25 H	0.0000000	2.5278983 *	4.3484367	6.0233139
26 H	2.5278983 *	0.0000000	2.5007995 *	4.4918805
27 H	4.3484367	2.5007995 *	0.0000000	2.1590256 *
28 H	6.0233139	4.4918805	2.1590256 *	0.0000000
29 H	10.5820501	9.5450397	7.1447739	5.6720657
30 H	11.6344109	10.1478139	7.6476312	5.9344936
31 H	10.6393108	8.8379886	6.4294681	4.6563672
32 H	8.2289635	6.4361447	4.0939785	2.2673826 *
33 H	8.8876371	8.2715494	6.1341012	5.0969923
34 H	6.3216245	6.5885129	5.2952363	4.4661373
35 H	6.7606873	7.3990696	6.2745960	5.7354735

H H H H

1 CO	4.6095102	6.4123484	6.6672065	5.2754489
2 C	9.9218644	11.4106277	10.8805880	8.6519514
3 C	9.7621608	11.4501439	11.1723827	9.0974446
4 C	8.5448889	10.3059597	10.2020248	8.2926109
5 C	7.3765917	9.0077392	8.8141751	6.8938474
6 C	7.5275131	8.8946924	8.3788588	6.2338665
7 C	8.9243530	10.2362909	9.5676666	7.2937463
8 C	9.4957214	10.5535292	9.6114601	7.2267223
9 C	8.8674703	9.6671942	8.5408535	6.1366496
10 C	7.4717887	8.2501614	7.2035992	4.8478652
11 C	6.7029525	7.7949432	7.0847897	4.8790506
12 N	5.2695384	6.4042814	5.9180735	3.9704911
13 C	4.7966071	5.4502553	4.6574824	2.6413378 *
14 C	3.5034065	3.9880092	3.4931652	2.1975436 *
15 C	2.1941343 *	3.4399536	3.9281893	3.4501924
16 C	1.1068508 *	2.1922549 *	3.4741414	3.9515518
17 C	2.2010358 *	1.1052545 *	2.1973854 *	3.4573085
18 C	3.4737433	2.2006577 *	1.1041416 *	2.1859142 *
19 C	3.9524698	3.4612027	2.1875246 *	1.1059296 *
20 O	2.6849653 *	4.6496563	5.3937951	4.6922578
21 N	6.2386034	7.9540878	8.0140342	6.3901883
22 H	10.9512056	12.3904220	11.7612711	9.4655424
23 H	10.6807495	12.4485501	12.2390240	10.1866539
24 H	8.6658141	10.5539756	10.6516883	8.9022132
25 H	10.5820501	11.6344109	10.6393108	8.2289635
26 H	9.5450397	10.1478139	8.8379886	6.4361447
27 H	7.1447739	7.6476312	6.4294681	4.0939785
28 H	5.6720657	5.9344936	4.6563672	2.2673826 *
29 H	0.0000000	2.5217573 *	4.3870948	5.0583842
30 H	2.5217573 *	0.0000000	2.5404501 *	4.3745079
31 H	4.3870948	2.5404501 *	0.0000000	2.5145101 *
32 H	5.0583842	4.3745079	2.5145101 *	0.0000000
33 H	2.3103918 *	4.6333065	5.8160426	5.4648872
34 H	6.2933504	7.7691317	7.6532637	6.0074045
35 H	6.5798671	8.4670710	8.7539923	7.2913057

H H H

1 CO	2.6586069 *	2.5005737 *	2.6216196 *
2 C	7.9417202	4.7735442	4.7379305
3 C	7.6879259	4.3299905	3.9175720
4 C	6.4887822	3.0665684	2.4861783 *
5 C	5.4263877	2.1111368 *	2.0893951 *
6 C	5.7240195	2.9532398 *	3.4251838
7 C	7.0917962	4.2379529	4.5640866
8 C	7.8344736	5.3625324	5.8897083

9 C	7.4532202	5.5394969	6.3027671
10 C	6.1698005	4.6666807	5.5564715
11 C	5.1844317	3.3188278	4.1529600
12 N	3.8893641	2.9870240 *	3.8834882
13 C	4.0145855	3.8305254	4.9365606
14 C	3.3290232	4.5243424	5.5043608
15 C	2.0462855 *	4.6737143	5.2898887
16 C	2.5109656 *	5.8658727	6.4042615
17 C	3.9308580	6.7929485	7.5553997
18 C	4.7302484	6.7182399	7.7358102
19 C	4.4860546	5.6959361	6.8256893
20 O	0.9917458 *	4.0208789	4.2220708
21 N	4.3819388	1.0440021 *	1.0392717 *
22 H	8.9761989	5.8497515	5.8208649
23 H	8.5595579	5.1863187	4.5850789
24 H	6.6005783	3.2277498	2.2121445 *
25 H	8.8876371	6.3216245	6.7606873
26 H	8.2715494	6.5885129	7.3990696
27 H	6.1341012	5.2952363	6.2745960
28 H	5.0969923	4.4661373	5.7354735
29 H	2.3103918 *	6.2933504	6.5798671
30 H	4.6333065	7.7691317	8.4670710
31 H	5.8160426	7.6532637	8.7539923
32 H	5.4648872	6.0074045	7.2913057
33 H	0.0000000	4.7326506	4.6632507
34 H	4.7326506	0.0000000	1.6671683 *
35 H	4.6632507	1.6671683 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.74 , TOTAL = 9312.6 SECONDS (155.2 MIN)
WALL CLOCK TIME: STEP = 0.73 , TOTAL = 8617.9 SECONDS (143.6 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 100.00%

..... END OF TWO-ELECTRON INTEGRALS

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 1.72 , TOTAL = 9314.3 SECONDS (155.2 MIN)
WALL CLOCK TIME: STEP = 1.73 , TOTAL = 8619.6 SECONDS (143.7 MIN)

CPU UTILIZATION: STEP = 99.37%, TOTAL = 100.00%

DIRECT SCF CALCULATION, SCHWRZ=T FDIFF=T

NONZERO BLOCKS

ITER	EX	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
1	0	-284.636975674	-284.636975674	0.003764268	198410688
2	1	-284.636978787	-0.000003113	0.000273355	142333068
3	2	-284.636978815	-0.000000028	0.000185743	123293967
4	3	-284.636978810	0.000000004	0.000076144	115981475
5	4	-284.636978803	0.000000007	0.000059679	110875235
6	5	-284.636978811	-0.000000008	0.000034333	103337924
7	6	-284.636978843	-0.000000033	0.000034390	102736459
8	7	-284.636978846	-0.000000003	0.000025352	125434925
9	8	-284.636978844	0.000000002	0.000062930	121490770
10	9	-284.636978845	-0.000000001	0.000064190	148761537

-----START SECOND ORDER SCF-----

11	10	-284.636978848	-0.000000002	0.000059646	198409514
12	11	-284.636978848	-0.000000001	0.000069206	198409455
13	12	-284.636978849	0.000000000	0.000043378	198409379
14	13	-284.636978849	0.000000000	0.000045939	198409388
15	14	-284.636978849	0.000000000	0.000013192	198409464
16	15	-284.636978849	0.000000000	0.000014269	198409464

-----DISABLING FDIFF OPTION-----

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 51.3 SECONDS (3.2 SEC/ITER)
 OF THE ABOVE TIME, DFT PART= 17.5 SECONDS (1.1 SEC/ITER)
 FOCK TIME ON FIRST ITERATION= 4.0, LAST ITERATION= 3.4
 TIME TO SOLVE SCF EQUATIONS= 2.4 SECONDS (0.1 SEC/ITER)

FINAL ENERGY IS -284.6369788491 AFTER 16 ITERATIONS
DFT EXCHANGE + CORRELATION ENERGY IS -46.6021365100
INTEGRATED TOTAL ELECTRON NUMBER IS 112.9998737844

SPIN SZ = 1.500
S-SQUARED = 3.760

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

..... END OF UDFT CALCULATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 54.93 , TOTAL = 9369.2 SECONDS (156.2 MIN)
WALL CLOCK TIME: STEP = 50.94 , TOTAL = 8670.6 SECONDS (144.5
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%
..... END OF 1-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 3.91 , TOTAL = 9373.1 SECONDS (156.2 MIN)
WALL CLOCK TIME: STEP = 3.89 , TOTAL = 8674.5 SECONDS (144.6
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 295954 WORDS.
USING 1271474 WORDS OF MEMORY.

..... END OF 2-ELECTRON GRADIENT

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 2.89 , TOTAL = 9376.0 SECONDS (156.3 MIN)
WALL CLOCK TIME: STEP = 2.70 , TOTAL = 8677.2 SECONDS (144.6
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

NSERCH=110 ENERGY= -284.6369788

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
------	------	-------	-------	-------

```

-----
1 CO      27.0 -0.0000023 -0.0000124 -0.0000220
2 C       6.0 -0.0000154 -0.0000094 -0.0000004
3 C       6.0 -0.0000144  0.0000055  0.0000117
4 C       6.0  0.0000117  0.0000018 -0.0000535
5 C       6.0  0.0000140 -0.0000033 -0.0000177
6 C       6.0  0.0000051  0.0000065  0.0000434
7 C       6.0  0.0000036  0.0000149  0.0000000
8 C       6.0  0.0000265  0.0000009 -0.0000343
9 C       6.0 -0.0000079  0.0000185 -0.0000486
10 C      6.0 -0.0000268  0.0000108  0.0000229
11 C      6.0 -0.0000099  0.0000087  0.0000393
12 N      7.0  0.0000142  0.0000119  0.0000082
13 C      6.0  0.0000398 -0.0000030  0.0000015
14 C      6.0  0.0000017 -0.0000165 -0.0000129
15 C      6.0 -0.0000007 -0.0000075 -0.0000243
16 C      6.0  0.0000037 -0.0000168 -0.0000053
17 C      6.0 -0.0000163 -0.0000018  0.0000156
18 C      6.0  0.0000122 -0.0000428  0.0000279
19 C      6.0  0.0000234 -0.0000233 -0.0000229
20 O      8.0 -0.0000108 -0.0000304 -0.0000206
21 N      7.0 -0.0000068  0.0000277 -0.0000024
22 H      1.0 -0.0000115  0.0000048 -0.0000409
23 H      1.0 -0.0000082 -0.0000150  0.0000272
24 H      1.0  0.0000134 -0.0000229  0.0000849
25 H      1.0  0.0000358 -0.0000315  0.0000493
26 H      1.0  0.0000320  0.0000246  0.0000352
27 H      1.0 -0.0000043  0.0000713 -0.0000322
28 H      1.0  0.0000000 -0.0000147 -0.0000049
29 H      1.0  0.0000106 -0.0000123  0.0000180
30 H      1.0 -0.0000598  0.0000043  0.0000233
31 H      1.0  0.0000126 -0.0000290  0.0000223
32 H      1.0 -0.0000111  0.0000121  0.0000037
33 H      1.0 -0.0000273  0.0000571 -0.0000381
34 H      1.0  0.0000285  0.0000144 -0.0000382
35 H      1.0 -0.0000555 -0.0000030 -0.0000152

```

MAXIMUM GRADIENT = 0.0000849 RMS GRADIENT = 0.0000254
 1 ***** EQUILIBRIUM GEOMETRY LOCATED *****

Co.inp

COORDINATES OF ALL ATOMS ARE (ANGS)

```

ATOM CHARGE X Y Z
-----
CO      27.0 0.1596841167 -1.7149970402 0.8965027875

```

C	6.0	4.9802664340	0.6147131425	0.5514391919
C	6.0	5.1720179545	-0.7270268484	0.1945093316
C	6.0	4.0285658312	-1.5388511176	-0.0949443459
C	6.0	2.7247000188	-1.0169757205	-0.0011884160
C	6.0	2.4655475047	0.3500358959	0.4343569907
C	6.0	3.6548401040	1.1746264956	0.6760492592
C	6.0	3.5192207504	2.5623322217	1.0521038981
C	6.0	2.2560889860	3.1467777057	1.2195661789
C	6.0	1.0837167190	2.3455690774	1.0490688395
C	6.0	1.1648482648	0.9902371361	0.6520488852
N	7.0	-0.0502444270	0.1928296652	0.6090908051
C	6.0	-1.2478565740	0.7137795684	0.3488309044
C	6.0	-2.5481174225	0.0418376775	0.4533403641
C	6.0	-2.8141765919	-1.2836339390	0.9428062009
C	6.0	-4.1104392170	-1.8195134178	1.0461031031
C	6.0	-5.2224205206	-1.0170765947	0.6464188720
C	6.0	-5.0135767940	0.2993782607	0.1478461451
C	6.0	-3.6985671901	0.8167742798	0.0571646770
O	8.0	-1.6905150214	-2.1299251671	1.3549050955
N	7.0	1.6094051906	-1.9394348597	-0.4282212923
H	1.0	5.8482429134	1.2701927713	0.7466759637
H	1.0	6.1861656807	-1.1554552093	0.1102377535
H	1.0	4.1829886945	-2.5836701215	-0.4292190095
H	1.0	4.4370962430	3.1544067599	1.2197836069
H	1.0	2.1574786564	4.2041423534	1.5225517350
H	1.0	0.1038675619	2.7969373819	1.2849518078
H	1.0	-1.2969452572	1.7664902362	0.0053840987
H	1.0	-4.2774911814	-2.8449681230	1.4277509449
H	1.0	-6.2441024528	-1.4311592802	0.7257222330
H	1.0	-5.8725682992	0.9196532662	-0.1628324871
H	1.0	-3.5393915532	1.8438028245	-0.3209303276
H	1.0	-2.0057500184	-2.9363198441	1.8385518795
H	1.0	1.2368885182	-1.6487737587	-1.3591819991
H	1.0	1.9965293778	-2.8956306780	-0.5543566756

INTERNUCLEAR DISTANCES (ANGS.)

	CO	C	C	C
1 CO	0.0000000	5.3651312	5.1567791	3.9977794
2 C	5.3651312	0.0000000	1.4015826 *	2.4415947 *
3 C	5.1567791	1.4015826 *	0.0000000	1.4318955 *
4 C	3.9977794	2.4415947 *	1.4318955 *	0.0000000
5 C	2.8057779 *	2.8382011 *	2.4721919 *	1.4075547 *
6 C	3.1296878	2.5313185 *	2.9227681 *	2.5082026 *

7 C	4.5403347	1.4442249 *	2.4799183 *	2.8455338 *
8 C	5.4411620	2.4856669 *	3.7798267	4.2889226
9 C	5.3043508	3.7787415	4.9557790	5.1792596
10 C	4.1671705	4.2926213	5.1851060	5.0069574
11 C	2.8962743 *	3.8351736	4.3835770	3.8929635
12 N	1.9407417 *	5.0484997	5.3188380	4.4867669
13 C	2.8600824 *	6.2322051	6.5813773	5.7542953
14 C	3.2580746	7.5507863	7.7626436	6.7861591
15 C	3.0053395	8.0318262	8.0404641	6.9256903
16 C	4.2740212	9.4239631	9.3852411	8.2233913
17 C	5.4329260	10.3327915	10.4082997	9.2953008
18 C	5.6018589	10.0069589	10.2372860	9.2302967
19 C	4.6904645	8.6952452	9.0049690	8.0796468
20 O	1.9507780 *	7.2579558	7.0999296	5.9295293
21 N	1.9766025 *	4.3412109	3.8144379	2.4746473 *
22 H	6.4260024	1.1050584 *	2.1796914 *	3.4511269
23 H	6.1032598	2.1868580 *	1.1041504 *	2.2009837 *
24 H	4.3242469	3.4390402	2.1941605 *	1.1078054 *
25 H	6.4893650	2.6817460 *	4.0812773	4.8910200
26 H	6.2784816	4.6685322	5.9302254	6.2529381
27 H	4.5289690	5.3925327	6.2684557	6.0088628
28 H	3.8777075	6.4053223	6.9354799	6.2686853
29 H	4.6095102	9.9218644	9.7621608	8.5448889
30 H	6.4123484	11.4106277	11.4501439	10.3059597
31 H	6.6672065	10.8805880	11.1723827	10.2020248
32 H	5.2754489	8.6519514	9.0974446	8.2926109
33 H	2.6586069 *	7.9417202	7.6879259	6.4887822
34 H	2.5005737 *	4.7735442	4.3299905	3.0665684
35 H	2.6216196 *	4.7379305	3.9175720	2.4861783 *

C C C C

1 CO	2.8057779 *	3.1296878	4.5403347	5.4411620
2 C	2.8382011 *	2.5313185 *	1.4442249 *	2.4856669 *
3 C	2.4721919 *	2.9227681 *	2.4799183 *	3.7798267
4 C	1.4075547 *	2.5082026 *	2.8455338 *	4.2889226
5 C	0.0000000	1.4579371 *	2.4752640 *	3.8147258
6 C	1.4579371 *	0.0000000	1.4672361 *	2.5270721 *
7 C	2.4752640 *	1.4672361 *	0.0000000	1.4441388 *
8 C	3.8147258	2.5270721 *	1.4441388 *	0.0000000
9 C	4.3642503	2.9124201 *	2.4781638 *	1.4018281 *
10 C	3.8862030	2.5038929 *	2.8497238 *	2.4451330 *
11 C	2.6246447 *	1.4659693 *	2.4969251 *	2.8591252 *
12 N	3.0881040	2.5267479 *	3.8335440	4.3071899
13 C	4.3473248	3.7321568	4.9351683	5.1610819
14 C	5.3972480	5.0231646	6.3094764	6.5972724

15 C	5.6250677	5.5500346	6.9254878	7.4104874
16 C	6.9613228	6.9516026	8.3307489	8.7984270
17 C	7.9734635	7.8114544	9.1438611	9.4547893
18 C	7.8508552	7.4847816	8.7284884	8.8739662
19 C	6.6801501	6.1932567	7.3880766	7.4922186
20 O	4.7509757	4.9265070	6.3208962	7.0178569
21 N	1.5090297 *	2.5920450 *	3.8859485	5.1092725
22 H	3.9429635	3.5194971	2.1966194 *	2.6809056 *
23 H	3.4660261	4.0267302	3.4866936	4.6713649
24 H	2.1827385 *	3.5074205	3.9528916	5.3959471
25 H	4.6715635	3.5168729	2.1970666 *	1.1050630 *
26 H	5.4684182	4.0166168	3.4837658	2.1843084 *
27 H	4.8030045	3.5054772	3.9512101	3.4313110
28 H	4.8909464	4.0431068	5.0319253	4.9924385
29 H	7.3765917	7.5275131	8.9243530	9.4957214
30 H	9.0077392	8.8946924	10.2362909	10.5535292
31 H	8.8141751	8.3788588	9.5676666	9.6114601
32 H	6.8938474	6.2338665	7.2937463	7.2267223
33 H	5.4263877	5.7240195	7.0917962	7.8344736
34 H	2.1111368 *	2.9532398 *	4.2379529	5.3625324
35 H	2.0893951 *	3.4251838	4.5640866	5.8897083

C C C N

1 CO	5.3043508	4.1671705	2.8962743 *	1.9407417 *
2 C	3.7787415	4.2926213	3.8351736	5.0484997
3 C	4.9557790	5.1851060	4.3835770	5.3188380
4 C	5.1792596	5.0069574	3.8929635	4.4867669
5 C	4.3642503	3.8862030	2.6246447 *	3.0881040
6 C	2.9124201 *	2.5038929 *	1.4659693 *	2.5267479 *
7 C	2.4781638 *	2.8497238 *	2.4969251 *	3.8335440
8 C	1.4018281 *	2.4451330 *	2.8591252 *	4.3071899
9 C	0.0000000	1.4301963 *	2.4826497 *	3.7970598
10 C	1.4301963 *	0.0000000	1.4146137 *	2.4725969 *
11 C	2.4826497 *	1.4146137 *	0.0000000	1.4540132 *
12 N	3.7970598	2.4725969 *	1.4540132 *	0.0000000
13 C	4.3537678	2.9307515 *	2.4473485 *	1.3316902 *
14 C	5.7713217	4.3419224	3.8373247	2.5072747 *
15 C	6.7388973	5.3269108	4.5921311	3.1512905
16 C	8.0763122	6.6578658	5.9898777	4.5525472
17 C	8.5787111	7.1579941	6.6952627	5.3119368
18 C	7.8806287	6.4943119	6.2373426	4.9858567
19 C	6.4990787	5.1177463	4.9027326	3.7422170
20 O	6.5907202	5.2744617	4.2874840	2.9397137 *
21 N	5.3854398	4.5628931	3.1539804	2.8943057 *
22 H	4.0802899	4.8937292	4.6927087	5.9976490

23 H	5.9317215	6.2588785	5.4873658	6.3999639
24 H	6.2665355	6.0073472	4.8011587	5.1679107
25 H	2.1810206 *	3.4537684	3.9640333	5.4111099
26 H	1.1043298 *	2.1980549 *	3.4745182	4.6689487
27 H	2.1814492 *	1.1043000 *	2.1887010 *	2.6947942 *
28 H	4.0004355	2.6631113 *	2.6610471 *	2.0964571 *
29 H	8.8674703	7.4717887	6.7029525	5.2695384
30 H	9.6671942	8.2501614	7.7949432	6.4042814
31 H	8.5408535	7.2035992	7.0847897	5.9180735
32 H	6.1366496	4.8478652	4.8790506	3.9704911
33 H	7.4532202	6.1698005	5.1844317	3.8893641
34 H	5.5394969	4.6666807	3.3188278	2.9870240 *
35 H	6.3027671	5.5564715	4.1529600	3.8834882

C C C C

1 CO	2.8600824 *	3.2580746	3.0053395	4.2740212
2 C	6.2322051	7.5507863	8.0318262	9.4239631
3 C	6.5813773	7.7626436	8.0404641	9.3852411
4 C	5.7542953	6.7861591	6.9256903	8.2233913
5 C	4.3473248	5.3972480	5.6250677	6.9613228
6 C	3.7321568	5.0231646	5.5500346	6.9516026
7 C	4.9351683	6.3094764	6.9254878	8.3307489
8 C	5.1610819	6.5972724	7.4104874	8.7984270
9 C	4.3537678	5.7713217	6.7388973	8.0763122
10 C	2.9307515 *	4.3419224	5.3269108	6.6578658
11 C	2.4473485 *	3.8373247	4.5921311	5.9898777
12 N	1.3316902 *	2.5072747 *	3.1512905	4.5525472
13 C	0.0000000	1.4673467 *	2.6068805 *	3.8856327
14 C	1.4673467 *	0.0000000	1.4377897 *	2.5013686 *
15 C	2.6068805 *	1.4377897 *	0.0000000	1.4064615 *
16 C	3.8856327	2.5013686 *	1.4064615 *	0.0000000
17 C	4.3452940	2.8827896 *	2.4410115 *	1.4283399 *
18 C	3.7937807	2.4976276 *	2.8240486 *	2.4722914 *
19 C	2.4701538 *	1.4425729 *	2.4450404 *	2.8456371 *
20 O	3.0487355	2.5029692 *	1.4658273 *	2.4592168 *
21 N	3.9758397	4.6890922	4.6773782	5.9080144
22 H	7.1289904	8.4908050	9.0331617	10.4312651
23 H	7.6691363	8.8226374	9.0396770	10.3603518
24 H	6.4009856	7.2787356	7.2479562	8.4582183
25 H	6.2477122	7.6856185	8.5061084	9.8909256
26 H	5.0156317	6.3726468	7.4275938	8.7062177
27 H	2.6538702 *	3.9134609	5.0282311	6.2553216
28 H	1.1084066 *	2.1772742 *	3.5332717	4.6752825
29 H	4.7966071	3.5034065	2.1941343 *	1.1068508 *
30 H	5.4502553	3.9880092	3.4399536	2.1922549 *

31 H	4.6574824	3.4931652	3.9281893	3.4741414
32 H	2.6413378 *	2.1975436 *	3.4501924	3.9515518
33 H	4.0145855	3.3290232	2.0462855 *	2.5109656 *
34 H	3.8305254	4.5243424	4.6737143	5.8658727
35 H	4.9365606	5.5043608	5.2898887	6.4042615

C C C O

1 CO	5.4329260	5.6018589	4.6904645	1.9507780 *
2 C	10.3327915	10.0069589	8.6952452	7.2579558
3 C	10.4082997	10.2372860	9.0049690	7.0999296
4 C	9.2953008	9.2302967	8.0796468	5.9295293
5 C	7.9734635	7.8508552	6.6801501	4.7509757
6 C	7.8114544	7.4847816	6.1932567	4.9265070
7 C	9.1438611	8.7284884	7.3880766	6.3208962
8 C	9.4547893	8.8739662	7.4922186	7.0178569
9 C	8.5787111	7.8806287	6.4990787	6.5907202
10 C	7.1579941	6.4943119	5.1177463	5.2744617
11 C	6.6952627	6.2373426	4.9027326	4.2874840
12 N	5.3119368	4.9858567	3.7422170	2.9397137 *
13 C	4.3452940	3.7937807	2.4701538 *	3.0487355
14 C	2.8827896 *	2.4976276 *	1.4425729 *	2.5029692 *
15 C	2.4410115 *	2.8240486 *	2.4450404 *	1.4658273 *
16 C	1.4283399 *	2.4722914 *	2.8456371 *	2.4592168 *
17 C	0.0000000	1.4231106 *	2.4560860 *	3.7702442
18 C	1.4231106 *	0.0000000	1.4160410 *	4.2896674
19 C	2.4560860 *	1.4160410 *	0.0000000	3.7946596
20 O	3.7702442	4.2896674	3.7946596	0.0000000
21 N	6.9770652	7.0148434	6.0005716	3.7557023
22 H	11.3049211	10.9215478	9.5824108	8.2923830
23 H	11.4220172	11.2939004	10.0797048	8.0337343
24 H	9.5954643	9.6551431	8.5975877	6.1552440
25 H	10.5373756	9.9305316	8.5443097	8.0925918
26 H	9.0824913	8.2801591	6.9220586	7.4132026
27 H	6.5820796	5.8068104	4.4594862	5.2439181
28 H	4.8547426	3.9982575	2.5831046 *	4.1422406
29 H	2.2010358 *	3.4737433	3.9524698	2.6849653 *
30 H	1.1052545 *	2.2006577 *	3.4612027	4.6496563
31 H	2.1973854 *	1.1041416 *	2.1875246 *	5.3937951
32 H	3.4573085	2.1859142 *	1.1059296 *	4.6922578
33 H	3.9308580	4.7302484	4.4860546	0.9917458 *
34 H	6.7929485	6.7182399	5.6959361	4.0208789
35 H	7.5553997	7.7358102	6.8256893	4.2220708

N H H H

1 CO	1.9766025 *	6.4260024	6.1032598	4.3242469
2 C	4.3412109	1.1050584 *	2.1868580 *	3.4390402
3 C	3.8144379	2.1796914 *	1.1041504 *	2.1941605 *
4 C	2.4746473 *	3.4511269	2.2009837 *	1.1078054 *
5 C	1.5090297 *	3.9429635	3.4660261	2.1827385 *
6 C	2.5920450 *	3.5194971	4.0267302	3.5074205
7 C	3.8859485	2.1966194 *	3.4866936	3.9528916
8 C	5.1092725	2.6809056 *	4.6713649	5.3959471
9 C	5.3854398	4.0802899	5.9317215	6.2665355
10 C	4.5628931	4.8937292	6.2588785	6.0073472
11 C	3.1539804	4.6927087	5.4873658	4.8011587
12 N	2.8943057 *	5.9976490	6.3999639	5.1679107
13 C	3.9758397	7.1289904	7.6691363	6.4009856
14 C	4.6890922	8.4908050	8.8226374	7.2787356
15 C	4.6773782	9.0331617	9.0396770	7.2479562
16 C	5.9080144	10.4312651	10.3603518	8.4582183
17 C	6.9770652	11.3049211	11.4220172	9.5954643
18 C	7.0148434	10.9215478	11.2939004	9.6551431
19 C	6.0005716	9.5824108	10.0797048	8.5975877
20 O	3.7557023	8.2923830	8.0337343	6.1552440
21 N	0.0000000	5.4451665	4.6745373	2.6529930 *
22 H	5.4451665	0.0000000	2.5304177 *	4.3598234
23 H	4.6745373	2.5304177 *	0.0000000	2.5186364 *
24 H	2.6529930 *	4.3598234	2.5186364 *	0.0000000
25 H	6.0546659	2.4011306 *	4.7817618	5.9757264
26 H	6.4691144	4.7782616	6.8520242	7.3475505
27 H	5.2568838	5.9681269	7.3481774	6.9662435
28 H	4.7295631	7.2006624	8.0340344	7.0101677
29 H	6.2386034	10.9512056	10.6807495	8.6658141
30 H	7.9540878	12.3904220	12.4485501	10.5539756
31 H	8.0140342	11.7612711	12.2390240	10.6516883
32 H	6.3901883	9.4655424	10.1866539	8.9022132
33 H	4.3819388	8.9761989	8.5595579	6.6005783
34 H	1.0440021 *	5.8497515	5.1863187	3.2277498
35 H	1.0392717 *	5.8208649	4.5850789	2.2121445 *

H H H H

1 CO	6.4893650	6.2784816	4.5289690	3.8777075
2 C	2.6817460 *	4.6685322	5.3925327	6.4053223
3 C	4.0812773	5.9302254	6.2684557	6.9354799
4 C	4.8910200	6.2529381	6.0088628	6.2686853
5 C	4.6715635	5.4684182	4.8030045	4.8909464
6 C	3.5168729	4.0166168	3.5054772	4.0431068
7 C	2.1970666 *	3.4837658	3.9512101	5.0319253
8 C	1.1050630 *	2.1843084 *	3.4313110	4.9924385

9 C	2.1810206 *	1.1043298 *	2.1814492 *	4.0004355
10 C	3.4537684	2.1980549 *	1.1043000 *	2.6631113 *
11 C	3.9640333	3.4745182	2.1887010 *	2.6610471 *
12 N	5.4111099	4.6689487	2.6947942 *	2.0964571 *
13 C	6.2477122	5.0156317	2.6538702 *	1.1084066 *
14 C	7.6856185	6.3726468	3.9134609	2.1772742 *
15 C	8.5061084	7.4275938	5.0282311	3.5332717
16 C	9.8909256	8.7062177	6.2553216	4.6752825
17 C	10.5373756	9.0824913	6.5820796	4.8547426
18 C	9.9305316	8.2801591	5.8068104	3.9982575
19 C	8.5443097	6.9220586	4.4594862	2.5831046 *
20 O	8.0925918	7.4132026	5.2439181	4.1422406
21 N	6.0546659	6.4691144	5.2568838	4.7295631
22 H	2.4011306 *	4.7782616	5.9681269	7.2006624
23 H	4.7817618	6.8520242	7.3481774	8.0340344
24 H	5.9757264	7.3475505	6.9662435	7.0101677
25 H	0.0000000	2.5278983 *	4.3484367	6.0233139
26 H	2.5278983 *	0.0000000	2.5007995 *	4.4918805
27 H	4.3484367	2.5007995 *	0.0000000	2.1590256 *
28 H	6.0233139	4.4918805	2.1590256 *	0.0000000
29 H	10.5820501	9.5450397	7.1447739	5.6720657
30 H	11.6344109	10.1478139	7.6476312	5.9344936
31 H	10.6393108	8.8379886	6.4294681	4.6563672
32 H	8.2289635	6.4361447	4.0939785	2.2673826 *
33 H	8.8876371	8.2715494	6.1341012	5.0969923
34 H	6.3216245	6.5885129	5.2952363	4.4661373
35 H	6.7606873	7.3990696	6.2745960	5.7354735

H H H H

1 CO	4.6095102	6.4123484	6.6672065	5.2754489
2 C	9.9218644	11.4106277	10.8805880	8.6519514
3 C	9.7621608	11.4501439	11.1723827	9.0974446
4 C	8.5448889	10.3059597	10.2020248	8.2926109
5 C	7.3765917	9.0077392	8.8141751	6.8938474
6 C	7.5275131	8.8946924	8.3788588	6.2338665
7 C	8.9243530	10.2362909	9.5676666	7.2937463
8 C	9.4957214	10.5535292	9.6114601	7.2267223
9 C	8.8674703	9.6671942	8.5408535	6.1366496
10 C	7.4717887	8.2501614	7.2035992	4.8478652
11 C	6.7029525	7.7949432	7.0847897	4.8790506
12 N	5.2695384	6.4042814	5.9180735	3.9704911
13 C	4.7966071	5.4502553	4.6574824	2.6413378 *
14 C	3.5034065	3.9880092	3.4931652	2.1975436 *
15 C	2.1941343 *	3.4399536	3.9281893	3.4501924
16 C	1.1068508 *	2.1922549 *	3.4741414	3.9515518

17 C	2.2010358 *	1.1052545 *	2.1973854 *	3.4573085
18 C	3.4737433	2.2006577 *	1.1041416 *	2.1859142 *
19 C	3.9524698	3.4612027	2.1875246 *	1.1059296 *
20 O	2.6849653 *	4.6496563	5.3937951	4.6922578
21 N	6.2386034	7.9540878	8.0140342	6.3901883
22 H	10.9512056	12.3904220	11.7612711	9.4655424
23 H	10.6807495	12.4485501	12.2390240	10.1866539
24 H	8.6658141	10.5539756	10.6516883	8.9022132
25 H	10.5820501	11.6344109	10.6393108	8.2289635
26 H	9.5450397	10.1478139	8.8379886	6.4361447
27 H	7.1447739	7.6476312	6.4294681	4.0939785
28 H	5.6720657	5.9344936	4.6563672	2.2673826 *
29 H	0.0000000	2.5217573 *	4.3870948	5.0583842
30 H	2.5217573 *	0.0000000	2.5404501 *	4.3745079
31 H	4.3870948	2.5404501 *	0.0000000	2.5145101 *
32 H	5.0583842	4.3745079	2.5145101 *	0.0000000
33 H	2.3103918 *	4.6333065	5.8160426	5.4648872
34 H	6.2933504	7.7691317	7.6532637	6.0074045
35 H	6.5798671	8.4670710	8.7539923	7.2913057

H H H

1 CO	2.6586069 *	2.5005737 *	2.6216196 *
2 C	7.9417202	4.7735442	4.7379305
3 C	7.6879259	4.3299905	3.9175720
4 C	6.4887822	3.0665684	2.4861783 *
5 C	5.4263877	2.1111368 *	2.0893951 *
6 C	5.7240195	2.9532398 *	3.4251838
7 C	7.0917962	4.2379529	4.5640866
8 C	7.8344736	5.3625324	5.8897083
9 C	7.4532202	5.5394969	6.3027671
10 C	6.1698005	4.6666807	5.5564715
11 C	5.1844317	3.3188278	4.1529600
12 N	3.8893641	2.9870240 *	3.8834882
13 C	4.0145855	3.8305254	4.9365606
14 C	3.3290232	4.5243424	5.5043608
15 C	2.0462855 *	4.6737143	5.2898887
16 C	2.5109656 *	5.8658727	6.4042615
17 C	3.9308580	6.7929485	7.5553997
18 C	4.7302484	6.7182399	7.7358102
19 C	4.4860546	5.6959361	6.8256893
20 O	0.9917458 *	4.0208789	4.2220708
21 N	4.3819388	1.0440021 *	1.0392717 *
22 H	8.9761989	5.8497515	5.8208649
23 H	8.5595579	5.1863187	4.5850789
24 H	6.6005783	3.2277498	2.2121445 *

25 H	8.8876371	6.3216245	6.7606873
26 H	8.2715494	6.5885129	7.3990696
27 H	6.1341012	5.2952363	6.2745960
28 H	5.0969923	4.4661373	5.7354735
29 H	2.3103918 *	6.2933504	6.5798671
30 H	4.6333065	7.7691317	8.4670710
31 H	5.8160426	7.6532637	8.7539923
32 H	5.4648872	6.0074045	7.2913057
33 H	0.0000000	4.7326506	4.6632507
34 H	4.7326506	0.0000000	1.6671683 *
35 H	4.6632507	1.6671683 *	0.0000000

* ... LESS THAN 3.000

NUCLEAR ENERGY = 931.4200141894
 ELECTRONIC ENERGY = -1216.0569930385
 TOTAL ENERGY = -284.6369788491

SPIN SZ = 1.500
 S-SQUARED = 3.760

 MOLECULAR ORBITALS

**** ALPHA SET ****

WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
 PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!

	1	2	3	4	5
	-4.2400	-2.8483	-2.8414	-2.8349	-1.3777
	A	A	A	A	A
1 CO 1 S	0.771104	-0.000255	0.003569	-0.005058	-0.017156
2 CO 1 X	0.000798	-0.322020	0.562916	0.547256	0.027991
3 CO 1 Y	-0.004245	0.456968	0.615681	-0.364721	0.005931
4 CO 1 Z	0.003610	0.640471	-0.155748	0.534661	-0.006457
5 CO 1 XX	-0.000479	-0.001105	0.000281	-0.000405	0.015906
6 CO 1 YY	0.000277	-0.000747	-0.000572	-0.000756	-0.007774
7 CO 1 ZZ	0.000202	0.001852	0.000292	0.001161	-0.008132
8 CO 1 XY	0.000074	0.001771	-0.002435	-0.001937	0.006212
9 CO 1 XZ	-0.001981	0.000465	0.001403	0.001238	-0.006789
10 CO 1 YZ	0.001809	-0.001197	0.002270	-0.002106	-0.001657
11 CO 1 XX	0.000288	0.000061	0.000508	-0.000774	0.011593

12 CO 1 YY -0.000629 -0.001020 -0.000796 0.000232 -0.006140
13 CO 1 ZZ 0.000340 0.000960 0.000288 0.000542 -0.005453
14 CO 1 XY 0.000009 0.000210 -0.000176 -0.000465 0.005097
15 CO 1 XZ 0.000143 -0.000074 0.000494 0.000671 -0.005899
16 CO 1 YZ -0.000442 -0.000301 0.000692 -0.001055 -0.000570
17 CO 1 S -0.042030 0.000949 -0.003109 0.003316 0.032416
18 CO 1 X 0.000599 0.004624 -0.004054 -0.003864 -0.026638
19 CO 1 Y -0.012130 -0.004770 -0.004443 0.003922 0.004012
20 CO 1 Z 0.007676 -0.003495 0.001765 -0.001710 0.008383
21 CO 1 S 0.000932 -0.000701 -0.000342 0.001573 0.008426
22 CO 1 X -0.000158 -0.000228 0.000665 0.000796 -0.010483
23 CO 1 Y 0.000345 0.000371 0.001153 -0.000190 -0.001753
24 CO 1 Z -0.000732 0.001399 -0.000232 0.000926 0.004604
25 CO 1 S 0.266689 0.000082 0.000883 -0.001370 -0.015066
26 CO 1 X 0.000482 -0.081021 0.143168 0.140007 0.001199
27 CO 1 Y -0.001055 0.114619 0.156411 -0.093338 -0.000773
28 CO 1 Z 0.000752 0.161302 -0.039926 0.137199 -0.000336
29 CO 1 XX -0.003054 0.001378 0.001441 -0.000293 0.014532
30 CO 1 YY -0.000724 -0.002686 -0.001610 0.001308 -0.000603
31 CO 1 ZZ 0.003778 0.001307 0.000170 -0.001015 -0.013929
32 CO 1 XY 0.001123 0.000602 -0.000463 -0.000867 0.005414
33 CO 1 XZ 0.005924 -0.002081 0.000459 0.000246 -0.002694
34 CO 1 YZ 0.002185 0.000568 0.000434 -0.000768 -0.007599
35 C 2 S -0.000182 0.000028 0.000000 0.000012 -0.000152
36 C 2 X -0.000023 -0.000004 0.000032 0.000000 -0.000086
37 C 2 Y 0.000073 -0.000010 0.000029 -0.000008 0.000076
38 C 2 Z 0.000056 -0.000012 0.000018 0.000013 -0.000008
39 C 2 S 0.019577 -0.004716 -0.000744 0.001481 -0.015352
40 C 2 X -0.007150 0.001683 0.000104 -0.000585 0.003254
41 C 2 Y -0.000814 0.000785 0.003422 -0.000666 -0.002148
42 C 2 Z -0.000167 0.000368 0.001012 -0.000209 -0.000107
43 C 3 S 0.000000 0.000019 -0.000022 0.000011 -0.000256
44 C 3 X 0.000166 -0.000059 0.000018 0.000029 -0.000119
45 C 3 Y 0.000119 -0.000054 0.000019 0.000025 -0.000217
46 C 3 Z 0.000007 -0.000009 0.000013 0.000013 -0.000071
47 C 3 S -0.016799 0.006407 0.002358 -0.003599 0.009397
48 C 3 X 0.007782 -0.002470 -0.000507 0.001241 -0.007642
49 C 3 Y -0.001568 0.000359 0.001807 -0.000017 0.002953
50 C 3 Z 0.000258 -0.000163 0.000637 0.000215 -0.000384
51 C 4 S -0.000350 0.000011 0.000018 0.000122 0.000124
52 C 4 X -0.000135 0.000082 -0.000004 -0.000113 0.000368
53 C 4 Y 0.000051 -0.000049 0.000017 -0.000001 0.000078
54 C 4 Z 0.000170 -0.000014 0.000011 0.000039 -0.000099
55 C 4 S 0.016471 -0.007507 -0.003368 0.006868 -0.028744
56 C 4 X 0.001871 -0.000818 0.002193 -0.000151 0.006378
57 C 4 Y 0.015953 -0.006239 -0.000195 0.003225 -0.009823

58	C	4	Z	0.004181	-0.001663	-0.000561	0.000486	-0.000132
59	C	5	S	-0.000305	-0.000126	-0.000060	-0.000074	0.001505
60	C	5	X	0.000803	-0.000056	-0.000004	0.000063	-0.001536
61	C	5	Y	0.000243	-0.000022	0.000071	0.000051	-0.000254
62	C	5	Z	0.000032	0.000028	0.000054	-0.000048	0.000004
63	C	5	S	-0.038443	0.010543	-0.000075	-0.001880	0.053530
64	C	5	X	-0.009890	0.008405	0.003826	-0.007977	0.010806
65	C	5	Y	-0.023753	0.009336	-0.002706	-0.001020	-0.001200
66	C	5	Z	-0.008735	0.003156	0.000398	-0.000311	-0.003879
67	C	6	S	-0.000244	-0.000020	-0.000143	0.000049	0.000277
68	C	6	X	-0.000029	0.000072	0.000216	0.000030	-0.000550
69	C	6	Y	0.000415	-0.000016	0.000184	0.000078	-0.000644
70	C	6	Z	-0.000091	-0.000022	-0.000004	-0.000005	-0.000367
71	C	6	S	0.023627	-0.001988	-0.003113	-0.006584	0.053641
72	C	6	X	-0.003392	-0.009265	-0.010336	0.009396	-0.005063
73	C	6	Y	-0.032425	0.009600	-0.004997	-0.001036	0.043283
74	C	6	Z	-0.007160	0.002837	-0.001713	-0.000260	0.016414
75	C	7	S	-0.000177	0.000025	-0.000051	0.000044	-0.000099
76	C	7	X	0.000126	-0.000016	0.000015	-0.000017	0.000320
77	C	7	Y	0.000068	-0.000055	-0.000009	-0.000006	0.000020
78	C	7	Z	0.000128	-0.000002	0.000086	0.000041	-0.000149
79	C	7	S	0.007262	0.002608	0.006877	-0.004439	-0.025976
80	C	7	X	-0.019037	0.002250	-0.006397	0.000933	0.023830
81	C	7	Y	0.003369	-0.003057	-0.006623	0.002432	0.001311
82	C	7	Z	-0.000937	-0.000825	-0.002309	0.000443	0.000347
83	C	8	S	-0.000007	0.000003	-0.000026	0.000006	-0.000226
84	C	8	X	0.000081	0.000008	0.000030	-0.000015	0.000189
85	C	8	Y	0.000030	0.000001	0.000016	0.000006	-0.000088
86	C	8	Z	-0.000009	0.000013	0.000012	0.000001	-0.000019
87	C	8	S	-0.012700	0.002554	0.004594	-0.000893	0.009007
88	C	8	X	0.009109	-0.000918	0.001153	-0.000353	-0.010011
89	C	8	Y	0.000035	-0.000517	-0.002100	0.000081	-0.001848
90	C	8	Z	0.000816	-0.000268	-0.000477	0.000153	-0.000945
91	C	9	S	-0.000125	-0.000030	0.000029	0.000051	-0.000198
92	C	9	X	-0.000091	0.000034	0.000053	-0.000009	-0.000040
93	C	9	Y	-0.000075	0.000023	0.000035	-0.000003	0.000142
94	C	9	Z	-0.000023	-0.000003	0.000010	0.000008	-0.000057
95	C	9	S	0.012164	-0.003900	-0.002432	-0.000127	-0.013319
96	C	9	X	0.004929	0.000319	0.000827	0.000168	-0.001181
97	C	9	Y	-0.006546	0.001086	0.001830	0.000246	0.001173
98	C	9	Z	-0.002337	0.000537	0.000671	-0.000029	0.001649
99	C	10	S	0.000126	0.000081	-0.000053	0.000065	-0.000060
100	C	10	X	-0.000026	-0.000003	-0.000048	-0.000059	0.000475
101	C	10	Y	0.000233	-0.000106	-0.000065	-0.000068	-0.000403
102	C	10	Z	0.000181	0.000032	0.000017	-0.000004	0.000224
103	C	10	S	-0.033082	0.004483	0.003762	0.003359	0.017574

104	C	10	X	-0.003594	0.004135	0.003282	-0.001280	0.008327
105	C	10	Y	0.013902	-0.000580	-0.000499	-0.000548	-0.004954
106	C	10	Z	0.004851	-0.000916	-0.001023	-0.000014	-0.003484
107	C	11	S	0.000525	0.000133	-0.000148	-0.000079	0.001498
108	C	11	X	-0.000218	-0.000107	0.000084	0.000059	-0.000358
109	C	11	Y	0.000110	0.000086	0.000260	0.000021	-0.000508
110	C	11	Z	-0.000286	-0.000075	-0.000057	-0.000012	0.000419
111	C	11	S	0.025213	-0.009070	-0.008481	0.006614	-0.032966
112	C	11	X	-0.001582	-0.009344	-0.001984	0.006846	-0.046890
113	C	11	Y	0.029142	-0.003298	0.000392	-0.004288	-0.010669
114	C	11	Z	0.006852	-0.000195	0.001345	-0.001668	-0.005454
115	N	12	S	-0.000629	0.001791	0.002605	-0.002339	0.012579
116	N	12	X	-0.000036	0.000099	0.000611	0.000123	-0.003577
117	N	12	Y	0.000595	-0.001642	-0.002432	0.002166	-0.000418
118	N	12	Z	-0.000007	0.000610	0.000295	-0.000142	0.000252
119	N	12	S	0.009821	0.000959	0.001894	-0.000781	-0.017246
120	N	12	X	0.005631	-0.002850	0.001924	-0.000489	0.003666
121	N	12	Y	-0.019176	-0.002626	-0.001327	0.002676	0.006253
122	N	12	Z	0.001061	0.001079	0.000177	0.000817	-0.002327
123	C	13	S	0.000801	-0.000088	0.000114	0.000078	0.012813
124	C	13	X	0.000246	-0.000013	0.000114	0.000032	-0.000872
125	C	13	Y	0.000749	0.000138	0.000085	-0.000227	-0.005597
126	C	13	Z	0.000040	-0.000110	0.000017	-0.000086	0.002143
127	C	13	S	0.014449	-0.002725	-0.001299	-0.005514	0.185716
128	C	13	X	0.006313	-0.001113	0.002259	0.001819	-0.094903
129	C	13	Y	0.000163	0.000867	0.000519	0.005085	-0.038074
130	C	13	Z	0.001919	-0.001003	0.000141	-0.001443	0.001393
131	C	14	S	0.000291	-0.000090	-0.000010	0.000002	0.032805
132	C	14	X	0.000141	-0.000122	0.000027	0.000140	0.003848
133	C	14	Y	0.000116	0.000113	-0.000027	-0.000125	-0.015652
134	C	14	Z	0.000066	-0.000020	0.000010	0.000009	0.006366
135	C	14	S	0.010830	-0.003614	0.005096	0.007313	0.149444
136	C	14	X	-0.009562	0.001356	0.004987	0.005859	-0.189605
137	C	14	Y	-0.006247	0.000382	-0.004129	-0.000120	-0.195201
138	C	14	Z	0.000437	0.000114	0.001915	0.000770	0.054237
139	C	15	S	0.000473	-0.000086	-0.000089	0.000070	0.183245
140	C	15	X	-0.000463	-0.000196	0.000120	0.000260	0.078108
141	C	15	Y	-0.000237	-0.000017	0.000083	-0.000023	-0.063921
142	C	15	Z	0.000057	0.000024	-0.000085	-0.000043	0.030909
143	C	15	S	-0.018574	-0.004387	0.004256	0.006052	-0.258933
144	C	15	X	0.009645	0.005056	-0.010973	-0.008568	0.002224
145	C	15	Y	-0.006761	0.003275	-0.005696	-0.002709	-0.193244
146	C	15	Z	0.003744	-0.001341	0.001688	0.000628	0.081109
147	C	16	S	-0.000312	-0.000103	0.000043	0.000067	0.034860
148	C	16	X	0.000016	0.000081	-0.000181	-0.000137	0.018562
149	C	16	Y	0.000033	0.000019	0.000001	0.000000	0.003870

150	C	16	Z	-0.000045	0.000033	0.000024	0.000037	0.000025
151	C	16	S	0.012305	0.006863	-0.012811	-0.010371	-0.015481
152	C	16	X	0.003948	0.003432	-0.005108	-0.003609	-0.030945
153	C	16	Y	0.007135	0.001722	-0.003467	-0.003203	0.054478
154	C	16	Z	-0.002434	-0.000299	0.000581	0.000620	-0.025149
155	C	17	S	0.000052	-0.000002	-0.000054	-0.000009	0.003816
156	C	17	X	-0.000009	-0.000042	0.000044	0.000046	0.001721
157	C	17	Y	0.000063	0.000047	-0.000058	-0.000047	-0.000682
158	C	17	Z	-0.000037	-0.000028	0.000020	0.000022	0.000446
159	C	17	S	-0.006584	-0.000632	0.003578	0.002598	-0.051997
160	C	17	X	-0.004076	-0.000553	0.001679	0.001487	-0.007887
161	C	17	Y	-0.002782	-0.001183	0.002353	0.001281	0.002140
162	C	17	Z	0.000806	0.000436	-0.000617	-0.000273	-0.001153
163	C	18	S	-0.000121	-0.000026	0.000043	0.000025	0.002477
164	C	18	X	0.000055	-0.000047	0.000042	0.000017	0.001412
165	C	18	Y	0.000003	-0.000033	0.000027	0.000017	0.000566
166	C	18	Z	-0.000010	0.000012	-0.000002	-0.000003	-0.000065
167	C	18	S	0.012394	0.000282	-0.001574	-0.003526	0.068970
168	C	18	X	0.004380	-0.000350	0.000100	-0.001028	0.019694
169	C	18	Y	-0.001148	-0.000383	0.002143	0.000585	-0.002466
170	C	18	Z	0.000738	0.000068	-0.000910	-0.000270	0.002245
171	C	19	S	-0.000086	-0.000086	0.000018	0.000074	0.004867
172	C	19	X	-0.000130	0.000035	-0.000034	-0.000001	0.000776
173	C	19	Y	0.000110	-0.000006	-0.000028	0.000007	0.000221
174	C	19	Z	-0.000046	-0.000013	0.000015	0.000035	0.000099
175	C	19	S	-0.010094	0.002146	0.003914	0.002856	-0.077606
176	C	19	X	0.005152	-0.000122	0.003051	-0.001044	0.040027
177	C	19	Y	0.004953	-0.001243	-0.000603	-0.001520	0.072462
178	C	19	Z	-0.001091	0.000553	0.000519	0.000255	-0.023786
179	O	20	S	-0.000117	0.001780	-0.003462	-0.001630	0.670656
180	O	20	X	0.000064	0.001489	-0.002930	-0.001164	-0.093616
181	O	20	Y	-0.000123	0.000615	-0.000476	-0.000570	-0.026726
182	O	20	Z	-0.000104	-0.000079	0.000692	0.000632	0.016971
183	O	20	S	0.003346	-0.000025	-0.000832	0.000549	0.140690
184	O	20	X	0.006586	-0.000873	0.000313	0.000202	0.016121
185	O	20	Y	0.003056	-0.000206	0.001755	0.000081	0.015434
186	O	20	Z	-0.000917	0.000152	-0.000399	0.000323	-0.006289
187	N	21	S	-0.000400	-0.002978	0.001911	0.000517	0.003782
188	N	21	X	-0.000264	0.002132	-0.001212	-0.000118	0.000352
189	N	21	Y	0.000043	-0.000197	0.000576	-0.000063	0.000560
190	N	21	Z	0.000301	-0.001888	0.001349	0.000629	0.000681
191	N	21	S	0.004108	0.000028	0.001532	-0.002179	0.000836
192	N	21	X	-0.008335	0.003801	-0.000830	0.000153	-0.012201
193	N	21	Y	0.001837	0.001750	0.001325	-0.002408	-0.004093
194	N	21	Z	0.004864	-0.000334	0.000132	-0.000132	-0.001622
195	H	22	S	-0.000035	0.000007	-0.000046	0.000005	0.000057

196	H	22	S	0.001262	-0.000409	-0.000976	0.000205	0.000966
197	H	23	S	0.000015	-0.000027	0.000005	0.000037	0.000041
198	H	23	S	-0.001775	0.000448	0.000446	-0.000138	0.003174
199	H	24	S	0.000205	-0.000106	0.000040	0.000074	-0.000026
200	H	24	S	0.006649	-0.002493	-0.000099	0.001090	-0.001727
201	H	25	S	-0.000069	0.000013	-0.000032	0.000013	0.000116
202	H	25	S	-0.002394	0.000276	-0.000248	0.000148	0.004090
203	H	26	S	0.000016	0.000029	-0.000021	0.000009	0.000128
204	H	26	S	0.002197	-0.000122	-0.000595	-0.000108	0.001551
205	H	27	S	0.000195	0.000067	0.000065	-0.000039	0.000272
206	H	27	S	-0.002863	0.001854	0.001351	-0.000859	0.003724
207	H	28	S	-0.000162	0.000033	0.000050	-0.000195	0.000376
208	H	28	S	-0.001751	-0.000351	-0.000030	-0.002391	0.002430
209	H	29	S	-0.000031	-0.000054	0.000034	0.000044	0.006710
210	H	29	S	0.002895	0.000643	-0.001127	-0.001057	0.033030
211	H	30	S	-0.000103	-0.000029	0.000021	0.000026	0.000652
212	H	30	S	-0.001464	-0.000271	0.000729	0.000449	0.004563
213	H	31	S	-0.000098	-0.000013	-0.000023	0.000031	-0.000450
214	H	31	S	0.001053	0.000043	-0.000503	-0.000310	0.000970
215	H	32	S	-0.000140	0.000006	-0.000067	0.000034	-0.000187
216	H	32	S	-0.001075	0.000512	-0.000144	0.000669	-0.033765
217	H	33	S	0.000890	-0.000045	0.000502	-0.000135	0.164146
218	H	33	S	0.000182	-0.000011	0.000676	-0.000171	-0.033939
219	H	34	S	-0.000651	0.000143	-0.000099	0.000243	-0.000231
220	H	34	S	-0.001196	0.001399	-0.000152	-0.000432	0.000115
221	H	35	S	-0.000010	0.000253	0.000202	-0.000418	0.000486
222	H	35	S	0.000133	0.001119	0.000740	-0.001095	0.001011

6	7	8	9	10
-1.2366	-1.2177	-1.1291	-1.1121	-1.0660
A	A	A	A	A

1	CO	1	S	-0.023215	-0.016082	0.004786	-0.009798	0.001955
2	CO	1	X	-0.004623	-0.023989	-0.007083	0.000311	0.008376
3	CO	1	Y	-0.026470	0.011075	0.001660	-0.002597	-0.002379
4	CO	1	Z	0.010403	0.018662	0.004965	0.006180	-0.004473
5	CO	1	XX	-0.008009	0.012137	-0.001912	-0.000023	0.001430
6	CO	1	YY	0.017330	-0.019404	-0.003246	0.000120	0.003257
7	CO	1	ZZ	-0.009321	0.007267	0.005158	-0.000097	-0.004686
8	CO	1	XY	-0.005883	-0.000006	-0.008741	-0.005741	-0.003771
9	CO	1	XZ	-0.004336	-0.022375	0.001796	-0.007855	0.007236
10	CO	1	YZ	-0.005026	0.004565	0.002547	-0.000067	-0.002930
11	CO	1	XX	-0.006143	0.009235	-0.002651	0.001449	0.000174
12	CO	1	YY	0.012289	-0.013504	-0.002265	0.000344	0.002576
13	CO	1	ZZ	-0.006146	0.004269	0.004917	-0.001793	-0.002750
14	CO	1	XY	-0.004853	-0.001542	-0.002403	-0.001624	-0.002612
15	CO	1	XZ	-0.003521	-0.014826	-0.000226	-0.005480	0.004752

16 CO 1 YZ -0.002701 0.003438 0.001619 -0.001102 -0.002210
17 CO 1 S 0.052097 0.046097 -0.011299 0.021476 -0.004092
18 CO 1 X -0.002683 0.046159 -0.022195 0.002165 -0.031679
19 CO 1 Y 0.023504 -0.004797 0.005514 -0.018136 0.007689
20 CO 1 Z -0.018753 -0.036184 0.018381 0.003173 0.016210
21 CO 1 S 0.020537 0.025559 0.011427 -0.055953 0.006347
22 CO 1 X 0.011612 0.011781 -0.025808 -0.022471 0.012577
23 CO 1 Y 0.004970 0.005442 0.005650 -0.027826 0.000515
24 CO 1 Z -0.007012 -0.008252 -0.001537 0.013485 -0.004972
25 CO 1 S -0.021712 -0.011493 0.002871 -0.006256 0.001009
26 CO 1 X 0.000722 -0.001284 0.003877 0.000528 0.000849
27 CO 1 Y -0.001836 -0.000210 -0.001052 0.001969 -0.000012
28 CO 1 Z 0.000533 -0.000071 -0.002486 -0.001290 -0.000398
29 CO 1 XX 0.007718 0.004484 0.013149 0.001953 0.009149
30 CO 1 YY 0.002250 -0.012673 0.002035 -0.009988 0.000435
31 CO 1 ZZ -0.009968 0.008188 -0.015185 0.008036 -0.009584
32 CO 1 XY -0.005344 0.007786 -0.017412 -0.012800 -0.003763
33 CO 1 XZ -0.011595 -0.028839 0.011378 0.000435 0.004624
34 CO 1 YZ -0.008440 -0.000213 0.001773 0.008678 -0.000721
35 C 2 S 0.006158 0.013288 -0.039432 -0.174940 0.193332
36 C 2 X -0.002370 -0.005000 0.012661 0.049544 -0.023224
37 C 2 Y -0.000429 -0.002194 0.001831 0.012405 -0.050812
38 C 2 Z -0.000106 -0.000859 0.000781 0.004336 -0.014348
39 C 2 S -0.055428 0.154186 -0.062031 -0.156896 -0.134560
40 C 2 X 0.027425 -0.054044 0.023334 0.055664 0.104152
41 C 2 Y -0.021127 -0.009781 -0.012711 -0.069739 0.018719
42 C 2 Z -0.004569 -0.003754 -0.001183 -0.017554 0.007231
43 C 3 S 0.006789 0.020902 -0.028264 -0.139217 0.251247
44 C 3 X -0.003000 -0.008808 0.008142 0.039032 -0.063457
45 C 3 Y -0.000117 -0.001089 -0.004781 -0.020235 0.018338
46 C 3 Z -0.000211 -0.000943 -0.000941 -0.003699 0.001507
47 C 3 S 0.034506 -0.100364 0.008186 -0.005183 0.010439
48 C 3 X -0.018938 0.039338 -0.023071 -0.047820 -0.010401
49 C 3 Y -0.029780 -0.009674 0.007945 -0.002768 -0.000010
50 C 3 Z -0.009637 -0.002403 -0.000350 -0.002249 0.000097
51 C 4 S 0.024138 0.081176 -0.026275 -0.138608 0.268155
52 C 4 X -0.009989 -0.035308 0.001991 0.008546 -0.004867
53 C 4 Y 0.003443 0.009008 -0.008859 -0.040459 0.058644
54 C 4 Z 0.000597 0.000815 -0.002786 -0.011939 0.017065
55 C 4 S 0.058155 0.124682 -0.094549 -0.141598 -0.045879
56 C 4 X -0.077464 0.004035 0.032593 0.035451 0.047114
57 C 4 Y -0.012729 0.095244 -0.011886 -0.024705 0.001394
58 C 4 Z -0.006029 0.033956 0.001980 -0.006338 0.002262
59 C 5 S 0.083906 0.242528 -0.035010 -0.150997 0.168305
60 C 5 X -0.022493 -0.063168 -0.008596 -0.042096 0.080840
61 C 5 Y -0.008319 -0.061788 -0.022830 -0.059375 0.003069

62	C	5	Z	-0.004480	-0.028693	-0.008864	-0.025070	0.007941
63	C	5	S	0.199992	-0.353257	0.009256	0.048907	-0.153427
64	C	5	X	-0.103540	-0.141142	0.070819	0.100615	0.010533
65	C	5	Y	0.156017	-0.212229	-0.071063	-0.066878	-0.154052
66	C	5	Z	0.039295	-0.089259	-0.026568	-0.011946	-0.049737
67	C	6	S	0.076966	0.059644	-0.108175	-0.295465	0.000077
68	C	6	X	-0.023503	0.004674	0.007561	-0.023504	0.067162
69	C	6	Y	-0.004333	-0.027324	-0.009647	-0.017253	-0.055123
70	C	6	Z	-0.000289	-0.009018	-0.005073	-0.007103	-0.017717
71	C	6	S	0.097718	-0.075111	0.242332	0.451333	0.027718
72	C	6	X	-0.029960	0.376013	-0.112935	-0.156952	0.120573
73	C	6	Y	0.332532	-0.298074	-0.019776	0.063797	-0.191700
74	C	6	Z	0.106979	-0.091109	0.008133	0.019816	-0.058397
75	C	7	S	0.021062	0.018893	-0.079599	-0.285978	0.056447
76	C	7	X	-0.004870	-0.002393	0.011616	0.022773	0.044666
77	C	7	Y	-0.001984	-0.005015	0.004014	0.015643	-0.050856
78	C	7	Z	-0.000787	-0.001489	0.000867	0.003617	-0.013323
79	C	7	S	-0.193254	-0.106353	0.074990	0.127717	-0.003190
80	C	7	X	0.139606	-0.091925	0.040221	0.177846	0.094918
81	C	7	Y	-0.067077	0.142498	-0.012125	0.042953	-0.145402
82	C	7	Z	-0.018340	0.039095	-0.007719	0.014249	-0.038818
83	C	8	S	0.010013	0.002450	-0.051651	-0.176208	-0.101662
84	C	8	X	-0.002573	0.000209	0.010806	0.028149	0.046405
85	C	8	Y	-0.003910	-0.001246	0.011189	0.041277	-0.011312
86	C	8	Z	-0.001022	-0.000191	0.002705	0.010381	-0.003748
87	C	8	S	0.132091	-0.092959	-0.013637	-0.038786	0.141450
88	C	8	X	-0.040162	0.015375	-0.014067	-0.080663	-0.032805
89	C	8	Y	-0.043693	0.030023	0.002218	0.037689	-0.096816
90	C	8	Z	-0.010951	0.007070	0.001420	0.010129	-0.026566
91	C	9	S	0.014930	-0.001465	-0.050210	-0.141785	-0.188669
92	C	9	X	-0.003332	0.000943	0.000666	-0.006706	0.012377
93	C	9	Y	-0.005557	0.000321	0.016032	0.042994	0.048553
94	C	9	Z	-0.001284	0.000124	0.003604	0.010583	0.011245
95	C	9	S	-0.097661	0.086401	0.002910	-0.094257	0.006961
96	C	9	X	-0.000126	-0.021456	0.001461	-0.017177	0.011838
97	C	9	Y	0.036903	-0.021047	-0.018779	-0.002237	0.011089
98	C	9	Z	0.008254	-0.004762	-0.002225	-0.000248	0.003699
99	C	10	S	0.064275	-0.015733	-0.077588	-0.144948	-0.247230
100	C	10	X	-0.003071	0.002020	-0.008922	-0.036266	-0.040912
101	C	10	Y	-0.028319	0.007341	0.020428	0.021894	0.034402
102	C	10	Z	-0.007751	0.001874	0.006891	0.007178	0.010794
103	C	10	S	0.080577	0.014386	-0.083673	-0.067569	-0.006487
104	C	10	X	0.084920	-0.087772	0.002406	0.069638	-0.017756
105	C	10	Y	-0.014330	-0.043752	0.022861	0.022880	-0.024727
106	C	10	Z	-0.004574	-0.008186	0.003267	0.003079	-0.005806
107	C	11	S	0.216240	-0.042908	-0.136920	-0.168176	-0.229067

108	C	11	X	-0.075477	0.033418	0.005358	-0.064255	-0.003608
109	C	11	Y	-0.042303	0.003859	0.007466	-0.013382	-0.040707
110	C	11	Z	-0.002753	-0.001892	-0.000921	-0.004793	-0.017315
111	C	11	S	-0.227247	0.383494	-0.101675	-0.206310	0.115850
112	C	11	X	-0.214229	0.281456	-0.111632	-0.216032	0.160932
113	C	11	Y	-0.036974	-0.116587	0.111795	0.102959	0.014609
114	C	11	Z	-0.014673	-0.041698	0.022853	0.039942	-0.004825
115	N	12	S	0.516056	-0.162879	-0.065577	0.098031	0.018420
116	N	12	X	-0.053764	0.029624	-0.051043	-0.064467	-0.100848
117	N	12	Y	0.089270	-0.032965	-0.019089	0.007869	-0.017850
118	N	12	Z	-0.024568	0.006665	-0.001696	-0.009923	-0.013175
119	N	12	S	-0.069145	0.030720	-0.020413	-0.018476	0.007964
120	N	12	X	0.042274	-0.041653	0.044350	0.030136	0.039685
121	N	12	Y	-0.052705	0.034982	0.010277	-0.046263	0.013240
122	N	12	Z	0.012735	0.006910	-0.015274	-0.007660	-0.000064
123	C	13	S	0.305879	-0.111927	0.115310	0.088761	0.159793
124	C	13	X	0.125634	-0.043058	-0.063504	0.051758	-0.003580
125	C	13	Y	-0.057201	0.020129	-0.025988	-0.016352	-0.033027
126	C	13	Z	0.028717	-0.011850	0.003616	0.010462	0.007581
127	C	13	S	0.008813	-0.057044	0.386733	0.009560	0.057131
128	C	13	X	0.072492	0.009679	-0.210343	0.003031	0.035360
129	C	13	Y	-0.024340	0.038883	-0.119545	-0.039631	-0.040367
130	C	13	Z	0.021852	-0.011730	0.014313	0.009356	0.015110
131	C	14	S	0.083233	-0.036076	0.330852	-0.065697	0.095771
132	C	14	X	0.031338	-0.011697	-0.033316	0.034948	0.040365
133	C	14	Y	0.007633	-0.002171	-0.018082	0.014661	0.018592
134	C	14	Z	0.000397	-0.000206	0.004231	-0.002663	-0.003497
135	C	14	S	-0.070348	0.050777	-0.258597	-0.079578	-0.102484
136	C	14	X	-0.006198	0.037786	-0.283133	0.012484	-0.007395
137	C	14	Y	0.140430	-0.024752	-0.184266	0.070524	0.065917
138	C	14	Z	-0.056720	0.010208	0.045787	-0.022978	-0.022714
139	C	15	S	0.018229	-0.013845	0.280764	-0.102328	-0.030961
140	C	15	X	0.002005	-0.002431	-0.049305	0.030705	0.042837
141	C	15	Y	0.015983	-0.005394	0.058871	-0.010373	0.025518
142	C	15	Z	-0.006316	0.002102	-0.027939	0.006792	-0.006766
143	C	15	S	0.101555	-0.033900	-0.149671	0.066006	0.033481
144	C	15	X	0.060890	-0.003519	0.054723	0.016798	0.052795
145	C	15	Y	0.109977	-0.017455	-0.017713	0.050762	0.069593
146	C	15	Z	-0.035134	0.008369	0.011690	-0.019600	-0.023631
147	C	16	S	0.003795	-0.004566	0.227596	-0.107769	-0.116348
148	C	16	X	0.000915	-0.000777	0.027501	-0.009367	0.003450
149	C	16	Y	0.002110	-0.001458	0.059062	-0.025862	-0.021732
150	C	16	Z	-0.000731	0.000318	-0.020791	0.009169	0.008713
151	C	16	S	0.069955	0.007367	0.048437	0.009615	0.071396
152	C	16	X	0.043656	-0.006124	0.008893	0.023768	0.038103
153	C	16	Y	-0.004956	0.011541	-0.019984	-0.004673	0.017465

154	C	16	Z	0.004178	-0.004992	0.009226	0.004704	-0.003832
155	C	17	S	0.003643	-0.002855	0.188541	-0.092899	-0.114730
156	C	17	X	0.001396	-0.001300	0.057012	-0.026134	-0.026474
157	C	17	Y	0.000230	-0.000068	0.015929	-0.006644	-0.003686
158	C	17	Z	0.000000	-0.000064	-0.001846	0.000671	-0.000540
159	C	17	S	0.002155	-0.009409	0.013256	0.009918	-0.011595
160	C	17	X	-0.008179	-0.003267	0.013452	-0.001354	-0.014353
161	C	17	Y	-0.012296	0.003070	0.006688	-0.012373	-0.008559
162	C	17	Z	0.004700	-0.001350	-0.002051	0.003955	0.002197
163	C	18	S	0.005125	-0.003614	0.186941	-0.084347	-0.076287
164	C	18	X	0.002818	-0.001719	0.050580	-0.019237	-0.005071
165	C	18	Y	-0.000131	0.000116	-0.027391	0.014565	0.021700
166	C	18	Z	0.000281	-0.000169	0.014910	-0.007273	-0.008865
167	C	18	S	0.037000	-0.009271	0.043045	-0.004663	0.052918
168	C	18	X	0.022338	-0.002995	0.004385	-0.004800	0.029316
169	C	18	Y	-0.007405	0.001227	0.010236	-0.004690	0.001165
170	C	18	Z	0.004400	-0.001486	-0.002895	0.001981	0.002058
171	C	19	S	0.020902	-0.010650	0.240530	-0.081596	-0.000910
172	C	19	X	0.006029	-0.002971	0.017304	0.004691	0.030070
173	C	19	Y	-0.005020	0.002349	-0.058530	0.021382	0.005474
174	C	19	Z	0.002584	-0.001346	0.024312	-0.007848	0.000437
175	C	19	S	-0.090821	0.030947	-0.031938	-0.008528	-0.046827
176	C	19	X	-0.006929	0.002085	0.049786	-0.017909	0.028041
177	C	19	Y	0.008852	-0.011397	0.079001	-0.011458	0.016499
178	C	19	Z	-0.003344	0.006379	-0.027365	0.001711	-0.004738
179	O	20	S	-0.032275	0.006661	-0.108228	0.033374	0.009809
180	O	20	X	0.006492	0.002689	-0.026627	0.015302	0.010720
181	O	20	Y	0.011593	-0.003619	0.062469	-0.016023	0.008120
182	O	20	Z	-0.005139	0.002195	-0.032276	0.009105	-0.003167
183	O	20	S	-0.020822	0.001284	-0.051795	0.016567	-0.009903
184	O	20	X	-0.014590	-0.000175	-0.025659	0.004560	-0.007825
185	O	20	Y	-0.011227	0.001601	-0.000749	-0.011944	-0.009154
186	O	20	Z	0.002479	-0.006343	0.002450	0.003753	0.005825
187	N	21	S	0.160140	0.560099	0.053720	0.133654	-0.094510
188	N	21	X	0.014448	0.058539	0.002041	-0.009568	0.026185
189	N	21	Y	0.008420	0.008588	-0.008966	-0.024520	0.017272
190	N	21	Z	-0.008433	-0.039882	-0.009229	-0.026438	0.024982
191	N	21	S	0.013520	0.014237	0.028524	0.032067	-0.037643
192	N	21	X	0.013079	-0.009432	-0.031934	-0.017793	-0.014341
193	N	21	Y	-0.024637	-0.017201	0.015614	0.015327	0.011908
194	N	21	Z	-0.015135	-0.022033	0.003268	0.005643	0.002054
195	H	22	S	0.000694	0.000415	-0.004613	-0.022453	0.029250
196	H	22	S	0.001670	0.009502	0.000653	0.013795	-0.038561
197	H	23	S	-0.000033	0.002036	-0.002838	-0.016470	0.038782
198	H	23	S	0.002209	-0.005662	0.009679	0.014613	0.003424
199	H	24	S	0.002863	0.014786	-0.002470	-0.017363	0.045558

200	H	24	S	0.001571	0.040624	-0.000785	-0.008965	0.001758
201	H	25	S	0.000215	0.000409	-0.006275	-0.022940	-0.014352
202	H	25	S	0.016985	-0.005333	0.007470	0.024400	0.033418
203	H	26	S	0.001297	-0.000905	-0.005683	-0.016867	-0.029750
204	H	26	S	-0.005080	0.001899	0.008622	0.003151	-0.004769
205	H	27	S	0.012032	-0.004771	-0.010429	-0.018134	-0.042681
206	H	27	S	0.034300	-0.025901	0.003485	0.028994	0.001685
207	H	28	S	0.040841	-0.015264	0.018686	0.014099	0.029200
208	H	28	S	0.008056	-0.013114	0.018807	0.016147	0.013390
209	H	29	S	-0.000921	-0.000178	0.030578	-0.016419	-0.021777
210	H	29	S	-0.003072	0.005143	-0.012879	-0.004875	0.004532
211	H	30	S	-0.000216	-0.000153	0.024946	-0.013249	-0.019293
212	H	30	S	-0.003530	-0.000117	0.015844	-0.008635	-0.008447
213	H	31	S	0.000283	-0.000265	0.023268	-0.011370	-0.012399
214	H	31	S	0.009937	-0.000775	-0.000267	-0.003791	0.004609
215	H	32	S	0.002947	-0.001516	0.034350	-0.011231	0.001868
216	H	32	S	0.007839	0.004174	-0.044843	0.003928	-0.007181
217	H	33	S	-0.015211	0.003175	-0.055020	0.013984	-0.004863
218	H	33	S	0.006850	0.003940	-0.008487	-0.010471	0.001356
219	H	34	S	0.040609	0.138673	0.014126	0.042367	-0.040056
220	H	34	S	-0.013410	-0.026166	-0.005696	0.020527	-0.008274
221	H	35	S	0.036024	0.141989	0.019936	0.047506	-0.028223
222	H	35	S	-0.012483	-0.022768	0.011639	0.010486	-0.004972

11	12	13	14	15
-1.0438	-1.0177	-1.0130	-0.9925	-0.9692
A	A	A	A	A

1	CO	1	S	0.000962	-0.005144	0.007213	0.009377	-0.005067
2	CO	1	X	0.003476	0.008080	-0.004043	0.003074	-0.006871
3	CO	1	Y	0.009865	0.005600	-0.002134	0.005913	0.000348
4	CO	1	Z	0.001997	-0.006364	-0.003442	-0.004721	0.006857
5	CO	1	XX	0.010575	0.011400	0.004603	0.001715	-0.006638
6	CO	1	YY	-0.016567	-0.005132	-0.001591	-0.004175	-0.001319
7	CO	1	ZZ	0.005992	-0.006267	-0.003013	0.002460	0.007957
8	CO	1	XY	-0.007113	0.017548	0.007707	-0.001436	0.000985
9	CO	1	XZ	-0.004916	-0.006954	0.009220	0.005957	-0.010647
10	CO	1	YZ	0.004068	-0.003708	-0.000173	0.002859	0.007638
11	CO	1	XX	0.006920	0.005714	0.002687	0.000963	-0.003424
12	CO	1	YY	-0.011092	-0.002554	-0.001579	-0.002393	-0.000624
13	CO	1	ZZ	0.004173	-0.003160	-0.001108	0.001430	0.004049
14	CO	1	XY	-0.003326	0.009437	0.004327	-0.000793	0.001873
15	CO	1	XZ	-0.003654	-0.003840	0.005085	0.003673	-0.006077
16	CO	1	YZ	0.002628	-0.001852	0.000498	0.001779	0.004792
17	CO	1	S	-0.002569	0.010259	-0.018530	-0.026304	0.016879
18	CO	1	X	-0.014326	0.001656	-0.001177	-0.004360	0.032202
19	CO	1	Y	-0.010348	-0.003389	0.017365	-0.018459	-0.002910

20	CO	1	Z	0.003386	0.002915	0.006723	0.006991	-0.019055
21	CO	1	S	0.009835	0.008982	0.023372	0.001863	-0.003503
22	CO	1	X	-0.002786	0.000761	0.003583	0.002675	-0.008543
23	CO	1	Y	0.007953	0.002221	0.013056	0.003145	-0.001527
24	CO	1	Z	-0.003413	-0.000284	-0.006381	-0.000825	0.001770
25	CO	1	S	0.000599	-0.004479	0.004713	0.006409	-0.002265
26	CO	1	X	0.001202	-0.001626	-0.000203	0.000320	-0.001462
27	CO	1	Y	-0.001471	-0.000371	-0.001403	0.000194	0.000699
28	CO	1	Z	-0.000716	0.000909	0.000409	0.000539	0.000597
29	CO	1	XX	0.007402	0.002238	0.000760	0.005121	-0.006631
30	CO	1	YY	-0.004402	0.000070	0.008511	-0.006785	-0.001337
31	CO	1	ZZ	-0.003000	-0.002309	-0.009271	0.001664	0.007968
32	CO	1	XY	-0.011961	0.014357	0.009521	-0.001265	-0.000561
33	CO	1	XZ	0.002074	-0.005627	0.004776	0.000943	-0.005860
34	CO	1	YZ	0.001889	-0.003940	-0.004941	0.003188	0.001350
35	C	2	S	0.020199	-0.073779	-0.226777	-0.060690	0.287693
36	C	2	X	-0.015764	0.011212	0.027850	0.057063	0.004465
37	C	2	Y	0.026962	-0.001002	0.006729	-0.070311	-0.058872
38	C	2	Z	0.007124	-0.000122	0.002129	-0.018128	-0.015527
39	C	2	S	0.082541	-0.005063	0.066476	0.068207	-0.150972
40	C	2	X	-0.054072	-0.004092	-0.047755	-0.043144	0.132279
41	C	2	Y	0.034306	-0.019676	-0.039293	-0.024700	0.055907
42	C	2	Z	0.008176	-0.004883	-0.010919	-0.009843	0.016827
43	C	3	S	-0.062420	-0.035470	-0.132976	0.214874	0.236049
44	C	3	X	0.020367	0.000389	0.005651	-0.052599	0.004362
45	C	3	Y	0.009756	-0.015209	-0.045741	-0.046885	0.079275
46	C	3	Z	0.003849	-0.004052	-0.011961	-0.016578	0.021314
47	C	3	S	0.023211	-0.018950	-0.077875	-0.014213	0.088572
48	C	3	X	0.005933	-0.002105	0.009803	0.027162	0.008709
49	C	3	Y	0.022644	-0.006039	-0.008584	-0.013338	-0.017145
50	C	3	Z	0.006544	-0.002721	-0.003415	-0.001161	-0.002461
51	C	4	S	-0.111650	0.018747	0.035115	0.317153	-0.110207
52	C	4	X	0.011917	-0.016966	-0.055610	0.012862	0.113195
53	C	4	Y	-0.020162	0.001295	-0.000403	0.026577	0.008568
54	C	4	Z	-0.005509	-0.000172	-0.001954	0.007652	0.006975
55	C	4	S	-0.020134	0.010156	0.055721	-0.062413	-0.079743
56	C	4	X	0.005538	-0.003050	0.004305	0.046824	-0.011602
57	C	4	Y	-0.005728	0.003099	0.034962	-0.053356	-0.021715
58	C	4	Z	-0.001730	0.002763	0.013382	-0.015655	-0.008940
59	C	5	S	-0.106210	0.067192	0.196190	0.050518	-0.276695
60	C	5	X	-0.025413	-0.000392	-0.004437	0.097289	-0.040263
61	C	5	Y	-0.013389	0.018341	0.052927	-0.094441	-0.004320
62	C	5	Z	-0.008219	0.007955	0.021769	-0.024080	-0.008609
63	C	5	S	0.006552	0.017119	-0.104886	-0.038555	0.170140
64	C	5	X	0.052707	-0.021148	-0.068214	0.080607	0.113704
65	C	5	Y	0.028546	-0.001336	-0.086365	-0.075532	0.131368

66	C	5	Z	0.010924	-0.004584	-0.034411	-0.016192	0.050575
67	C	6	S	-0.046201	0.077419	0.233765	-0.253357	-0.082569
68	C	6	X	0.029014	-0.024822	-0.060932	-0.036387	-0.055881
69	C	6	Y	0.043046	-0.017101	-0.043638	-0.022603	0.072927
70	C	6	Z	0.011001	-0.004133	-0.010675	-0.006926	0.024868
71	C	6	S	-0.061000	0.036143	-0.023015	0.009462	-0.102187
72	C	6	X	-0.088060	0.003520	0.072049	-0.009654	-0.189645
73	C	6	Y	-0.040690	0.031161	-0.110562	-0.131083	0.172773
74	C	6	Z	-0.010693	0.011340	-0.035233	-0.043985	0.045122
75	C	7	S	0.125174	-0.067938	-0.167228	-0.288586	0.009356
76	C	7	X	-0.003537	-0.023347	-0.076100	0.019837	0.078837
77	C	7	Y	0.047476	-0.020487	-0.050339	0.018259	-0.047028
78	C	7	Z	0.013242	-0.006099	-0.015062	0.004928	-0.010907
79	C	7	S	0.067629	-0.023409	-0.000509	0.014864	0.060750
80	C	7	X	-0.129423	0.025079	-0.045715	-0.060218	0.105730
81	C	7	Y	0.051497	0.001632	0.049057	0.015608	-0.229648
82	C	7	Z	0.011578	0.000065	0.012216	0.005218	-0.056339
83	C	8	S	0.211231	-0.090393	-0.214922	-0.042880	-0.180229
84	C	8	X	-0.041880	0.007602	0.011654	-0.056420	0.051349
85	C	8	Y	-0.015676	0.009695	0.025046	0.075778	-0.018730
86	C	8	Z	-0.003365	0.002306	0.006088	0.021046	-0.005432
87	C	8	S	-0.081115	0.011037	-0.035847	0.001479	0.150036
88	C	8	X	0.067929	-0.024597	-0.029772	-0.025890	-0.039717
89	C	8	Y	0.047195	-0.005011	0.008923	-0.008520	-0.104849
90	C	8	Z	0.013854	-0.001584	0.001982	-0.000790	-0.031035
91	C	9	S	0.200402	-0.055234	-0.118226	0.234171	-0.166746
92	C	9	X	0.019731	-0.016935	-0.042229	-0.060017	-0.052744
93	C	9	Y	-0.043504	0.008600	0.016137	-0.036461	0.016565
94	C	9	Z	-0.010558	0.002170	0.004291	-0.006452	0.004551
95	C	9	S	0.043874	-0.016206	-0.002186	0.002964	-0.051788
96	C	9	X	0.011080	-0.008916	-0.018360	-0.002038	0.033648
97	C	9	Y	0.002094	-0.004878	-0.018242	0.025328	-0.006610
98	C	9	Z	-0.001065	-0.000301	-0.003737	0.003723	-0.001218
99	C	10	S	0.102518	0.011804	0.040498	0.316060	0.082648
100	C	10	X	0.043796	-0.008823	-0.014437	0.033347	-0.040371
101	C	10	Y	0.028381	-0.019924	-0.047495	0.010759	-0.076277
102	C	10	Z	0.005514	-0.005091	-0.012450	0.001529	-0.018654
103	C	10	S	-0.079975	0.013100	0.009983	-0.086884	0.089102
104	C	10	X	-0.005432	0.001512	-0.030725	-0.056370	0.024147
105	C	10	Y	0.041609	-0.009818	-0.012432	0.072030	0.014768
106	C	10	Z	0.013857	-0.004131	-0.004713	0.027840	-0.000252
107	C	11	S	-0.089508	0.079625	0.194930	0.040818	0.224002
108	C	11	X	0.044577	0.012553	0.054651	-0.056705	-0.049744
109	C	11	Y	0.065525	-0.012296	-0.024489	0.114093	0.008411
110	C	11	Z	0.009627	-0.001105	-0.003320	0.032884	0.015608
111	C	11	S	-0.027588	-0.006775	0.110322	0.127558	-0.137914

112	C	11	X	0.030767	-0.044992	0.057086	0.072201	-0.121938
113	C	11	Y	0.103361	-0.026689	-0.056483	0.099559	-0.056454
114	C	11	Z	0.028201	-0.007937	-0.012249	0.027179	-0.001287
115	N	12	S	-0.124727	-0.024779	-0.088644	-0.035333	0.007346
116	N	12	X	-0.086148	0.048014	0.100073	-0.002353	0.160501
117	N	12	Y	-0.019865	0.004400	-0.010228	0.028980	0.022481
118	N	12	Z	-0.003908	0.004552	0.014326	0.006975	0.023681
119	N	12	S	-0.030956	-0.007733	-0.013249	0.001237	0.002918
120	N	12	X	0.040981	-0.023377	-0.038062	0.022187	-0.041698
121	N	12	Y	0.003155	0.005722	0.022131	-0.013367	-0.000009
122	N	12	Z	-0.002813	-0.002642	-0.001177	0.003694	0.002559
123	C	13	S	0.192719	-0.012827	-0.059059	0.002567	-0.177173
124	C	13	X	-0.097340	-0.039371	-0.095828	-0.004744	-0.037037
125	C	13	Y	-0.026268	0.026258	0.006310	0.015295	0.027818
126	C	13	Z	-0.000453	-0.011693	-0.009390	-0.000635	-0.007682
127	C	13	S	-0.028278	0.041006	-0.104394	-0.040815	-0.123586
128	C	13	X	0.077381	-0.058941	0.007078	0.090346	-0.002755
129	C	13	Y	-0.008481	-0.023853	0.048423	0.016792	0.048640
130	C	13	Z	0.014788	0.001014	-0.012931	0.012180	-0.012723
131	C	14	S	0.280917	0.039426	0.180013	0.005466	0.064517
132	C	14	X	0.039469	-0.054003	-0.010514	-0.002271	-0.073261
133	C	14	Y	0.034874	0.110217	-0.039671	0.000953	-0.031760
134	C	14	Z	-0.008428	-0.046450	0.014664	0.000655	0.005792
135	C	14	S	-0.112881	0.010650	0.016618	0.062683	0.099388
136	C	14	X	0.085575	-0.093912	0.072542	0.041901	0.032417
137	C	14	Y	0.095820	-0.024953	0.007637	0.050408	0.009938
138	C	14	Z	-0.031152	0.000043	0.002971	-0.021584	-0.004631
139	C	15	S	-0.010634	-0.319557	0.175091	0.006533	0.091254
140	C	15	X	0.092364	0.052914	0.033991	-0.000398	0.021728
141	C	15	Y	0.078890	0.039849	0.045786	-0.000111	0.028481
142	C	15	Z	-0.023786	-0.009648	-0.016438	0.000212	-0.010183
143	C	15	S	0.057906	-0.101910	-0.007889	0.042300	-0.016596
144	C	15	X	0.047932	-0.002214	0.031708	-0.008303	0.012735
145	C	15	Y	0.104866	0.019180	0.004021	0.018482	-0.014528
146	C	15	Z	-0.035101	-0.005900	-0.000331	-0.004940	0.007662
147	C	16	S	-0.253343	-0.269957	-0.054560	-0.000501	-0.075755
148	C	16	X	0.020647	-0.083015	0.065959	0.003201	0.047590
149	C	16	Y	-0.040085	-0.015913	-0.013595	-0.000822	-0.005817
150	C	16	Z	0.017010	-0.000464	0.010342	0.000604	0.005763
151	C	16	S	0.081619	0.060951	0.024648	-0.005593	-0.004664
152	C	16	X	0.049825	0.016326	0.013083	-0.000143	0.000727
153	C	16	Y	0.036206	0.076881	0.013310	-0.003903	0.019769
154	C	16	Z	-0.010803	-0.029538	-0.003256	0.000256	-0.007312
155	C	17	S	-0.257313	0.057016	-0.209649	-0.009299	-0.135633
156	C	17	X	-0.053682	-0.026536	-0.020669	-0.000501	-0.012210
157	C	17	Y	0.001008	0.091029	-0.028336	-0.001776	0.009899

158	C	17	Z	-0.004430	-0.037640	0.009572	0.000612	-0.004708
159	C	17	S	-0.018130	-0.050003	-0.015550	-0.000888	-0.013992
160	C	17	X	-0.009022	-0.039542	0.018858	-0.000555	0.027628
161	C	17	Y	0.000812	-0.003604	0.006981	0.001819	0.011616
162	C	17	Z	-0.000512	-0.001035	-0.001442	0.000108	-0.002332
163	C	18	S	-0.125967	0.321326	-0.183141	-0.007536	-0.015460
164	C	18	X	0.010983	0.071732	-0.001745	0.000865	0.030923
165	C	18	Y	0.054044	0.009106	0.040707	0.002329	0.036880
166	C	18	Z	-0.020173	0.002640	-0.016157	-0.000851	-0.011883
167	C	18	S	0.066210	0.069244	-0.006460	0.015881	-0.036817
168	C	18	X	0.049267	-0.006707	0.022583	0.014232	-0.009815
169	C	18	Y	0.009264	0.012136	-0.007997	-0.001608	-0.007225
170	C	18	Z	-0.000074	-0.005841	0.005151	0.000910	0.001827
171	C	19	S	0.096206	0.346472	-0.006863	0.002644	0.102095
172	C	19	X	0.075673	-0.047929	0.068087	0.002547	0.010778
173	C	19	Y	-0.006177	-0.032317	-0.003819	-0.000158	-0.015920
174	C	19	Z	0.008967	0.008717	0.007130	0.000423	0.006979
175	C	19	S	-0.016399	-0.055855	0.026735	-0.027432	0.011561
176	C	19	X	0.058656	0.006512	0.013712	0.006238	-0.029541
177	C	19	Y	0.015343	0.091665	-0.012382	0.004216	0.008323
178	C	19	Z	0.000212	-0.034234	0.006200	0.001215	-0.004641
179	O	20	S	0.009387	0.105779	-0.044181	-0.000672	-0.014421
180	O	20	X	0.018835	0.086935	-0.033830	-0.005161	-0.019472
181	O	20	Y	0.032288	-0.115658	0.081607	0.000104	0.047517
182	O	20	Z	-0.013996	0.061635	-0.042711	0.000178	-0.024574
183	O	20	S	0.005224	0.067650	-0.030098	0.000114	0.001525
184	O	20	X	-0.005422	0.019968	-0.014106	-0.003509	-0.000565
185	O	20	Y	-0.007565	-0.012304	0.012068	-0.000382	0.008958
186	O	20	Z	0.002657	0.006924	-0.003691	-0.000512	-0.006840
187	N	21	S	0.064978	-0.035041	-0.090709	-0.030901	0.096381
188	N	21	X	-0.015261	0.008924	0.031235	0.035454	-0.071528
189	N	21	Y	-0.023547	0.019734	0.054232	-0.016607	-0.061505
190	N	21	Z	-0.020908	0.016280	0.041951	0.009207	-0.060923
191	N	21	S	0.050062	-0.024567	-0.060569	-0.005180	0.079962
192	N	21	X	-0.001331	0.001832	-0.011426	0.003745	0.006795
193	N	21	Y	0.003393	-0.004856	-0.002141	0.013485	0.000749
194	N	21	Z	-0.000477	-0.000840	-0.002020	0.002399	-0.003906
195	H	22	S	0.005333	-0.014794	-0.046022	-0.014550	0.060885
196	H	22	S	0.006074	0.007842	0.024011	0.023083	-0.060708
197	H	23	S	-0.010780	-0.006182	-0.023913	0.043367	0.050278
198	H	23	S	0.001496	0.001116	0.000580	-0.011392	-0.019220
199	H	24	S	-0.020100	0.003336	0.006189	0.073752	-0.026729
200	H	24	S	-0.000886	0.000860	0.009403	-0.023305	-0.002220
201	H	25	S	0.035579	-0.017747	-0.043808	-0.010869	-0.034972
202	H	25	S	-0.036675	0.010709	0.011864	0.016745	0.038649
203	H	26	S	0.032708	-0.009768	-0.021493	0.047397	-0.035466

204	H	26	S	-0.006237	0.003968	0.007074	-0.012258	0.012664
205	H	27	S	0.018421	0.002818	0.005919	0.074240	0.020845
206	H	27	S	-0.003075	0.002340	-0.013973	-0.036030	-0.004850
207	H	28	S	0.045377	0.008991	-0.009778	0.007821	-0.038488
208	H	28	S	0.011806	0.014249	-0.017841	0.006403	-0.013172
209	H	29	S	-0.051002	-0.058880	-0.012706	-0.000015	-0.020640
210	H	29	S	0.013826	0.038706	0.003827	-0.000250	0.009906
211	H	30	S	-0.046303	0.010020	-0.041414	-0.002046	-0.032079
212	H	30	S	-0.003131	-0.011961	0.010453	0.001077	0.015867
213	H	31	S	-0.021884	0.060911	-0.035121	-0.001569	-0.003258
214	H	31	S	0.009435	-0.014164	0.011814	0.005860	0.001841
215	H	32	S	0.022846	0.073202	-0.000730	0.000730	0.022178
216	H	32	S	-0.009709	-0.045590	0.002549	0.003254	-0.004344
217	H	33	S	-0.019389	0.077899	-0.052070	0.000268	-0.028851
218	H	33	S	-0.000245	0.002878	-0.002989	0.003023	-0.005758
219	H	34	S	0.026401	-0.015470	-0.042458	-0.022947	0.062647
220	H	34	S	-0.000505	-0.003594	-0.019161	0.000005	0.013778
221	H	35	S	0.026049	-0.018338	-0.047043	0.007004	0.047212
222	H	35	S	0.004858	-0.004484	-0.009536	0.009007	0.014581

16	17	18	19	20
-0.9310	-0.9071	-0.8804	-0.8744	-0.8617

A	A	A	A	A
---	---	---	---	---

1	CO	1	S	0.014020	-0.012255	-0.029171	-0.021822	0.010089
2	CO	1	X	-0.001538	0.019690	0.012612	-0.006539	-0.009921
3	CO	1	Y	0.024525	-0.000058	-0.005573	-0.017583	0.000152
4	CO	1	Z	-0.002611	0.000984	-0.000405	0.007478	0.013067
5	CO	1	XX	0.013762	0.050548	0.016456	-0.000683	-0.049296
6	CO	1	YY	-0.038003	-0.037297	0.008833	0.015922	0.003866
7	CO	1	ZZ	0.024241	-0.013251	-0.025290	-0.015240	0.045430
8	CO	1	XY	0.007896	-0.018558	0.029771	0.018361	-0.042731
9	CO	1	XZ	-0.010280	-0.006057	-0.026652	-0.017653	0.008159
10	CO	1	YZ	0.005639	0.007564	-0.008177	-0.024489	0.009962
11	CO	1	XX	0.006421	0.027052	0.007533	-0.000451	-0.023832
12	CO	1	YY	-0.020147	-0.020245	0.004468	0.008021	0.001121
13	CO	1	ZZ	0.013726	-0.006807	-0.012001	-0.007570	0.022711
14	CO	1	XY	0.003716	-0.009137	0.015889	0.008956	-0.022136
15	CO	1	XZ	-0.005096	-0.003977	-0.014092	-0.009270	0.004783
16	CO	1	YZ	0.003390	0.003530	-0.003825	-0.012495	0.005439
17	CO	1	S	-0.040841	0.033609	0.077684	0.057083	-0.024507
18	CO	1	X	0.004961	-0.033802	0.006802	0.006741	0.004055
19	CO	1	Y	-0.034318	0.012795	0.036234	0.030643	-0.009020
20	CO	1	Z	0.002274	0.001077	-0.012949	-0.009874	-0.011335
21	CO	1	S	0.014272	-0.004118	0.011337	0.000267	0.007278
22	CO	1	X	-0.001869	0.009952	-0.007732	-0.000788	0.012236
23	CO	1	Y	0.006250	0.002551	0.003142	-0.002112	0.003965

24	CO	1	Z	-0.002298	-0.003267	0.000913	0.001805	-0.007559
25	CO	1	S	0.009085	-0.009040	-0.021761	-0.017520	0.007622
26	CO	1	X	0.000876	-0.000490	-0.001945	-0.000147	0.000468
27	CO	1	Y	-0.001646	-0.001836	-0.001427	0.000051	-0.000078
28	CO	1	Z	-0.000208	0.000099	0.001353	-0.000460	-0.001666
29	CO	1	XX	0.005624	0.015954	-0.007197	-0.001712	-0.008198
30	CO	1	YY	-0.012082	-0.004795	0.015801	0.006911	-0.003482
31	CO	1	ZZ	0.006458	-0.011159	-0.008604	-0.005200	0.011680
32	CO	1	XY	0.003601	-0.020228	0.004803	0.012663	-0.006493
33	CO	1	XZ	-0.003691	0.007635	-0.005291	-0.006432	-0.002176
34	CO	1	YZ	0.000720	0.003834	-0.007864	-0.011479	0.002050
35	C	2	S	0.075746	0.033646	-0.098217	0.162027	-0.192938
36	C	2	X	-0.003968	-0.002342	0.052950	0.063877	0.034391
37	C	2	Y	-0.023322	-0.014873	-0.051470	-0.087816	-0.101803
38	C	2	Z	-0.006274	-0.003985	-0.012969	-0.022090	-0.027449
39	C	2	S	-0.095454	-0.033536	0.168597	-0.057563	0.141302
40	C	2	X	0.065410	0.028579	-0.087641	0.066945	-0.085391
41	C	2	Y	0.008809	0.019219	-0.036013	-0.014183	-0.099623
42	C	2	Z	0.004116	0.006007	-0.012711	-0.000823	-0.028728
43	C	3	S	0.029208	0.007503	0.164928	0.116855	0.203472
44	C	3	X	0.010755	0.005685	-0.004115	0.049003	-0.015645
45	C	3	Y	0.038868	0.023246	-0.057899	0.117047	-0.081162
46	C	3	Z	0.011325	0.006886	-0.017320	0.034794	-0.024741
47	C	3	S	0.025678	0.018023	-0.086039	-0.113816	-0.131460
48	C	3	X	-0.008865	-0.003685	0.086332	0.086326	0.102104
49	C	3	Y	-0.009867	0.001516	-0.029945	-0.031951	-0.071595
50	C	3	Z	-0.002783	0.000583	-0.004637	-0.006197	-0.015110
51	C	4	S	-0.101166	-0.058583	0.082933	-0.250101	0.045329
52	C	4	X	0.024156	0.006041	0.103055	0.023452	0.160334
53	C	4	Y	0.009529	0.009783	-0.004289	0.060318	0.026986
54	C	4	Z	0.003877	0.003640	0.003040	0.019858	0.012849
55	C	4	S	-0.042675	-0.034342	0.057357	0.243652	0.041309
56	C	4	X	-0.013627	0.002019	0.025066	-0.055502	0.002818
57	C	4	Y	-0.001183	-0.000491	0.011914	0.147059	0.004859
58	C	4	Z	-0.000829	-0.000614	0.005648	0.044323	0.001713
59	C	5	S	-0.045330	-0.001041	-0.125714	0.120816	-0.188888
60	C	5	X	-0.030453	-0.017825	-0.013345	-0.157369	0.008166
61	C	5	Y	0.046982	0.032525	0.003217	0.131255	0.114117
62	C	5	Z	0.010164	0.010063	0.001535	0.031611	0.021406
63	C	5	S	0.121630	0.010410	-0.060534	0.005858	0.103150
64	C	5	X	0.043822	0.044168	0.022731	-0.165580	0.051987
65	C	5	Y	0.082370	0.015309	-0.025539	0.102974	0.096648
66	C	5	Z	0.026559	0.006523	-0.007398	0.018682	0.025263
67	C	6	S	0.110084	0.062215	0.027139	0.074962	0.220145
68	C	6	X	0.009779	0.021873	-0.118560	-0.029664	-0.012713
69	C	6	Y	0.026612	0.001280	0.046138	-0.167034	0.083911

70	C	6	Z	0.005132	-0.000975	0.019905	-0.051579	0.019854
71	C	6	S	0.040536	-0.051418	-0.125847	-0.089979	0.008571
72	C	6	X	-0.155800	-0.097368	0.059888	0.004378	-0.099891
73	C	6	Y	0.140977	-0.021558	-0.105478	0.154345	0.097653
74	C	6	Z	0.043787	-0.006444	-0.037044	0.053343	0.036326
75	C	7	S	0.006160	-0.003531	-0.100456	-0.198663	-0.062150
76	C	7	X	-0.011442	-0.010933	-0.054796	0.042424	-0.175743
77	C	7	Y	-0.082791	-0.053271	0.070940	-0.081499	-0.035775
78	C	7	Z	-0.023001	-0.014722	0.019373	-0.022519	-0.013626
79	C	7	S	0.006329	0.060294	0.030880	-0.063396	-0.033910
80	C	7	X	0.091981	-0.006495	-0.125242	0.127358	-0.015257
81	C	7	Y	-0.131629	-0.080930	0.103899	-0.110392	0.038980
82	C	7	Z	-0.034731	-0.022763	0.030470	-0.031095	0.008961
83	C	8	S	-0.223180	-0.121524	0.151861	-0.068960	-0.018459
84	C	8	X	0.020022	-0.002451	-0.032428	-0.073438	-0.078105
85	C	8	Y	-0.016793	-0.001818	0.036723	0.121424	0.029819
86	C	8	Z	-0.005228	-0.000708	0.010439	0.033608	0.007348
87	C	8	S	0.101496	0.053885	-0.088939	0.214479	0.028687
88	C	8	X	-0.062551	-0.025101	0.052502	-0.105098	-0.038225
89	C	8	Y	-0.070994	-0.040087	0.060799	-0.064129	0.015214
90	C	8	Z	-0.020442	-0.010454	0.014858	-0.016772	0.003277
91	C	9	S	-0.092044	-0.003115	0.032040	0.274174	0.063224
92	C	9	X	-0.094938	-0.060845	0.108964	-0.027194	0.033418
93	C	9	Y	-0.004428	-0.006056	0.002054	0.027826	-0.009896
94	C	9	Z	-0.000406	-0.000425	-0.001353	0.010444	-0.004329
95	C	9	S	-0.026764	-0.011924	-0.027173	-0.164325	-0.098868
96	C	9	X	0.001048	0.004196	0.007776	-0.017731	-0.019464
97	C	9	Y	-0.015253	0.005598	0.029610	0.152650	0.054471
98	C	9	Z	-0.001615	0.000463	0.008201	0.040716	0.016721
99	C	10	S	0.177227	0.107191	-0.196508	0.001532	-0.111401
100	C	10	X	-0.014351	0.007163	0.035179	0.063744	0.067474
101	C	10	Y	-0.035820	0.005738	-0.025328	0.138645	0.019547
102	C	10	Z	-0.011804	0.000692	-0.006977	0.037652	-0.001057
103	C	10	S	-0.046072	-0.036916	0.130614	0.170884	0.064444
104	C	10	X	-0.019488	-0.024109	0.073150	0.067188	0.077546
105	C	10	Y	0.035076	0.035043	-0.060106	-0.023615	-0.039323
106	C	10	Z	0.005678	0.012438	-0.022143	-0.007846	-0.018080
107	C	11	S	0.053564	-0.024289	0.120310	-0.141123	-0.026233
108	C	11	X	0.084023	0.054030	0.040780	0.013597	0.157947
109	C	11	Y	0.112372	0.063796	-0.133036	-0.094306	-0.034751
110	C	11	Z	0.014643	0.009741	-0.022343	-0.026222	-0.030416
111	C	11	S	-0.108230	-0.022006	0.021552	-0.095525	-0.154032
112	C	11	X	-0.119917	0.019159	0.070581	-0.027963	-0.104354
113	C	11	Y	0.042051	0.059735	-0.107347	-0.041776	-0.017950
114	C	11	Z	0.018452	0.017841	-0.026965	-0.019992	-0.009101
115	N	12	S	-0.188578	-0.055411	0.014364	0.062788	-0.028215

116	N	12	X	-0.101261	-0.101623	0.156311	-0.011889	-0.127504
117	N	12	Y	0.036394	-0.023015	-0.071698	-0.081518	-0.023529
118	N	12	Z	-0.014531	-0.002362	0.021759	-0.010583	-0.036017
119	N	12	S	-0.090927	-0.068125	0.025530	0.016899	-0.027734
120	N	12	X	-0.014319	0.023491	-0.013210	-0.000119	-0.018293
121	N	12	Y	-0.006806	0.001260	0.029857	-0.006576	-0.013185
122	N	12	Z	-0.004384	-0.000183	0.003049	-0.003217	-0.008513
123	C	13	S	0.283680	0.050932	-0.057964	-0.042895	0.111415
124	C	13	X	-0.098809	0.019567	-0.149625	0.014294	0.052190
125	C	13	Y	0.044254	-0.060167	-0.045046	-0.049105	-0.003487
126	C	13	Z	-0.019658	0.022075	-0.005125	0.005408	-0.006651
127	C	13	S	0.046758	-0.045223	-0.110845	0.065863	0.140780
128	C	13	X	-0.013492	0.082558	0.001253	-0.065741	-0.090053
129	C	13	Y	0.027340	-0.029231	0.039923	-0.032220	-0.036857
130	C	13	Z	-0.008576	0.021540	-0.017152	0.002056	-0.004838
131	C	14	S	0.060647	-0.036251	0.199401	0.008817	-0.137341
132	C	14	X	0.113268	0.117307	0.037103	-0.022132	0.044704
133	C	14	Y	0.116909	-0.112123	-0.010111	-0.005631	0.041748
134	C	14	Z	-0.030182	0.050975	0.006225	-0.002616	-0.014097
135	C	14	S	-0.049372	-0.150431	-0.062997	-0.050569	-0.033768
136	C	14	X	0.065906	0.093713	0.148908	-0.063531	-0.138624
137	C	14	Y	-0.112334	0.144746	-0.003911	-0.032208	-0.079089
138	C	14	Z	0.044907	-0.045761	0.016778	0.006639	0.022926
139	C	15	S	-0.170250	0.053124	-0.100487	-0.009181	0.038281
140	C	15	X	-0.073670	0.222964	0.045482	-0.035239	-0.013706
141	C	15	Y	-0.015223	0.050368	0.150332	0.014471	-0.139426
142	C	15	Z	0.004698	-0.011458	-0.055909	-0.008343	0.053917
143	C	15	S	-0.005118	0.065899	0.062230	-0.024383	-0.117652
144	C	15	X	-0.096179	0.061223	-0.061526	0.015655	0.051092
145	C	15	Y	-0.043419	0.109421	0.003615	-0.009092	-0.030400
146	C	15	Z	0.013930	-0.039902	-0.006901	0.004233	0.013801
147	C	16	S	0.154091	-0.208133	-0.030090	0.026478	0.034851
148	C	16	X	-0.085274	-0.073521	-0.139695	0.007063	0.083539
149	C	16	Y	-0.000351	0.027187	0.040297	0.001323	-0.044456
150	C	16	Z	-0.005729	-0.018417	-0.027206	0.000103	0.024223
151	C	16	S	-0.059294	0.167438	0.027055	-0.003299	0.002228
152	C	16	X	-0.039985	0.024098	-0.044143	0.005508	0.032228
153	C	16	Y	-0.043141	0.107012	0.045411	-0.011714	-0.025749
154	C	16	Z	0.011561	-0.040469	-0.021257	0.005401	0.013748
155	C	17	S	0.163757	0.200412	0.206864	-0.028576	-0.105366
156	C	17	X	0.021848	-0.053892	-0.005734	0.012543	-0.005003
157	C	17	Y	-0.066830	0.094443	-0.039461	-0.012851	0.029060
158	C	17	Z	0.027730	-0.041827	0.014600	0.006033	-0.011504
159	C	17	S	0.001591	-0.063807	-0.101624	0.006396	0.077678
160	C	17	X	-0.052202	-0.087130	-0.100698	0.015879	0.057058
161	C	17	Y	-0.010462	-0.015876	-0.024538	-0.002378	0.014372

162	C	17	Z	0.000881	-0.000174	0.001518	0.001881	-0.001905
163	C	18	S	-0.126213	0.191135	-0.123394	-0.023160	0.103852
164	C	18	X	-0.051593	-0.079355	-0.061645	0.016429	0.019886
165	C	18	Y	-0.051874	-0.081979	-0.096701	0.011590	0.061483
166	C	18	Z	0.016102	0.025350	0.032463	-0.003319	-0.022228
167	C	18	S	0.114409	-0.056824	0.039138	-0.018343	-0.011394
168	C	18	X	0.076097	-0.068375	0.040217	-0.009223	-0.032587
169	C	18	Y	0.002283	0.019637	-0.032682	-0.007791	0.037172
170	C	18	Z	0.004323	-0.013338	0.016182	0.002785	-0.016416
171	C	19	S	-0.123570	-0.211576	-0.139188	0.028048	0.061054
172	C	19	X	0.082713	-0.084365	0.113408	0.004910	-0.081938
173	C	19	Y	0.024756	-0.007364	-0.032564	-0.005666	0.043473
174	C	19	Z	-0.001676	-0.004708	0.021785	0.002054	-0.023867
175	C	19	S	0.020334	0.085150	0.086522	0.003945	-0.025358
176	C	19	X	0.119277	-0.053684	0.031000	-0.016655	0.006780
177	C	19	Y	-0.001268	-0.117935	-0.065257	0.013002	0.040467
178	C	19	Z	0.012752	0.040416	0.027188	-0.007230	-0.016932
179	O	20	S	0.018594	0.040262	0.048499	-0.004175	-0.036633
180	O	20	X	0.048868	0.033136	0.162559	0.032239	-0.141877
181	O	20	Y	-0.165833	0.304583	-0.040339	-0.044293	0.039202
182	O	20	Z	0.089602	-0.165144	0.022030	0.022933	-0.018395
183	O	20	S	0.010706	0.039551	0.045611	-0.012535	-0.034881
184	O	20	X	0.023557	-0.000937	0.064755	0.007642	-0.050563
185	O	20	Y	-0.027743	0.061347	-0.005796	-0.010299	0.009723
186	O	20	Z	0.015492	-0.033087	0.002375	0.005676	-0.004506
187	N	21	S	0.027656	0.006363	0.014415	-0.005446	0.044181
188	N	21	X	-0.025324	-0.015044	-0.061120	-0.041596	-0.138556
189	N	21	Y	-0.011548	0.003644	-0.015229	0.184238	-0.075610
190	N	21	Z	-0.020984	0.002334	-0.024269	0.037947	-0.128883
191	N	21	S	0.037936	0.030250	-0.000507	-0.016355	0.042833
192	N	21	X	0.004142	-0.005419	-0.016144	0.000778	-0.026972
193	N	21	Y	-0.002007	0.007834	-0.004370	0.017379	-0.020553
194	N	21	Z	-0.001751	0.000473	-0.007507	0.006549	-0.027252
195	H	22	S	0.013659	0.004771	-0.025671	0.046702	-0.073924
196	H	22	S	-0.023011	-0.015966	0.030492	-0.014928	0.044575
197	H	23	S	0.006210	0.000875	0.054927	0.033815	0.069182
198	H	23	S	-0.001988	-0.000876	-0.031919	-0.032909	-0.040930
199	H	24	S	-0.031050	-0.021068	0.032714	-0.106815	0.012658
200	H	24	S	0.004094	-0.000595	0.000277	0.042767	-0.000814
201	H	25	S	-0.057468	-0.035226	0.042723	-0.016887	-0.024971
202	H	25	S	0.038117	0.016000	-0.029981	0.042382	0.002978
203	H	26	S	-0.022890	-0.000846	0.006679	0.092332	0.015312
204	H	26	S	0.011054	-0.001675	-0.013452	-0.052951	-0.017513
205	H	27	S	0.053117	0.030341	-0.082446	0.001298	-0.055472
206	H	27	S	-0.004098	-0.016231	0.025426	0.016333	0.034122
207	H	28	S	0.110881	-0.009005	-0.037800	-0.037103	0.035070

208	H	28	S	-0.008452	0.018829	-0.024014	0.002543	0.004171
209	H	29	S	0.050626	-0.075222	-0.019769	0.008095	0.027025
210	H	29	S	-0.015901	0.033617	0.013445	-0.005609	-0.006823
211	H	30	S	0.046497	0.061289	0.070945	-0.010822	-0.036662
212	H	30	S	-0.023841	-0.033400	-0.035228	0.004323	0.017271
213	H	31	S	-0.033628	0.057272	-0.042431	-0.008740	0.040993
214	H	31	S	0.019354	-0.026084	0.019737	-0.001449	-0.020843
215	H	32	S	-0.022007	-0.069991	-0.053459	0.006222	0.035603
216	H	32	S	-0.002108	0.050521	0.018397	-0.010553	-0.015762
217	H	33	S	0.101207	-0.188408	0.014022	0.022939	-0.011342
218	H	33	S	0.010156	-0.005225	0.001755	-0.000736	0.001812
219	H	34	S	0.022023	0.004158	0.029271	0.019591	0.101142
220	H	34	S	0.002372	-0.001161	-0.000750	0.000983	0.008664
221	H	35	S	0.008647	-0.003653	0.003552	-0.116823	0.034071
222	H	35	S	0.000707	-0.000064	0.005405	-0.021154	0.004333

21	22	23	24	25
-0.8421	-0.8252	-0.8099	-0.8032	-0.7892

A	A	A	A	A
---	---	---	---	---

1	CO	1	S	0.010648	-0.051265	-0.003685	-0.013160	0.021429
2	CO	1	X	-0.007950	0.046096	0.014037	0.013069	0.003386
3	CO	1	Y	0.005958	-0.001114	0.010508	0.029578	0.036050
4	CO	1	Z	0.000686	-0.004508	0.006962	-0.010373	-0.006996
5	CO	1	XX	0.067190	0.117444	0.048298	0.192770	0.071028
6	CO	1	YY	-0.069089	-0.039182	-0.128449	-0.147420	-0.113519
7	CO	1	ZZ	0.001899	-0.078262	0.080152	-0.045350	0.042491
8	CO	1	XY	0.029699	0.018036	0.070654	0.044521	0.045530
9	CO	1	XZ	-0.000819	-0.054638	-0.056698	-0.074079	-0.023250
10	CO	1	YZ	0.011447	0.004206	-0.028756	0.011991	0.060609
11	CO	1	XX	0.034879	0.057445	0.022438	0.092740	0.032022
12	CO	1	YY	-0.034380	-0.019016	-0.060720	-0.070118	-0.051807
13	CO	1	ZZ	-0.000499	-0.038429	0.038281	-0.022622	0.019785
14	CO	1	XY	0.015943	0.009713	0.034944	0.019823	0.022167
15	CO	1	XZ	-0.000926	-0.027327	-0.028744	-0.036053	-0.010421
16	CO	1	YZ	0.005396	0.001301	-0.013086	0.004413	0.028978
17	CO	1	S	-0.021804	0.139310	0.011314	0.031892	-0.058037
18	CO	1	X	0.005303	-0.022498	0.003220	-0.001624	0.021847
19	CO	1	Y	0.001821	0.025364	0.012758	-0.020665	-0.026525
20	CO	1	Z	0.002365	-0.013635	-0.031915	0.015283	0.008999
21	CO	1	S	-0.004536	0.003183	0.006094	-0.025206	0.002429
22	CO	1	X	0.000045	0.009994	0.004948	-0.002119	-0.002020
23	CO	1	Y	0.003832	0.003628	0.006318	-0.011476	-0.003216
24	CO	1	Z	-0.001865	-0.003417	-0.006246	0.010525	-0.002179
25	CO	1	S	0.009991	-0.038117	-0.001477	-0.010783	0.017463
26	CO	1	X	-0.000618	-0.007213	-0.002069	-0.002720	-0.004150
27	CO	1	Y	-0.000688	-0.001480	-0.002036	-0.002867	-0.002497

28 CO 1 Z -0.000151 0.002430 0.000987 0.000617 0.000402
29 CO 1 XX 0.009913 0.017465 -0.015872 0.034085 0.002650
30 CO 1 YY -0.009251 -0.001933 -0.013527 -0.018488 -0.010074
31 CO 1 ZZ -0.000662 -0.015532 0.029398 -0.015597 0.007424
32 CO 1 XY 0.006747 -0.016097 0.011415 0.003996 0.008711
33 CO 1 XZ 0.003706 -0.011871 -0.011266 -0.006791 -0.000381
34 CO 1 YZ 0.004747 0.002698 -0.016822 0.004218 0.017155
35 C 2 S 0.063610 -0.046684 -0.104627 -0.011055 -0.021605
36 C 2 X 0.058557 -0.048416 -0.035285 0.085006 -0.046170
37 C 2 Y -0.003539 0.004595 0.023278 -0.053561 -0.040305
38 C 2 Z 0.000446 0.000445 0.002929 -0.011323 -0.011837
39 C 2 S 0.040858 -0.064542 -0.001861 0.040886 -0.121363
40 C 2 X -0.012251 0.022593 -0.033999 -0.012595 0.032647
41 C 2 Y 0.005146 0.012782 -0.018772 -0.053252 -0.020033
42 C 2 Z 0.001826 0.003608 -0.005111 -0.014882 -0.004328
43 C 3 S 0.051313 -0.033109 0.017323 0.129801 -0.028742
44 C 3 X 0.036798 -0.031987 -0.036497 0.071710 -0.048529
45 C 3 Y 0.027698 -0.025699 -0.078721 0.007732 0.027368
46 C 3 Z 0.009135 -0.007624 -0.027388 0.007351 0.007408
47 C 3 S -0.035455 0.071555 -0.046653 -0.040773 0.008212
48 C 3 X 0.039519 -0.044141 0.037323 0.042114 -0.033884
49 C 3 Y 0.001815 0.003888 -0.007600 -0.032487 0.010867
50 C 3 Z 0.001472 -0.000643 -0.000955 -0.007371 0.002137
51 C 4 S -0.042455 0.036315 0.069218 -0.078318 -0.035298
52 C 4 X -0.001475 0.009515 0.060409 0.047692 -0.017751
53 C 4 Y -0.009346 0.005869 0.036673 -0.024915 0.072135
54 C 4 Z -0.001784 0.004702 -0.001386 0.006547 0.026147
55 C 4 S 0.099129 -0.118624 0.126485 -0.008311 -0.090083
56 C 4 X -0.004839 0.002390 -0.009678 -0.002100 0.015781
57 C 4 Y 0.050206 -0.072356 0.000095 0.007259 -0.005706
58 C 4 Z 0.015655 -0.021947 -0.000614 0.003672 -0.000818
59 C 5 S 0.066585 -0.053680 0.018781 0.014231 -0.015444
60 C 5 X -0.085780 0.054547 -0.016136 -0.126588 0.104133
61 C 5 Y -0.034996 0.021047 0.080285 -0.061015 0.122187
62 C 5 Z -0.009856 0.021245 -0.039884 0.022246 0.060905
63 C 5 S -0.043838 0.088575 0.234608 0.051820 0.019192
64 C 5 X -0.062227 0.100121 -0.069470 0.034013 0.058094
65 C 5 Y -0.008844 0.055186 0.185878 0.028044 -0.027317
66 C 5 Z -0.005809 0.025961 0.039416 0.020400 -0.002784
67 C 6 S -0.065805 0.027715 -0.062342 0.037689 0.069813
68 C 6 X -0.118822 0.085727 0.054457 -0.078780 0.103896
69 C 6 Y -0.049399 0.026198 -0.043979 0.037801 -0.082504
70 C 6 Z -0.014488 0.013001 -0.037867 0.016755 -0.022673
71 C 6 S -0.008485 -0.042647 -0.176985 0.148167 0.107672
72 C 6 X 0.059174 -0.123712 -0.053817 -0.017948 -0.044783
73 C 6 Y 0.016501 0.027601 0.246972 0.106341 0.000795

74	C	6	Z	0.005451	0.006286	0.080469	0.030568	-0.000477
75	C	7	S	-0.097815	0.073865	0.052299	-0.065342	-0.022094
76	C	7	X	0.061073	-0.035162	0.005526	-0.058951	-0.012015
77	C	7	Y	0.088132	-0.057865	0.061015	0.066642	-0.111449
78	C	7	Z	0.024961	-0.015209	0.010049	0.018931	-0.031088
79	C	7	S	0.004063	0.042940	-0.087731	-0.011436	0.061429
80	C	7	X	-0.026779	0.015083	0.030752	0.046400	0.088212
81	C	7	Y	0.058648	-0.087475	-0.048224	0.088111	-0.037566
82	C	7	Z	0.015011	-0.022485	-0.016379	0.026843	-0.009040
83	C	8	S	0.153210	-0.090652	0.085685	0.073938	-0.000098
84	C	8	X	0.026450	-0.019220	0.053661	-0.005008	-0.040871
85	C	8	Y	0.034859	-0.023557	-0.044977	-0.006396	0.103497
86	C	8	Z	0.009745	-0.006238	-0.013738	-0.002026	0.027815
87	C	8	S	-0.076760	0.099455	0.039392	-0.106511	0.107877
88	C	8	X	0.059495	-0.042225	0.052007	0.011352	-0.064807
89	C	8	Y	0.051101	-0.040686	-0.002515	0.048789	0.013257
90	C	8	Z	0.012870	-0.010938	-0.000653	0.011912	0.002018
91	C	9	S	-0.032288	0.033364	-0.110109	-0.080154	0.129200
92	C	9	X	0.096127	-0.060625	0.015117	0.061319	0.057684
93	C	9	Y	0.010935	-0.000980	-0.016317	-0.038931	0.085767
94	C	9	Z	0.000054	0.001947	-0.006640	-0.014373	0.021772
95	C	9	S	0.061904	-0.056276	0.073399	0.020781	-0.055495
96	C	9	X	-0.003476	-0.008481	-0.006231	0.000589	-0.049508
97	C	9	Y	-0.025628	0.035905	-0.045566	-0.050510	0.064325
98	C	9	Z	-0.003528	0.008675	-0.011564	-0.012060	0.021819
99	C	10	S	-0.093590	0.045700	0.062159	-0.032317	-0.102459
100	C	10	X	-0.033395	0.017142	-0.077882	0.010439	-0.051458
101	C	10	Y	-0.058603	0.052556	-0.044450	-0.088080	0.058648
102	C	10	Z	-0.018372	0.016758	-0.013771	-0.032199	0.014116
103	C	10	S	0.060935	0.000427	0.037099	-0.003464	0.011910
104	C	10	X	0.019296	0.006063	-0.036874	0.009672	0.027493
105	C	10	Y	-0.068359	0.016947	-0.036432	-0.023979	-0.050255
106	C	10	Z	-0.027404	0.007197	-0.008943	-0.010483	-0.022200
107	C	11	S	0.117439	-0.084611	-0.025415	0.043456	-0.022821
108	C	11	X	-0.035664	-0.000118	-0.083004	0.101552	-0.151531
109	C	11	Y	-0.046148	0.006725	0.087010	0.081241	-0.091129
110	C	11	Z	-0.015594	0.009846	0.004599	-0.004569	-0.030641
111	C	11	S	-0.032350	-0.096185	-0.147508	-0.110286	-0.123264
112	C	11	X	-0.022708	-0.012244	-0.070995	-0.088023	-0.010139
113	C	11	Y	-0.106014	0.055094	-0.074626	-0.025472	0.000265
114	C	11	Z	-0.026379	0.016742	-0.027558	-0.006431	0.002084
115	N	12	S	-0.102103	0.074840	-0.040137	-0.075081	-0.031189
116	N	12	X	0.130480	-0.039900	-0.028100	-0.181442	0.134371
117	N	12	Y	0.087815	-0.058380	0.102588	0.093596	0.231665
118	N	12	Z	-0.008451	0.011743	-0.034627	-0.039549	-0.023236
119	N	12	S	-0.058767	0.056770	-0.074670	-0.113680	-0.015148

120	N	12	X	-0.013250	0.007582	-0.024688	-0.007093	0.018644
121	N	12	Y	0.033677	0.008356	0.039662	0.020115	0.068286
122	N	12	Z	-0.005542	-0.000925	-0.001308	-0.008705	-0.012356
123	C	13	S	0.136693	-0.094749	0.008246	0.075705	0.040083
124	C	13	X	-0.113302	0.058585	0.081606	0.153171	0.058536
125	C	13	Y	0.169506	-0.038876	0.068699	0.008057	0.251328
126	C	13	Z	-0.062303	0.012786	-0.013473	0.013391	-0.059042
127	C	13	S	0.036152	-0.066023	-0.098368	0.012898	-0.116300
128	C	13	X	-0.018682	-0.013274	0.031349	0.026606	0.079040
129	C	13	Y	0.022286	-0.011728	0.013076	-0.043292	0.026921
130	C	13	Z	-0.012727	0.001726	0.000854	0.011405	-0.000457
131	C	14	S	-0.103798	-0.065771	-0.017957	-0.063821	-0.017869
132	C	14	X	0.083074	-0.080687	-0.065143	-0.044569	-0.116368
133	C	14	Y	0.162546	0.076963	-0.057077	-0.104268	-0.031922
134	C	14	Z	-0.053377	-0.046041	0.014671	0.033397	0.006820
135	C	14	S	0.004635	-0.069198	0.021142	-0.096087	0.019675
136	C	14	X	-0.034969	0.028237	0.058549	0.011032	0.087974
137	C	14	Y	-0.068379	0.061837	0.064894	0.103373	0.104097
138	C	14	Z	0.026811	-0.019805	-0.020335	-0.034778	-0.026992
139	C	15	S	-0.042948	-0.133808	0.029174	0.043289	0.060175
140	C	15	X	0.091146	0.019426	-0.044353	-0.136336	-0.031794
141	C	15	Y	-0.194021	-0.026689	0.062154	0.085366	0.048487
142	C	15	Z	0.072224	-0.012480	-0.032837	-0.052670	-0.025301
143	C	15	S	-0.103747	0.142566	0.099868	0.159604	0.135102
144	C	15	X	-0.006870	-0.063872	-0.022774	0.014879	-0.037511
145	C	15	Y	0.000086	0.068531	0.015024	0.056274	0.040187
146	C	15	Z	-0.004567	-0.034227	-0.005176	-0.026063	-0.021933
147	C	16	S	0.071905	0.177242	-0.004177	0.048833	-0.069746
148	C	16	X	-0.024416	-0.121333	0.016621	0.078915	0.028070
149	C	16	Y	-0.074053	-0.038626	0.044776	0.057602	0.089341
150	C	16	Z	0.024370	-0.000582	-0.017257	-0.018282	-0.033665
151	C	16	S	0.050438	-0.039565	-0.027483	-0.035889	-0.017912
152	C	16	X	0.010473	-0.025974	-0.022836	0.003132	-0.025209
153	C	16	Y	-0.007893	-0.071575	-0.001979	-0.043666	0.018144
154	C	16	Z	0.004284	0.022743	-0.003399	0.017590	-0.008248
155	C	17	S	0.029779	-0.006520	-0.027288	-0.127514	0.027208
156	C	17	X	-0.027789	0.059687	0.033051	0.082839	0.019706
157	C	17	Y	-0.038356	-0.162693	0.008756	0.033213	0.041938
158	C	17	Z	0.012179	0.066716	-0.001096	-0.006863	-0.015010
159	C	17	S	-0.001808	-0.017916	-0.011329	0.064199	-0.035726
160	C	17	X	-0.036176	0.002632	0.010488	0.070734	-0.023751
161	C	17	Y	-0.012303	-0.018121	0.017536	0.038749	0.015794
162	C	17	Z	0.001762	0.008155	-0.005077	-0.009547	-0.008290
163	C	18	S	0.004041	-0.174111	-0.009298	0.053970	-0.029146
164	C	18	X	-0.016170	0.098137	0.024832	0.055214	0.002123
165	C	18	Y	0.032362	0.066878	-0.006367	0.033616	-0.065521

166	C	18	Z	-0.013756	-0.018797	0.004350	-0.008947	0.025964
167	C	18	S	0.165214	0.038458	-0.053865	-0.135212	0.004730
168	C	18	X	0.067055	0.056851	-0.003021	-0.043363	0.034238
169	C	18	Y	0.016389	-0.040507	-0.003994	0.025986	-0.007237
170	C	18	Z	-0.000837	0.020588	0.000701	-0.013954	0.005387
171	C	19	S	0.071729	0.216524	-0.011937	-0.029673	-0.045087
172	C	19	X	0.014456	0.046581	-0.014964	-0.098440	0.037934
173	C	19	Y	0.094258	0.052580	-0.034094	-0.049214	-0.054984
174	C	19	Z	-0.034193	-0.018336	0.011593	0.009672	0.025742
175	C	19	S	-0.084673	-0.025386	0.004466	0.014882	-0.049971
176	C	19	X	0.108831	-0.002844	-0.033363	-0.066539	0.005400
177	C	19	Y	0.083642	0.052927	-0.031730	-0.059703	-0.027339
178	C	19	Z	-0.023262	-0.022418	0.009580	0.016650	0.010933
179	O	20	S	0.024939	0.108222	0.023462	0.025215	0.026337
180	O	20	X	-0.083009	0.289679	0.127549	0.258936	0.058902
181	O	20	Y	0.237245	0.211678	0.000414	-0.049587	0.017316
182	O	20	Z	-0.152038	-0.162975	-0.009450	-0.000529	-0.025647
183	O	20	S	0.040007	0.109020	0.034777	0.011831	0.050783
184	O	20	X	-0.039097	0.103153	0.057253	0.093846	0.028525
185	O	20	Y	0.061717	0.050699	0.005192	-0.019271	0.006875
186	O	20	Z	-0.039969	-0.049508	-0.010287	0.001032	-0.009923
187	N	21	S	-0.009704	0.005622	0.003677	0.020717	0.000643
188	N	21	X	0.046798	-0.052321	-0.226849	0.118586	-0.043348
189	N	21	Y	0.109642	-0.078138	0.338830	-0.017086	-0.240656
190	N	21	Z	0.072479	0.007660	-0.192228	0.237507	-0.034670
191	N	21	S	-0.012318	0.024188	0.004163	0.038976	0.002872
192	N	21	X	0.009547	0.002477	-0.023894	0.029634	-0.025101
193	N	21	Y	0.029566	-0.012662	0.057759	0.009968	-0.054090
194	N	21	Z	0.018447	-0.003082	-0.053699	0.073213	-0.007985
195	H	22	S	0.038948	-0.030938	-0.039602	0.010992	-0.033792
196	H	22	S	0.007551	-0.013166	0.013228	0.022176	0.000595
197	H	23	S	0.024044	-0.017926	0.005274	0.070362	-0.033028
198	H	23	S	-0.009835	0.009640	-0.013864	-0.008446	0.009104
199	H	24	S	-0.012599	0.011247	0.005272	-0.015467	-0.046790
200	H	24	S	0.014378	-0.025519	-0.013184	0.004007	-0.006395
201	H	25	S	0.066219	-0.043054	0.034694	0.023598	0.009558
202	H	25	S	-0.022079	0.012303	-0.022522	-0.003387	0.014772
203	H	26	S	-0.010302	0.013085	-0.045805	-0.046347	0.081243
204	H	26	S	0.006162	-0.011318	0.008760	0.016287	-0.012641
205	H	27	S	-0.026297	0.019186	0.047810	-0.033796	0.005763
206	H	27	S	0.027401	-0.001133	0.000333	0.006084	0.038550
207	H	28	S	0.141394	-0.050860	0.038983	0.024422	0.148936
208	H	28	S	0.012815	0.006980	0.015870	0.020485	0.038408
209	H	29	S	0.058173	0.085839	-0.026094	-0.017850	-0.078269
210	H	29	S	0.003363	-0.022743	-0.007660	-0.028181	-0.010615
211	H	30	S	0.024054	0.002017	-0.023476	-0.083760	-0.005367

212	H	30	S	-0.013752	-0.000116	0.004787	0.017270	-0.005452
213	H	31	S	0.012827	-0.072271	-0.012370	0.011125	-0.029887
214	H	31	S	0.007701	0.021205	0.004272	-0.010029	0.011773
215	H	32	S	0.070333	0.103329	-0.019364	-0.038028	-0.037394
216	H	32	S	-0.023551	-0.010301	0.015639	0.027294	0.017879
217	H	33	S	-0.146241	-0.177662	-0.020161	-0.012083	-0.026043
218	H	33	S	-0.011332	-0.007216	0.005239	-0.000763	-0.003090
219	H	34	S	-0.033790	-0.002628	0.227983	-0.159783	-0.017448
220	H	34	S	-0.009997	0.004374	0.024827	-0.008305	-0.001313
221	H	35	S	-0.059417	0.036336	-0.243312	0.031151	0.137570
222	H	35	S	-0.002741	0.005437	-0.038399	0.010470	0.021937

	26	27	28	29	30
	-0.7644	-0.7586	-0.7504	-0.7399	-0.7273
	A	A	A	A	A

1	CO	1	S	0.039526	0.038208	-0.008599	0.000249	-0.008409
2	CO	1	X	-0.025248	0.044842	0.010510	0.029377	0.008010
3	CO	1	Y	0.002485	0.013523	0.006939	-0.002606	-0.002488
4	CO	1	Z	0.001037	-0.019783	-0.005082	-0.007981	0.000611
5	CO	1	XX	-0.075220	-0.012710	-0.015441	0.007198	-0.097760
6	CO	1	YY	-0.014984	-0.022616	-0.005991	0.237509	0.093764
7	CO	1	ZZ	0.090204	0.035326	0.021432	-0.244706	0.003995
8	CO	1	XY	-0.117098	0.056482	-0.065659	0.169814	-0.105259
9	CO	1	XZ	0.041938	0.182989	-0.067974	0.298653	0.015141
10	CO	1	YZ	0.025052	-0.058218	0.073065	-0.068245	0.007605
11	CO	1	XX	-0.035046	-0.006024	-0.008923	0.002850	-0.043719
12	CO	1	YY	-0.006727	-0.011405	-0.001994	0.108056	0.041725
13	CO	1	ZZ	0.041773	0.017429	0.010917	-0.110907	0.001994
14	CO	1	XY	-0.055897	0.025085	-0.029553	0.077587	-0.049335
15	CO	1	XZ	0.020991	0.083874	-0.031136	0.136726	0.007968
16	CO	1	YZ	0.011180	-0.026259	0.034384	-0.030472	0.003738
17	CO	1	S	-0.109907	-0.104552	0.021454	0.007781	0.019107
18	CO	1	X	-0.016626	-0.036887	-0.025397	-0.008652	-0.000744
19	CO	1	Y	-0.031448	-0.015065	-0.000517	-0.000852	0.001498
20	CO	1	Z	0.018091	-0.000778	0.004902	-0.001540	0.007010
21	CO	1	S	0.002528	-0.001481	-0.002810	0.004694	-0.006807
22	CO	1	X	-0.010887	0.005490	0.001479	0.000452	-0.005483
23	CO	1	Y	0.000666	0.001771	-0.005792	-0.001411	-0.006069
24	CO	1	Z	0.004935	-0.007286	0.001142	-0.006099	-0.000166
25	CO	1	S	0.029894	0.031103	-0.007939	0.002336	-0.008815
26	CO	1	X	0.006233	-0.003568	0.000529	-0.003234	-0.002768
27	CO	1	Y	0.002270	-0.002255	-0.000824	-0.001316	-0.001911
28	CO	1	Z	-0.001996	0.002172	0.000980	-0.000020	0.000372
29	CO	1	XX	0.008471	-0.023000	0.004564	-0.001172	-0.009832
30	CO	1	YY	-0.016560	0.000078	-0.000852	0.033134	0.015588
31	CO	1	ZZ	0.008088	0.022923	-0.003713	-0.031963	-0.005756

32 CO 1 XY -0.022360 -0.005410 -0.020155 0.017014 -0.006945
33 CO 1 XZ 0.015966 0.033054 -0.004799 0.039754 0.001421
34 CO 1 YZ 0.011729 -0.004616 0.007013 -0.007056 0.001324
35 C 2 S -0.079622 0.173945 -0.013174 -0.106887 0.041486
36 C 2 X 0.048158 0.094644 0.019093 0.016068 0.094457
37 C 2 Y -0.089710 0.003737 -0.059353 -0.075794 0.155593
38 C 2 Z -0.023649 -0.000855 -0.015043 -0.021400 0.043309
39 C 2 S -0.109049 0.050217 -0.174911 -0.165027 -0.078988
40 C 2 X 0.028403 0.012024 0.019425 0.047450 0.003126
41 C 2 Y -0.056984 -0.055582 0.027150 0.021934 0.087447
42 C 2 Z -0.013871 -0.014781 0.007337 0.005674 0.023695
43 C 3 S 0.124166 -0.112716 0.001030 0.122530 -0.043031
44 C 3 X 0.052441 0.015856 -0.053929 0.051355 0.057314
45 C 3 Y 0.012500 0.143908 0.064779 -0.013283 -0.090346
46 C 3 Z 0.005756 0.033605 0.017770 -0.004167 -0.023817
47 C 3 S -0.023600 -0.067292 0.053836 0.056361 0.038311
48 C 3 X 0.023520 -0.010017 -0.023282 0.003366 -0.006344
49 C 3 Y -0.020706 -0.014075 0.065542 0.016531 0.080388
50 C 3 Z -0.004049 -0.003936 0.019874 0.006232 0.020619
51 C 4 S -0.115764 0.021563 -0.051130 -0.110634 0.063254
52 C 4 X 0.023750 -0.182092 -0.070828 0.035234 0.060914
53 C 4 Y 0.065698 -0.019654 0.158966 0.074721 -0.099215
54 C 4 Z 0.022436 -0.040485 0.050005 0.014897 -0.026086
55 C 4 S -0.005903 0.237978 -0.029937 -0.055172 -0.095145
56 C 4 X -0.006534 -0.102640 0.034174 0.023792 0.122686
57 C 4 Y 0.012420 0.061137 -0.018341 -0.000937 -0.004782
58 C 4 Z 0.002457 0.004273 -0.008007 -0.003981 0.008691
59 C 5 S 0.072325 0.041864 0.087986 0.049069 -0.003268
60 C 5 X -0.062493 0.139170 0.129102 -0.042391 -0.015746
61 C 5 Y 0.034484 -0.055428 0.142554 0.053385 0.159019
62 C 5 Z 0.007405 -0.095022 0.062764 -0.017427 0.056796
63 C 5 S 0.212778 -0.151550 0.196423 0.150028 0.089480
64 C 5 X -0.004061 -0.267419 -0.000410 0.030580 0.077453
65 C 5 Y 0.100324 0.016529 0.041697 0.053834 -0.153710
66 C 5 Z 0.033809 -0.013648 0.022734 0.022119 -0.049264
67 C 6 S 0.017868 0.020423 -0.004313 0.004077 0.137177
68 C 6 X 0.070104 -0.109804 0.035917 0.078901 -0.165224
69 C 6 Y -0.035563 0.075704 -0.144820 -0.058436 -0.137818
70 C 6 Z -0.021520 -0.010892 -0.033030 -0.022376 -0.043826
71 C 6 S 0.134991 0.065866 -0.115773 -0.031355 0.319348
72 C 6 X -0.089735 0.332322 0.055591 -0.146988 -0.182481
73 C 6 Y 0.259879 0.045589 0.103152 0.104051 -0.051030
74 C 6 Z 0.083289 0.014361 0.026635 0.024158 -0.013675
75 C 7 S -0.028403 -0.141137 -0.134779 0.017821 -0.103865
76 C 7 X -0.090551 0.023691 0.027543 -0.070445 0.118647
77 C 7 Y 0.036933 -0.034415 0.004007 0.054613 0.092360

78	C	7	Z	0.005374	-0.017970	0.003354	0.011004	0.024481
79	C	7	S	-0.053972	-0.188198	-0.039441	0.067695	0.028742
80	C	7	X	0.164408	0.105729	0.089329	0.077789	-0.038830
81	C	7	Y	-0.040803	0.186517	-0.034299	-0.145999	-0.067467
82	C	7	Z	-0.013252	0.046254	-0.007726	-0.036912	-0.019128
83	C	8	S	0.089509	-0.023101	0.163307	0.085135	0.078463
84	C	8	X	-0.006694	-0.065636	0.059799	0.041176	0.213629
85	C	8	Y	-0.006234	0.094346	0.111156	-0.041144	0.037759
86	C	8	Z	-0.003156	0.021932	0.032193	-0.011431	0.010749
87	C	8	S	0.067013	-0.168537	0.032973	0.168956	-0.010814
88	C	8	X	-0.036823	-0.023915	0.007016	-0.035320	0.072787
89	C	8	Y	-0.002220	0.029686	0.008062	-0.024198	-0.029181
90	C	8	Z	0.000876	0.010170	0.002864	-0.008167	-0.008355
91	C	9	S	-0.087991	0.059061	-0.095712	-0.095083	-0.078035
92	C	9	X	0.063458	0.079806	0.133074	0.001083	-0.069985
93	C	9	Y	-0.049471	-0.010300	-0.005133	-0.032658	0.078836
94	C	9	Z	-0.016673	-0.009928	-0.001047	-0.007157	0.023581
95	C	9	S	-0.042785	-0.002588	-0.015446	-0.046359	0.015985
96	C	9	X	-0.009340	0.035769	0.025906	-0.033379	0.063470
97	C	9	Y	-0.018662	-0.007647	-0.013309	0.003461	-0.030408
98	C	9	Z	-0.007057	-0.005455	-0.006012	0.004030	-0.006960
99	C	10	S	0.028048	-0.104108	0.042474	0.081987	0.095104
100	C	10	X	-0.039344	0.113369	-0.097523	-0.094903	-0.118429
101	C	10	Y	-0.083643	-0.104461	-0.153317	0.011849	0.091912
102	C	10	Z	-0.025244	-0.051536	-0.027525	0.015603	0.031749
103	C	10	S	0.030971	0.046100	0.141562	0.011472	-0.076753
104	C	10	X	0.006960	0.010477	-0.016641	-0.013097	0.034648
105	C	10	Y	-0.020223	0.001626	-0.027473	-0.023816	0.100191
106	C	10	Z	-0.001900	-0.000299	-0.003261	-0.008598	0.021990
107	C	11	S	-0.035663	0.125094	0.069916	-0.075064	-0.018449
108	C	11	X	-0.031625	0.128587	-0.069209	-0.061637	0.133809
109	C	11	Y	0.129118	0.045913	0.118280	0.031411	-0.053633
110	C	11	Z	0.019063	-0.035621	0.066351	0.026643	-0.036327
111	C	11	S	-0.244378	0.228491	0.000753	-0.193984	-0.036545
112	C	11	X	-0.134320	0.057643	0.038942	-0.035376	-0.195778
113	C	11	Y	0.000561	-0.088584	-0.128071	0.027218	0.125919
114	C	11	Z	-0.005533	-0.039855	-0.022965	0.019194	0.040679
115	N	12	S	0.020672	-0.042818	-0.032105	0.019331	-0.039094
116	N	12	X	-0.153790	-0.123374	-0.023284	0.039760	-0.102826
117	N	12	Y	0.101462	0.063776	-0.004676	-0.083372	-0.099992
118	N	12	Z	-0.012026	-0.072397	0.093942	0.026388	-0.025533
119	N	12	S	0.004799	-0.063752	-0.060235	0.028108	-0.100287
120	N	12	X	-0.001829	-0.011262	-0.026490	0.013746	-0.009517
121	N	12	Y	-0.006566	0.013753	0.012912	-0.020914	-0.056011
122	N	12	Z	0.003170	-0.014638	0.043420	0.003191	-0.022976
123	C	13	S	-0.096443	0.027193	-0.019155	-0.007485	0.036470

124	C	13	X	0.198660	0.109867	-0.082199	-0.054035	0.039316
125	C	13	Y	-0.024932	-0.036153	-0.136822	0.011660	-0.002911
126	C	13	Z	0.041688	-0.008933	0.085954	-0.022508	-0.009796
127	C	13	S	-0.126435	0.007955	-0.087224	0.019215	0.182709
128	C	13	X	0.026585	0.002306	0.070064	0.003816	-0.083044
129	C	13	Y	0.009204	-0.015025	0.025792	0.014996	-0.073014
130	C	13	Z	0.006247	-0.000568	0.014510	-0.001851	0.020467
131	C	14	S	0.002366	-0.027677	0.054831	0.004844	-0.067903
132	C	14	X	-0.179549	-0.036069	0.138585	0.011215	-0.017430
133	C	14	Y	-0.009053	-0.042311	-0.038033	0.016075	0.011224
134	C	14	Z	-0.003182	-0.008500	0.052169	-0.053109	-0.004689
135	C	14	S	0.050740	-0.025844	0.155254	-0.024101	-0.171664
136	C	14	X	0.087245	0.017406	0.057147	-0.011606	-0.130248
137	C	14	Y	0.043935	0.014785	0.017408	-0.008996	-0.067149
138	C	14	Z	-0.007583	-0.006516	-0.005522	-0.015144	0.008863
139	C	15	S	-0.025158	-0.020769	-0.032507	-0.002878	-0.022454
140	C	15	X	0.149306	0.015102	0.015824	-0.034607	-0.006140
141	C	15	Y	0.026914	0.026477	0.058973	-0.066022	-0.014282
142	C	15	Z	0.031696	-0.042950	0.010638	-0.104698	0.020329
143	C	15	S	0.041561	0.052683	0.023381	-0.023166	-0.083251
144	C	15	X	-0.093809	-0.029397	-0.005917	0.031646	0.025962
145	C	15	Y	0.016122	0.000450	-0.039452	0.016685	0.022350
146	C	15	Z	-0.008844	-0.005145	0.025943	-0.018382	-0.003227
147	C	16	S	-0.109264	0.010392	0.093675	0.002785	-0.007943
148	C	16	X	-0.155382	-0.049861	-0.026821	0.044421	-0.030655
149	C	16	Y	0.038022	0.023775	-0.117681	0.000537	0.104955
150	C	16	Z	-0.018007	-0.023422	0.053918	-0.038743	-0.038094
151	C	16	S	-0.088721	-0.040581	-0.023792	0.034689	0.035667
152	C	16	X	-0.025078	-0.017935	-0.016028	0.026700	0.021763
153	C	16	Y	0.021350	-0.009543	-0.020217	-0.004325	0.006282
154	C	16	Z	-0.008174	-0.001891	0.006215	-0.009710	0.001078
155	C	17	S	0.163094	0.001021	-0.080331	-0.012117	0.013606
156	C	17	X	-0.041284	0.045087	-0.019967	0.011666	0.115408
157	C	17	Y	-0.101473	-0.041299	-0.039779	0.033278	0.000185
158	C	17	Z	0.039119	0.016164	0.017719	-0.027135	0.010939
159	C	17	S	-0.064228	-0.000776	0.016557	0.011917	0.009711
160	C	17	X	-0.040142	0.009621	0.027424	0.001744	0.001739
161	C	17	Y	-0.053530	0.000020	0.008369	0.000932	-0.005208
162	C	17	Z	0.017260	0.001366	0.000388	0.001893	0.002105
163	C	18	S	-0.194927	-0.038180	0.087471	0.018952	-0.038473
164	C	18	X	0.075956	0.063740	-0.036897	-0.016995	0.113347
165	C	18	Y	-0.063736	0.008851	0.115280	-0.025048	-0.042139
166	C	18	Z	0.032517	-0.000972	-0.044793	-0.000800	0.026343
167	C	18	S	0.012968	-0.027398	-0.031689	0.010477	0.036660
168	C	18	X	0.022066	0.002303	-0.032131	0.000269	0.028662
169	C	18	Y	-0.070626	-0.004440	0.013955	0.003546	0.008940

170	C	18	Z	0.030786	0.001345	-0.008681	-0.005913	-0.000675
171	C	19	S	0.148892	0.040102	-0.028587	-0.026681	0.029193
172	C	19	X	0.110316	-0.026437	-0.092133	0.017353	-0.036744
173	C	19	Y	-0.010597	-0.016508	0.047873	-0.019863	-0.033462
174	C	19	Z	0.016067	-0.002469	-0.018642	-0.007231	0.010495
175	C	19	S	0.050605	0.016827	0.028717	-0.009694	-0.043968
176	C	19	X	-0.027995	-0.015164	-0.033318	0.011767	0.037770
177	C	19	Y	0.003581	-0.014657	-0.004593	-0.001072	0.028795
178	C	19	Z	-0.004947	0.002563	0.002721	0.003343	-0.006741
179	O	20	S	-0.006073	0.034488	-0.010475	0.015782	0.024749
180	O	20	X	-0.251341	0.053131	0.088609	0.044441	-0.013663
181	O	20	Y	0.057129	-0.011299	-0.006315	-0.141063	0.053144
182	O	20	Z	0.063055	-0.079185	0.084199	-0.289654	0.025831
183	O	20	S	0.017674	0.051904	-0.038142	0.019768	0.034154
184	O	20	X	-0.106551	0.043266	0.043444	0.020486	-0.007848
185	O	20	Y	0.027885	0.000948	0.000218	-0.068540	0.024382
186	O	20	Z	0.029310	-0.036103	0.033878	-0.121294	0.011964
187	N	21	S	0.014769	-0.067033	-0.014597	-0.015933	-0.037189
188	N	21	X	0.076012	0.071337	-0.103953	0.166779	-0.066743
189	N	21	Y	0.004449	-0.002923	-0.151335	-0.046768	-0.146422
190	N	21	Z	0.046445	-0.293129	-0.056900	-0.128745	-0.063786
191	N	21	S	0.042424	-0.111661	-0.014352	-0.003358	-0.083170
192	N	21	X	0.015407	0.044279	-0.047486	0.065942	-0.061439
193	N	21	Y	0.011441	-0.034509	-0.053433	-0.013608	-0.040627
194	N	21	Z	0.021348	-0.115147	-0.024315	-0.052517	-0.027695
195	H	22	S	-0.037213	0.104062	-0.010336	-0.059576	0.112369
196	H	22	S	0.010710	0.031885	0.001935	-0.023560	0.017421
197	H	23	S	0.066639	-0.063524	-0.035094	0.074876	0.028577
198	H	23	S	0.001821	-0.001893	0.007715	0.013800	0.027483
199	H	24	S	-0.080937	0.011567	-0.115452	-0.082636	0.094475
200	H	24	S	-0.011110	0.020197	-0.048319	-0.018422	0.031133
201	H	25	S	0.028552	-0.003587	0.120018	0.036668	0.139636
202	H	25	S	0.014749	0.021056	0.019571	0.013188	0.024974
203	H	26	S	-0.059278	0.013929	-0.045619	-0.054420	0.013738
204	H	26	S	0.001545	0.009474	-0.000276	-0.011760	0.026815
205	H	27	S	0.008247	-0.126381	0.019709	0.087112	0.130357
206	H	27	S	-0.003426	-0.039525	-0.021950	0.024349	0.045203
207	H	28	S	-0.065643	-0.018024	-0.093850	0.016119	0.027633
208	H	28	S	-0.000332	-0.005396	-0.022365	-0.002676	0.029696
209	H	29	S	-0.052086	-0.007996	0.114790	-0.011475	-0.067100
210	H	29	S	0.010400	-0.005373	0.025970	-0.005438	-0.025718
211	H	30	S	0.102142	-0.011581	-0.014989	-0.018164	-0.050962
212	H	30	S	0.001240	0.000853	0.010929	-0.005235	-0.019123
213	H	31	S	-0.124152	-0.036027	0.086639	0.007349	-0.078837
214	H	31	S	0.001916	-0.003968	0.009242	-0.000982	-0.021621
215	H	32	S	0.057546	0.006401	0.003717	-0.017883	-0.008128

216	H	32	S	0.004231	0.008515	0.003529	-0.003274	-0.020776
217	H	33	S	0.030150	-0.019611	0.021528	-0.024017	-0.014750
218	H	33	S	-0.002478	0.003195	0.006742	-0.005311	-0.008947
219	H	34	S	-0.043839	0.131932	0.023021	0.020422	0.012998
220	H	34	S	-0.003769	0.005556	0.001234	0.004308	-0.003358
221	H	35	S	0.012340	0.009282	0.062842	0.070529	0.080803
222	H	35	S	0.007031	-0.013050	0.005522	0.007965	0.027947

		31	32	33	34	35		
		-0.7241	-0.7165	-0.7010	-0.6997	-0.6941		
		A	A	A	A	A		

1	CO	1	S	0.033451	0.026483	0.004054	0.033648	-0.007102
2	CO	1	X	-0.008278	0.029544	0.014624	-0.011446	-0.023852
3	CO	1	Y	0.020571	-0.010268	0.004990	0.001739	0.005790
4	CO	1	Z	-0.001498	-0.042212	-0.004648	-0.000071	0.022886
5	CO	1	XX	0.099190	-0.085728	0.068513	0.137781	-0.134254
6	CO	1	YY	-0.219614	0.184701	0.158859	0.053631	0.282744
7	CO	1	ZZ	0.120424	-0.098972	-0.227372	-0.191412	-0.148490
8	CO	1	XY	0.111667	0.041366	0.079130	0.091284	-0.045378
9	CO	1	XZ	0.150097	0.046335	-0.155582	-0.015935	-0.102159
10	CO	1	YZ	-0.060864	-0.020395	0.227294	0.373104	0.115317
11	CO	1	XX	0.043992	-0.039392	0.031891	0.061087	-0.061942
12	CO	1	YY	-0.098730	0.081734	0.069059	0.022758	0.126186
13	CO	1	ZZ	0.054738	-0.042342	-0.100950	-0.083845	-0.064244
14	CO	1	XY	0.050190	0.019407	0.035455	0.040366	-0.018441
15	CO	1	XZ	0.069273	0.017218	-0.069545	-0.004380	-0.044625
16	CO	1	YZ	-0.025889	-0.010461	0.102308	0.169848	0.049844
17	CO	1	S	-0.092673	-0.072551	-0.016127	-0.097460	0.010724
18	CO	1	X	-0.002714	-0.009355	0.007832	0.001790	0.009876
19	CO	1	Y	-0.018350	0.007669	-0.006727	-0.008962	0.003725
20	CO	1	Z	0.015534	0.037416	-0.007479	0.008877	-0.010728
21	CO	1	S	-0.007228	-0.013576	0.006999	0.001665	-0.008480
22	CO	1	X	-0.001994	-0.000926	0.013411	-0.003393	-0.006777
23	CO	1	Y	-0.005064	0.004311	0.006072	-0.002137	-0.011873
24	CO	1	Z	-0.001996	0.008490	-0.005777	0.002245	0.005036
25	CO	1	S	0.024571	0.022690	0.002651	0.026186	-0.008443
26	CO	1	X	0.004533	-0.002383	-0.004903	0.002658	0.005601
27	CO	1	Y	-0.001997	0.001129	-0.000976	0.002457	-0.003257
28	CO	1	Z	-0.001290	0.004761	0.000093	-0.002823	-0.004673
29	CO	1	XX	0.017789	-0.023417	-0.003617	0.027276	-0.014921
30	CO	1	YY	-0.028423	0.034050	0.021692	-0.001041	0.044616
31	CO	1	ZZ	0.010633	-0.010633	-0.018075	-0.026235	-0.029695
32	CO	1	XY	0.014568	0.005250	0.014085	0.012972	-0.004813
33	CO	1	XZ	0.029384	0.014361	-0.030800	0.004335	-0.004059
34	CO	1	YZ	-0.005906	0.002137	0.030443	0.057656	0.014089
35	C	2	S	-0.015898	-0.039429	0.040107	0.018248	0.014821

36	C	2	X	-0.021380	0.040796	0.120725	-0.049923	-0.078753
37	C	2	Y	0.074518	-0.043189	0.049546	0.043369	-0.015714
38	C	2	Z	0.017731	-0.014151	0.016275	0.014790	-0.004356
39	C	2	S	0.036758	-0.050775	-0.134851	0.184615	0.199368
40	C	2	X	-0.004380	0.044228	0.072557	-0.055237	-0.094067
41	C	2	Y	0.011409	-0.013088	-0.045067	-0.069695	0.022241
42	C	2	Z	0.002360	-0.003335	-0.009300	-0.019430	0.005247
43	C	3	S	0.006510	0.065230	-0.030031	-0.024524	-0.018970
44	C	3	X	0.042628	0.105182	0.090285	0.006742	-0.109484
45	C	3	Y	-0.091426	0.009518	0.005389	-0.049119	0.009460
46	C	3	Z	-0.025547	-0.000967	0.002624	-0.013238	0.002050
47	C	3	S	-0.024805	-0.018184	-0.015265	-0.119086	-0.024210
48	C	3	X	0.003404	0.008898	-0.017640	0.021195	0.030475
49	C	3	Y	-0.004752	-0.011514	-0.007592	-0.048311	-0.004079
50	C	3	Z	-0.001221	-0.003318	-0.002841	-0.012595	-0.001215
51	C	4	S	0.013346	-0.065892	0.022225	0.018966	0.027501
52	C	4	X	0.103042	-0.014141	-0.040952	0.074094	0.026876
53	C	4	Y	-0.101079	-0.035967	-0.079710	-0.096989	0.046795
54	C	4	Z	-0.028321	-0.036403	-0.032461	-0.029446	0.025425
55	C	4	S	-0.112696	-0.008271	0.037669	-0.029990	0.041470
56	C	4	X	0.067183	0.008452	-0.023002	0.018597	-0.005741
57	C	4	Y	0.016169	0.039902	-0.010655	0.027960	0.013959
58	C	4	Z	0.008682	0.007139	-0.007120	0.010762	0.009869
59	C	5	S	-0.047990	0.018406	0.016340	-0.041008	-0.022371
60	C	5	X	-0.096096	-0.040953	0.030633	-0.089199	-0.014907
61	C	5	Y	0.036774	-0.043274	0.043698	-0.008573	-0.035744
62	C	5	Z	0.001626	-0.084377	0.001270	-0.014762	0.012017
63	C	5	S	-0.107051	-0.118420	0.219025	-0.161028	-0.170457
64	C	5	X	0.108668	-0.009452	-0.067307	0.053697	0.011289
65	C	5	Y	-0.149806	-0.072366	0.105443	-0.079592	-0.045147
66	C	5	Z	-0.044372	-0.034546	0.027580	-0.032131	-0.018347
67	C	6	S	0.067193	0.020388	0.059024	0.028234	-0.041989
68	C	6	X	-0.022112	0.052964	-0.002029	0.026633	-0.042535
69	C	6	Y	-0.022337	0.047515	-0.018003	0.014283	0.024198
70	C	6	Z	-0.021975	-0.000059	-0.000411	0.035215	0.013253
71	C	6	S	0.243570	0.056806	0.181542	0.075958	-0.214273
72	C	6	X	-0.157279	-0.037240	-0.077481	0.060462	0.117818
73	C	6	Y	-0.156828	-0.110525	0.292174	-0.156689	-0.211068
74	C	6	Z	-0.054759	-0.034429	0.097086	-0.034477	-0.056300
75	C	7	S	0.043893	0.054443	-0.044855	0.027453	-0.002585
76	C	7	X	0.038121	-0.092829	-0.038370	0.027445	0.051067
77	C	7	Y	-0.010988	0.015481	0.024791	-0.097767	-0.024925
78	C	7	Z	-0.008119	-0.002478	0.008106	-0.012675	-0.002948
79	C	7	S	0.136456	0.152310	-0.083692	0.098577	0.009725
80	C	7	X	-0.076960	0.022875	0.203506	-0.094123	-0.202065
81	C	7	Y	-0.020586	-0.024689	-0.051913	0.182896	0.105330

82	C	7	Z	-0.006023	-0.008444	-0.016005	0.049842	0.025208
83	C	8	S	-0.028262	-0.011794	0.002085	-0.044585	-0.008584
84	C	8	X	0.066327	-0.030620	-0.005835	-0.008749	-0.022424
85	C	8	Y	0.007580	-0.049039	-0.002625	0.076170	0.020732
86	C	8	Z	-0.000453	-0.014693	0.000986	0.028905	0.005519
87	C	8	S	-0.025946	0.050312	0.069382	-0.237946	-0.121330
88	C	8	X	0.034756	-0.044851	-0.042575	0.058270	0.063318
89	C	8	Y	0.001304	0.023676	-0.035705	0.089082	0.048591
90	C	8	Z	0.000470	0.007081	-0.007078	0.027543	0.012999
91	C	9	S	0.037314	0.007046	-0.009569	0.057321	0.012786
92	C	9	X	-0.050495	-0.015756	-0.000759	0.049016	0.024106
93	C	9	Y	0.106773	0.014608	-0.022126	0.098527	-0.013224
94	C	9	Z	0.027481	0.006719	-0.002474	0.038711	-0.007510
95	C	9	S	-0.022593	-0.011555	-0.054704	0.106774	0.115707
96	C	9	X	0.028355	-0.062137	0.003137	0.008627	-0.014066
97	C	9	Y	0.008797	0.006581	0.014274	-0.043678	-0.027159
98	C	9	Z	-0.001100	0.002875	0.002393	-0.012713	-0.006261
99	C	10	S	-0.010821	-0.018585	0.001780	-0.055453	-0.018245
100	C	10	X	-0.068140	-0.048439	0.009611	-0.022649	0.033693
101	C	10	Y	0.095861	0.069164	0.001378	-0.058908	-0.033351
102	C	10	Z	0.019520	0.031511	0.010642	0.019497	-0.021728
103	C	10	S	-0.107501	-0.103656	0.049164	-0.046927	-0.024740
104	C	10	X	0.054616	-0.018462	0.049643	-0.043539	-0.057040
105	C	10	Y	0.091721	-0.023743	-0.016439	0.001038	-0.042369
106	C	10	Z	0.024626	-0.001896	-0.001952	0.014787	-0.012191
107	C	11	S	-0.006089	-0.051246	-0.041525	0.032715	0.027206
108	C	11	X	-0.034022	-0.046198	0.045898	-0.021960	0.041722
109	C	11	Y	-0.077887	-0.066716	0.016968	0.014659	0.016172
110	C	11	Z	-0.062954	0.012083	0.031705	0.094514	-0.008359
111	C	11	S	-0.012132	-0.040599	-0.245489	0.090378	0.187985
112	C	11	X	-0.088976	0.077108	-0.175544	0.060991	0.161725
113	C	11	Y	0.143831	0.075923	-0.007007	-0.008393	-0.055292
114	C	11	Z	0.043638	0.018315	-0.000582	0.002369	-0.025821
115	N	12	S	-0.024978	-0.006398	0.015370	-0.019397	-0.051468
116	N	12	X	-0.012426	0.090445	-0.095506	-0.062924	0.034028
117	N	12	Y	0.168651	0.011705	0.022443	0.123338	-0.058921
118	N	12	Z	-0.093548	0.094967	0.093019	0.219638	-0.017353
119	N	12	S	-0.067646	-0.010444	0.041711	-0.023695	-0.106700
120	N	12	X	0.027705	0.041529	-0.043867	0.003015	0.009410
121	N	12	Y	0.018257	0.003464	0.001495	0.037569	-0.003042
122	N	12	Z	-0.038979	0.033847	0.038054	0.095844	-0.005657
123	C	13	S	-0.033129	0.026835	-0.034989	0.025585	0.058723
124	C	13	X	0.102854	-0.043289	0.112063	-0.018727	0.007526
125	C	13	Y	-0.048962	0.139591	0.052944	-0.059388	0.125417
126	C	13	Z	-0.001271	0.041288	0.059732	0.167823	-0.074899
127	C	13	S	-0.207572	-0.052368	-0.174020	0.176526	-0.067416

128	C	13	X	0.136104	0.126514	-0.055108	-0.029358	0.145689
129	C	13	Y	-0.027951	-0.029472	0.056579	-0.020975	-0.072110
130	C	13	Z	0.028692	0.041179	-0.014698	0.030137	0.027136
131	C	14	S	0.078618	-0.027303	-0.025379	0.036018	-0.075987
132	C	14	X	0.011031	0.036589	-0.106984	0.025559	0.093277
133	C	14	Y	-0.181784	-0.060386	-0.019853	0.067288	-0.230903
134	C	14	Z	0.041779	0.137534	0.028941	0.029965	0.044162
135	C	14	S	0.246928	0.050390	-0.091901	0.070750	-0.047988
136	C	14	X	0.114508	0.021662	0.113903	-0.103556	0.004852
137	C	14	Y	0.170776	0.147476	0.119645	-0.164937	0.263465
138	C	14	Z	-0.065309	-0.026232	-0.026084	0.062304	-0.105746
139	C	15	S	0.022264	0.006122	0.129958	-0.088468	0.074150
140	C	15	X	0.126068	0.037885	-0.125181	0.071197	0.101713
141	C	15	Y	0.145197	0.166660	0.013919	-0.048743	0.129344
142	C	15	Z	-0.090428	0.136032	-0.001570	0.012426	-0.135504
143	C	15	S	0.226973	0.187836	0.268346	-0.307059	0.381736
144	C	15	X	-0.052590	-0.018199	0.012722	-0.000594	0.011233
145	C	15	Y	-0.035738	0.042335	0.034002	-0.070166	0.121196
146	C	15	Z	0.003702	0.016823	-0.008987	0.030479	-0.071850
147	C	16	S	0.014374	0.049298	-0.059678	0.011164	-0.022832
148	C	16	X	-0.115289	-0.092150	0.161058	-0.071679	-0.163197
149	C	16	Y	-0.179462	0.026393	0.029455	-0.050227	0.121874
150	C	16	Z	0.044727	0.056494	0.007656	0.010073	-0.100020
151	C	16	S	-0.119554	-0.006306	-0.006193	-0.007087	-0.028902
152	C	16	X	-0.063767	-0.047243	-0.060323	0.063692	-0.057183
153	C	16	Y	-0.015117	-0.001511	-0.029552	0.031332	-0.049331
154	C	16	Z	-0.003166	0.014752	0.006825	-0.012204	0.007048
155	C	17	S	-0.013223	-0.042728	0.063408	-0.020143	0.032130
156	C	17	X	-0.145255	0.068910	-0.246668	0.098723	0.080897
157	C	17	Y	-0.139128	-0.059162	-0.000068	0.023054	-0.190827
158	C	17	Z	0.036135	0.059581	-0.015802	0.000017	0.062539
159	C	17	S	-0.048738	-0.028924	0.035811	-0.021655	0.041307
160	C	17	X	0.012020	-0.009260	-0.000997	0.007186	0.005088
161	C	17	Y	-0.020174	0.019589	0.069733	-0.066671	0.035360
162	C	17	Z	0.008605	-0.006952	-0.026365	0.029414	-0.015523
163	C	18	S	0.015741	0.028685	-0.065664	0.023875	-0.040838
164	C	18	X	-0.059337	0.042741	-0.217654	0.127204	0.102871
165	C	18	Y	0.154793	0.095274	0.021868	-0.046103	0.148043
166	C	18	Z	-0.070414	-0.010545	-0.020767	0.034919	-0.063091
167	C	18	S	-0.075759	0.041320	-0.242780	0.141429	-0.026763
168	C	18	X	-0.050685	0.050322	-0.075350	0.013105	0.066374
169	C	18	Y	-0.049469	0.014162	0.009666	-0.023140	0.028452
170	C	18	Z	0.013753	0.004537	-0.008935	0.009292	-0.009656
171	C	19	S	0.015682	-0.023070	0.039160	-0.000305	0.014642
172	C	19	X	-0.065541	-0.119214	0.156491	-0.051698	-0.202384
173	C	19	Y	0.056417	0.034924	0.184044	-0.131585	0.132291

174	C	19	Z	-0.037834	0.019044	-0.045196	0.065676	-0.090406
175	C	19	S	0.012968	-0.137181	0.142178	-0.010220	-0.214643
176	C	19	X	-0.136380	-0.001994	-0.110160	0.064699	-0.050900
177	C	19	Y	-0.006066	0.025010	-0.094159	0.055748	0.025963
178	C	19	Z	-0.009690	-0.005518	0.027718	-0.010579	-0.017455
179	O	20	S	-0.038273	0.025821	-0.019218	-0.009269	-0.022468
180	O	20	X	-0.028849	0.096121	0.094991	-0.126062	-0.082979
181	O	20	Y	-0.128747	0.200884	-0.045659	-0.045920	-0.153256
182	O	20	Z	-0.039173	0.336114	0.006440	-0.106656	-0.105052
183	O	20	S	-0.063214	0.029030	-0.036181	0.001120	-0.026861
184	O	20	X	0.003643	0.062734	0.044277	-0.057167	-0.023260
185	O	20	Y	-0.039173	0.096382	-0.024684	-0.011633	-0.061339
186	O	20	Z	-0.023414	0.146917	-0.000048	-0.049758	-0.049185
187	N	21	S	-0.000151	-0.033270	-0.023087	0.016257	0.032422
188	N	21	X	0.067317	0.195201	-0.054501	0.020152	-0.054883
189	N	21	Y	-0.026638	0.038490	-0.008015	0.094025	0.049951
190	N	21	Z	-0.005407	-0.154749	-0.071699	-0.023848	0.087976
191	N	21	S	0.008233	-0.030299	-0.052890	0.037099	0.055488
192	N	21	X	-0.005966	0.074646	0.004003	0.007669	-0.036730
193	N	21	Y	0.018364	0.014788	-0.028477	0.039663	0.019560
194	N	21	Z	0.006036	-0.062554	-0.036911	-0.001066	0.047321
195	H	22	S	0.009008	-0.016683	0.089624	0.001680	-0.035293
196	H	22	S	-0.000354	-0.012743	0.028222	0.028381	-0.001906
197	H	23	S	0.042502	0.076557	0.031672	0.004287	-0.067644
198	H	23	S	0.014086	0.018447	0.021493	-0.003650	-0.036228
199	H	24	S	0.078752	-0.001178	0.058158	0.077336	-0.019896
200	H	24	S	0.044629	0.025253	0.018488	0.047748	-0.008219
201	H	25	S	0.018568	-0.035231	0.001143	0.001365	-0.009213
202	H	25	S	-0.004892	-0.002739	0.026208	-0.025253	-0.034909
203	H	26	S	0.074862	0.012152	-0.015855	0.080967	-0.004560
204	H	26	S	0.021301	-0.001839	-0.003464	0.038086	-0.002370
205	H	27	S	0.055273	0.047200	0.002234	-0.027959	-0.031907
206	H	27	S	0.027338	0.032669	0.025130	-0.025691	-0.016240
207	H	28	S	-0.046743	0.096528	0.009002	-0.071505	0.136546
208	H	28	S	0.043007	0.063489	-0.000692	-0.041488	0.101266
209	H	29	S	0.130291	0.027361	-0.064689	0.048914	-0.090741
210	H	29	S	0.053990	0.000686	-0.046017	0.045667	-0.059335
211	H	30	S	0.097118	-0.039319	0.159804	-0.066933	0.014835
212	H	30	S	0.039739	-0.008256	0.063850	-0.030849	0.010627
213	H	31	S	0.088264	0.025350	0.078670	-0.067469	-0.005053
214	H	31	S	0.033928	0.022240	0.023013	-0.028672	0.021966
215	H	32	S	0.036185	-0.000142	0.149807	-0.100630	0.094751
216	H	32	S	0.020590	0.008506	0.097959	-0.072587	0.054122
217	H	33	S	0.067228	-0.008453	0.000179	0.015395	0.061636
218	H	33	S	0.018593	0.005319	0.008855	-0.004074	0.008207
219	H	34	S	-0.022295	0.034686	0.049605	0.031813	-0.017607

220 H 34 S -0.004230 0.007569 0.005973 0.008104 0.001315
221 H 35 S 0.043586 0.018610 -0.012875 -0.053253 -0.044106
222 H 35 S 0.020201 0.003939 -0.008885 -0.012987 -0.014830

36 37 38 39 40
-0.6910 -0.6838 -0.6797 -0.6680 -0.6609
A A A A A

1 CO 1 S 0.004939 -0.005249 -0.023417 0.024569 -0.056505
2 CO 1 X 0.002348 -0.005825 0.014310 0.008408 -0.021160
3 CO 1 Y -0.005897 -0.004927 0.000698 -0.005728 -0.010335
4 CO 1 Z -0.012928 -0.002436 -0.001959 -0.001435 0.007786
5 CO 1 XX 0.131630 -0.003596 -0.209999 0.073857 -0.098931
6 CO 1 YY -0.063917 -0.308688 0.023991 -0.092926 -0.032714
7 CO 1 ZZ -0.067714 0.312284 0.186008 0.019068 0.131646
8 CO 1 XY 0.082835 0.081765 -0.238223 0.010367 0.157491
9 CO 1 XZ 0.164119 0.113197 -0.098217 -0.130327 0.216353
10 CO 1 YZ -0.163891 0.103580 -0.114290 0.197846 -0.126843
11 CO 1 XX 0.057981 -0.002449 -0.090238 0.032931 -0.045220
12 CO 1 YY -0.028205 -0.136015 0.011973 -0.041807 -0.012754
13 CO 1 ZZ -0.029775 0.138464 0.078265 0.008875 0.057974
14 CO 1 XY 0.034236 0.036775 -0.101318 0.005808 0.066501
15 CO 1 XZ 0.071342 0.052365 -0.043135 -0.056010 0.094264
16 CO 1 YZ -0.072369 0.051345 -0.051877 0.087547 -0.052105
17 CO 1 S -0.008227 0.014344 0.075271 -0.082762 0.176350
18 CO 1 X 0.009010 0.022539 -0.002685 -0.012988 0.023083
19 CO 1 Y -0.008553 0.019354 0.013659 0.007114 0.027824
20 CO 1 Z 0.013012 -0.003493 -0.014578 0.002434 -0.011293
21 CO 1 S -0.010406 -0.009335 0.009326 -0.002904 0.011015
22 CO 1 X -0.002361 0.002576 0.003104 0.007322 0.003050
23 CO 1 Y -0.003394 -0.007698 0.004485 0.001051 -0.002415
24 CO 1 Z 0.005359 -0.001064 -0.007218 -0.005414 0.001452
25 CO 1 S 0.004902 -0.003796 -0.015406 0.017644 -0.043577
26 CO 1 X -0.000828 -0.000003 -0.001391 -0.000909 0.001330
27 CO 1 Y 0.002384 0.000901 -0.001080 0.001541 -0.001190
28 CO 1 Z 0.002230 0.001590 0.002859 -0.000864 0.000976
29 CO 1 XX 0.031205 -0.014174 -0.039585 -0.003137 -0.010990
30 CO 1 YY -0.017213 -0.032982 0.007843 -0.008253 -0.001987
31 CO 1 ZZ -0.013992 0.047156 0.031742 0.011390 0.012978
32 CO 1 XY 0.013114 0.018443 -0.043783 -0.002859 0.040410
33 CO 1 XZ 0.020537 0.015357 -0.015861 -0.012961 0.018564
34 CO 1 YZ -0.026732 0.013742 -0.021958 0.032312 -0.025587
35 C 2 S -0.011062 -0.012356 0.007616 -0.056405 0.039073
36 C 2 X -0.198702 0.110078 0.073497 0.007119 0.035616
37 C 2 Y -0.015097 0.014562 -0.063262 -0.161034 -0.076800
38 C 2 Z -0.008154 0.018230 -0.015218 -0.051814 0.030414
39 C 2 S 0.292345 -0.219810 -0.032056 -0.185645 0.040131

40	C	2	X	-0.145037	0.109291	0.054301	0.019839	-0.041262
41	C	2	Y	-0.011573	0.015495	-0.109265	0.139029	0.018588
42	C	2	Z	-0.008624	0.008905	-0.028728	0.035266	0.012297
43	C	3	S	-0.001912	0.014318	-0.007744	0.067460	-0.030756
44	C	3	X	-0.148273	0.112741	0.168943	-0.065076	-0.104703
45	C	3	Y	-0.043127	0.002195	0.065840	0.132989	0.080467
46	C	3	Z	-0.017672	0.014060	0.022366	0.025123	0.062859
47	C	3	S	-0.044231	0.045658	-0.106370	0.182149	0.012215
48	C	3	X	0.021517	-0.027418	-0.025508	0.003590	0.019814
49	C	3	Y	-0.031320	0.026879	-0.022413	0.080472	0.016125
50	C	3	Z	-0.007582	0.008841	-0.008091	0.022265	0.012590
51	C	4	S	0.001830	-0.014724	-0.021865	-0.010507	0.053854
52	C	4	X	0.132874	-0.072749	-0.085222	-0.150139	-0.036703
53	C	4	Y	0.021174	-0.016422	-0.176914	0.178125	0.000369
54	C	4	Z	0.010583	0.008298	-0.066736	0.026001	0.073806
55	C	4	S	-0.067447	-0.018956	-0.176041	0.245053	0.088730
56	C	4	X	0.014819	0.016191	0.057813	-0.082043	-0.028477
57	C	4	Y	0.002946	-0.018634	0.018516	0.055738	0.008780
58	C	4	Z	0.002195	-0.003387	0.008253	0.004098	0.019264
59	C	5	S	-0.075613	0.051869	-0.024046	-0.008726	-0.050115
60	C	5	X	-0.108664	0.056909	-0.003172	0.130435	0.033302
61	C	5	Y	-0.029159	0.017443	-0.098630	-0.196205	-0.099856
62	C	5	Z	-0.019959	0.045894	-0.048810	-0.103674	0.119798
63	C	5	S	-0.263761	0.213352	-0.261793	-0.371906	-0.111565
64	C	5	X	0.119281	-0.039262	0.170383	-0.199192	-0.032968
65	C	5	Y	-0.071476	0.025388	-0.203473	-0.048223	-0.020633
66	C	5	Z	-0.018228	0.017164	-0.058713	-0.034284	0.023836
67	C	6	S	-0.004615	-0.011378	0.065421	0.003725	0.027276
68	C	6	X	-0.027884	0.041831	0.170859	-0.153266	-0.074956
69	C	6	Y	0.033793	-0.058465	0.139273	0.224111	0.053855
70	C	6	Z	0.017328	0.036454	0.040617	0.040183	0.184582
71	C	6	S	-0.007195	-0.034687	0.377190	0.045791	0.032880
72	C	6	X	0.144193	-0.114854	-0.023841	0.206191	0.099721
73	C	6	Y	-0.252200	0.140097	-0.258546	-0.177771	-0.053562
74	C	6	Z	-0.083456	0.057478	-0.091189	-0.058768	0.025417
75	C	7	S	0.015606	0.018750	0.031581	0.015614	-0.053998
76	C	7	X	0.112595	-0.067290	-0.165048	-0.083029	-0.046948
77	C	7	Y	-0.139656	0.087146	-0.159005	0.110240	-0.021991
78	C	7	Z	-0.033100	0.048264	-0.045382	0.014614	0.090039
79	C	7	S	0.027872	0.031065	0.404471	-0.036355	-0.062692
80	C	7	X	-0.233164	0.144943	0.048946	0.065371	-0.014342
81	C	7	Y	0.260154	-0.198213	0.211610	-0.005304	0.081427
82	C	7	Z	0.074728	-0.049441	0.063422	-0.004475	0.046178
83	C	8	S	-0.006646	-0.006426	0.001473	0.035246	0.029575
84	C	8	X	0.081382	-0.059545	-0.012534	0.184050	0.012248
85	C	8	Y	0.152174	-0.124577	0.152954	-0.063268	0.022453

86	C	8	Z	0.043779	-0.019449	0.042385	-0.023738	0.058454
87	C	8	S	-0.298828	0.206994	-0.262618	0.166048	-0.003475
88	C	8	X	0.079108	-0.046233	-0.047600	-0.171730	-0.049971
89	C	8	Y	0.119317	-0.083611	0.174859	0.035688	0.052032
90	C	8	Z	0.031553	-0.018527	0.045889	0.008698	0.021441
91	C	9	S	0.017927	0.006208	-0.004862	-0.052003	-0.037264
92	C	9	X	0.064864	-0.054838	0.150361	-0.127740	0.025829
93	C	9	Y	0.140783	-0.082372	0.182551	0.161480	-0.018553
94	C	9	Z	0.040081	-0.002817	0.051958	0.044172	0.043922
95	C	9	S	0.056950	-0.030180	-0.048279	-0.237646	-0.028329
96	C	9	X	0.042584	-0.026813	-0.024597	-0.076851	-0.060422
97	C	9	Y	-0.040006	0.024264	-0.047332	0.031526	0.001506
98	C	9	Z	-0.012074	0.007773	-0.012024	0.008036	0.014051
99	C	10	S	-0.011170	-0.001608	-0.027078	-0.005088	0.000255
100	C	10	X	-0.055824	0.037038	-0.219275	-0.129097	-0.048960
101	C	10	Y	-0.098013	0.064592	-0.076062	0.190793	0.017823
102	C	10	Z	-0.018452	0.059583	0.003559	0.056858	0.094501
103	C	10	S	0.016021	-0.022420	-0.143306	-0.198045	-0.025508
104	C	10	X	-0.015002	0.002873	0.003430	0.000837	-0.012456
105	C	10	Y	0.035931	-0.011057	0.033367	0.105195	-0.065514
106	C	10	Z	0.012903	0.010351	0.010121	0.031192	-0.002896
107	C	11	S	0.080280	-0.036694	-0.001173	0.028429	-0.045407
108	C	11	X	0.041559	-0.090116	-0.060461	0.139681	0.151918
109	C	11	Y	0.068265	-0.094962	0.065755	-0.176029	-0.061800
110	C	11	Z	0.030741	0.073264	0.046097	-0.084240	0.151516
111	C	11	S	0.306786	-0.151342	0.062769	0.382343	0.022318
112	C	11	X	0.026528	-0.006420	0.017642	0.099766	0.043433
113	C	11	Y	-0.073464	0.043342	0.100631	0.127508	-0.041701
114	C	11	Z	-0.013199	0.027208	0.049850	0.026153	0.022145
115	N	12	S	-0.020505	0.031572	0.002018	0.002339	0.000246
116	N	12	X	-0.078358	0.082705	0.028018	-0.031028	-0.082417
117	N	12	Y	-0.019993	0.069962	-0.051763	0.014356	-0.094857
118	N	12	Z	0.026701	0.135536	0.051598	-0.046159	0.179072
119	N	12	S	-0.046523	0.024793	0.017704	0.004907	-0.023403
120	N	12	X	-0.052812	0.029541	-0.018175	0.026368	-0.028486
121	N	12	Y	-0.023088	0.032154	0.001765	-0.010781	-0.011651
122	N	12	Z	0.016083	0.055408	0.016729	-0.023056	0.080490
123	C	13	S	0.001384	0.014191	-0.031967	0.003173	0.023094
124	C	13	X	-0.021196	-0.123162	-0.054369	0.024712	0.072961
125	C	13	Y	-0.114968	-0.089175	0.007416	-0.076836	0.169770
126	C	13	Z	0.067372	0.103945	-0.001173	-0.001656	0.098200
127	C	13	S	0.063894	0.166210	-0.137492	0.069200	0.004766
128	C	13	X	-0.053158	-0.030782	0.073607	0.006941	-0.002034
129	C	13	Y	-0.014921	-0.106837	0.055559	-0.029451	0.006319
130	C	13	Z	0.015020	0.042926	0.002583	0.013906	0.027779
131	C	14	S	-0.060429	-0.038019	0.000356	0.002368	-0.033795

132	C	14	X	0.089407	0.200007	0.022770	0.014929	-0.137507
133	C	14	Y	0.056846	0.011447	-0.008417	0.003355	-0.024338
134	C	14	Z	0.037637	0.039922	-0.042318	-0.026529	0.103331
135	C	14	S	-0.192201	-0.170746	0.061525	0.008223	-0.026803
136	C	14	X	-0.086380	-0.205877	0.067973	-0.035900	0.014841
137	C	14	Y	0.069047	0.101583	0.070344	-0.025732	0.009554
138	C	14	Z	-0.032985	-0.049461	-0.040829	-0.006338	0.027457
139	C	15	S	0.058311	0.024246	-0.000910	-0.002440	0.026020
140	C	15	X	-0.114966	-0.040296	-0.024888	-0.011204	0.020096
141	C	15	Y	-0.037592	-0.030254	-0.029304	-0.028237	0.057226
142	C	15	Z	0.091734	-0.013101	-0.093914	-0.016365	0.039118
143	C	15	S	0.059937	0.032123	0.069471	-0.032030	0.070833
144	C	15	X	0.119740	0.173031	0.023406	0.005108	-0.041982
145	C	15	Y	0.114901	0.120267	0.031428	-0.020546	-0.017928
146	C	15	Z	-0.009940	-0.037296	-0.029128	0.005482	0.017731
147	C	16	S	-0.019949	0.006409	0.014917	-0.006482	-0.032492
148	C	16	X	0.091662	-0.014050	0.018680	0.016981	0.001448
149	C	16	Y	0.200248	0.213098	0.010922	0.004184	-0.071289
150	C	16	Z	-0.032239	-0.092333	-0.051067	-0.014431	0.063949
151	C	16	S	0.160278	0.219627	0.047175	-0.006437	-0.102694
152	C	16	X	0.031852	0.048556	-0.001364	0.004781	-0.028123
153	C	16	Y	-0.014697	-0.002118	-0.000396	-0.003730	-0.006060
154	C	16	Z	0.014792	0.001261	-0.014034	-0.002276	0.006466
155	C	17	S	0.060239	0.039144	-0.006665	0.009754	-0.001257
156	C	17	X	0.013139	0.139327	0.017844	-0.007482	-0.109485
157	C	17	Y	0.016857	-0.038397	-0.001476	0.004746	-0.015874
158	C	17	Z	0.012724	0.024318	-0.021906	-0.011103	0.024153
159	C	17	S	0.079500	0.053291	-0.006476	0.011682	-0.023926
160	C	17	X	-0.015118	-0.032093	-0.011230	0.006291	0.025963
161	C	17	Y	0.052583	0.033665	0.016866	-0.001138	-0.012080
162	C	17	Z	-0.018562	-0.014585	-0.008868	-0.000275	0.013516
163	C	18	S	-0.059115	-0.028026	0.005809	-0.009618	-0.011988
164	C	18	X	-0.051407	0.025088	-0.032686	0.005613	0.035202
165	C	18	Y	-0.013408	0.031855	0.001820	-0.015960	0.020103
166	C	18	Z	0.015429	-0.007160	-0.020593	-0.001649	0.026297
167	C	18	S	-0.084476	0.035131	-0.010436	-0.007157	-0.026106
168	C	18	X	0.017106	0.081777	0.017609	-0.007047	-0.040191
169	C	18	Y	0.045668	0.043609	0.003679	-0.001039	-0.022348
170	C	18	Z	-0.013762	-0.011109	-0.005458	-0.002002	0.010709
171	C	19	S	0.035412	0.001366	-0.013713	0.012523	0.021127
172	C	19	X	0.038580	-0.071620	0.013985	0.008427	-0.021391
173	C	19	Y	0.195283	0.183893	0.023882	0.005397	-0.062070
174	C	19	Z	-0.048678	-0.065832	-0.031384	-0.014780	0.076793
175	C	19	S	-0.067321	-0.257760	-0.031103	0.004147	0.075433
176	C	19	X	-0.016160	0.007252	-0.007232	-0.001100	-0.022787
177	C	19	Y	-0.002820	0.072346	-0.011317	0.009528	-0.012004

178	C	19	Z	0.005964	-0.024077	0.002833	-0.005112	0.014257
179	O	20	S	-0.008728	-0.006690	0.023510	-0.007087	-0.011670
180	O	20	X	0.023566	-0.031230	0.063904	-0.018447	-0.004287
181	O	20	Y	0.045553	-0.073915	-0.060513	-0.019939	-0.013469
182	O	20	Z	0.121473	-0.058631	-0.127040	-0.012438	-0.031676
183	O	20	S	-0.027007	-0.015783	0.029218	-0.003359	-0.018940
184	O	20	X	0.000764	-0.004370	0.037912	-0.000578	-0.013414
185	O	20	Y	0.012365	-0.033018	-0.037246	-0.004533	-0.007385
186	O	20	Z	0.059679	-0.030756	-0.061587	-0.010293	-0.013665
187	N	21	S	0.027781	-0.015767	-0.000273	-0.007961	0.039591
188	N	21	X	0.112066	-0.052286	0.010671	0.056712	-0.117179
189	N	21	Y	0.048284	-0.042928	0.088574	0.047600	0.033066
190	N	21	Z	0.006159	-0.011622	0.037596	-0.034111	0.082610
191	N	21	S	0.077288	-0.051145	0.024827	-0.029195	0.024883
192	N	21	X	0.048392	-0.026154	0.023743	0.032407	-0.050484
193	N	21	Y	0.045077	-0.035796	0.049675	-0.003195	-0.009173
194	N	21	Z	0.011836	-0.012906	0.017388	-0.021965	0.039634
195	H	22	S	-0.098320	0.049650	0.015253	-0.085656	0.012502
196	H	22	S	0.002782	-0.012525	0.029806	-0.063742	0.011603
197	H	23	S	-0.067805	0.065673	0.073288	-0.038554	-0.097199
198	H	23	S	-0.034878	0.035661	0.048283	-0.021558	-0.044408
199	H	24	S	0.000819	-0.006037	0.104527	-0.143758	0.004945
200	H	24	S	0.006467	-0.010677	0.066998	-0.054805	-0.004203
201	H	25	S	0.083462	-0.071718	0.047767	0.086233	0.035056
202	H	25	S	-0.013807	-0.000344	0.017693	0.075230	0.018457
203	H	26	S	0.087926	-0.040779	0.103006	0.085993	-0.022530
204	H	26	S	0.046412	-0.026003	0.068637	0.040851	-0.008517
205	H	27	S	-0.008000	-0.000170	0.096525	0.136104	0.065371
206	H	27	S	-0.027390	0.005940	0.048508	0.052428	0.056227
207	H	28	S	-0.077794	-0.067138	0.005363	-0.044793	0.113426
208	H	28	S	-0.021543	0.013704	0.003502	0.001952	0.046894
209	H	29	S	-0.154410	-0.153269	-0.014484	-0.011160	0.047526
210	H	29	S	-0.092244	-0.089272	-0.009519	-0.006086	0.030935
211	H	30	S	0.016136	-0.051786	-0.014236	0.007602	0.071318
212	H	30	S	-0.002532	-0.035750	-0.005283	0.003748	0.042697
213	H	31	S	-0.009440	-0.011746	0.022634	-0.012729	-0.021144
214	H	31	S	-0.002361	0.009501	0.016582	-0.007615	-0.012714
215	H	32	S	0.144921	0.118126	0.017613	0.011376	-0.043648
216	H	32	S	0.061892	0.031155	0.019047	-0.004613	-0.015516
217	H	33	S	0.000211	0.020607	-0.016715	0.009434	-0.004610
218	H	33	S	-0.007731	-0.000952	0.002769	0.005081	-0.000081
219	H	34	S	-0.014839	0.006758	-0.007834	0.012072	0.008861
220	H	34	S	0.010452	-0.006278	-0.002389	-0.005950	0.002266
221	H	35	S	0.007647	0.009577	-0.057756	-0.036621	-0.044092
222	H	35	S	0.006061	-0.001430	-0.011482	-0.039599	-0.016746

			41	42	43	44	45
			-0.6593	-0.6518	-0.6397	-0.6328	-0.6243
			A	A	A	A	A
1	CO	1 S	0.016973	0.002731	-0.043331	-0.037323	-0.043407
2	CO	1 X	-0.040697	-0.027720	-0.008509	-0.016674	-0.015896
3	CO	1 Y	-0.006896	-0.004492	-0.017055	-0.001182	0.011700
4	CO	1 Z	0.030633	0.014780	0.014460	0.017329	0.026956
5	CO	1 XX	0.216527	0.503542	0.000591	-0.020880	-0.054293
6	CO	1 YY	0.020156	-0.126218	-0.054768	0.064362	0.029496
7	CO	1 ZZ	-0.236684	-0.377324	0.054177	-0.043483	0.024796
8	CO	1 XY	0.417840	-0.437686	0.032843	0.080920	0.027486
9	CO	1 XZ	-0.185225	0.196491	0.309424	0.209955	0.114531
10	CO	1 YZ	-0.191537	-0.100001	0.403198	0.151787	0.013647
11	CO	1 XX	0.089651	0.222343	0.000575	-0.009531	-0.023679
12	CO	1 YY	0.010831	-0.055644	-0.026631	0.025868	0.013281
13	CO	1 ZZ	-0.100482	-0.166699	0.026056	-0.016337	0.010399
14	CO	1 XY	0.179785	-0.198327	0.013582	0.033261	0.011928
15	CO	1 XZ	-0.086245	0.088650	0.136594	0.090323	0.050790
16	CO	1 YZ	-0.085747	-0.043339	0.179121	0.067766	0.006793
17	CO	1 S	-0.056389	-0.007941	0.130717	0.111732	0.131136
18	CO	1 X	0.015654	0.015772	-0.006806	-0.008635	-0.000820
19	CO	1 Y	0.008999	0.008071	0.018242	0.011102	-0.006478
20	CO	1 Z	-0.023634	-0.013155	-0.013456	-0.010952	-0.025547
21	CO	1 S	0.010883	0.012511	-0.003254	-0.003879	0.005777
22	CO	1 X	0.005581	-0.011764	-0.007654	-0.008350	0.000864
23	CO	1 Y	0.005862	0.003028	-0.000268	-0.000770	-0.005536
24	CO	1 Z	-0.001020	0.001117	0.010372	0.008742	-0.004453
25	CO	1 S	0.010244	0.000262	-0.033517	-0.029250	-0.033877
26	CO	1 X	0.007808	0.006087	0.002610	0.004409	0.003075
27	CO	1 Y	0.001134	0.000744	0.002525	-0.001379	-0.002403
28	CO	1 Z	-0.005315	-0.002861	-0.001302	-0.001963	-0.003195
29	CO	1 XX	0.033121	0.079882	0.005287	-0.003185	-0.008567
30	CO	1 YY	0.000216	-0.021718	-0.008699	0.012368	0.009893
31	CO	1 ZZ	-0.033337	-0.058164	0.003412	-0.009184	-0.001326
32	CO	1 XY	0.069787	-0.070479	-0.001100	0.011589	-0.001834
33	CO	1 XZ	-0.027330	0.031083	0.050059	0.038537	0.010608
34	CO	1 YZ	-0.035999	-0.015580	0.060238	0.018091	0.001744
35	C	2 S	0.023104	0.011179	0.052485	-0.075187	-0.011664
36	C	2 X	0.123300	0.082699	-0.010993	0.029379	0.066511
37	C	2 Y	-0.045036	-0.005620	-0.116336	0.131348	0.073468
38	C	2 Z	-0.002311	0.011095	-0.049548	0.086077	-0.082981
39	C	2 S	-0.098260	-0.084298	0.120947	-0.214872	-0.102734
40	C	2 X	0.065339	0.040260	-0.000555	0.034693	0.016324
41	C	2 Y	-0.041536	-0.017686	-0.028284	-0.019711	0.007887
42	C	2 Z	-0.008312	0.000147	-0.010072	0.005604	-0.017635
43	C	3 S	-0.039173	-0.020086	-0.036128	0.030746	-0.006261

44	C	3	X	0.069721	0.010027	-0.056493	0.175563	0.019617
45	C	3	Y	0.081453	0.030640	0.130495	-0.164299	-0.012199
46	C	3	Z	0.036310	0.018592	0.023842	0.014003	-0.077717
47	C	3	S	-0.064032	-0.009984	-0.046548	0.014014	0.011566
48	C	3	X	0.002659	0.008837	0.014615	-0.053071	-0.006190
49	C	3	Y	-0.000555	-0.004077	-0.055805	0.082185	0.041751
50	C	3	Z	0.002255	-0.000063	-0.020105	0.032969	-0.006868
51	C	4	S	0.030220	0.032349	0.019026	-0.018960	0.021584
52	C	4	X	-0.097742	-0.054352	0.022552	-0.110595	-0.030072
53	C	4	Y	-0.085081	0.001390	-0.138984	0.095575	0.075138
54	C	4	Z	-0.004371	0.014718	-0.048251	0.105800	-0.051010
55	C	4	S	0.024705	0.136427	-0.021375	-0.079161	-0.014545
56	C	4	X	-0.001100	-0.054040	-0.048308	0.114452	0.039779
57	C	4	Y	0.037966	0.009514	0.038111	-0.083489	-0.027041
58	C	4	Z	0.016892	0.007028	0.013069	-0.001372	-0.022043
59	C	5	S	-0.037861	-0.012495	-0.050768	0.062665	0.006034
60	C	5	X	0.102060	0.072251	-0.071769	0.128080	0.063350
61	C	5	Y	-0.002494	-0.008026	0.003774	-0.093507	0.010211
62	C	5	Z	0.061797	0.031437	-0.003111	0.099702	-0.080002
63	C	5	S	-0.142616	0.041033	-0.178418	0.284648	0.110471
64	C	5	X	0.009809	-0.097824	0.036461	0.022051	0.035430
65	C	5	Y	-0.085646	0.097530	-0.054221	-0.016155	0.019233
66	C	5	Z	-0.016086	0.026853	-0.019214	0.031586	-0.017434
67	C	6	S	0.031034	0.002604	0.015884	-0.052749	-0.015069
68	C	6	X	0.110408	0.012104	0.038060	0.089829	0.034014
69	C	6	Y	0.040183	0.019726	0.017960	0.041361	0.096837
70	C	6	Z	0.024457	0.036539	-0.045782	0.102977	-0.170892
71	C	6	S	0.161336	-0.036055	0.006765	0.079998	0.002158
72	C	6	X	-0.044367	-0.006712	-0.047157	0.135229	-0.011921
73	C	6	Y	-0.079206	0.128183	-0.119877	0.115831	0.073701
74	C	6	Z	-0.027065	0.052057	-0.054755	0.058733	-0.034157
75	C	7	S	-0.025045	-0.005205	-0.033095	0.067112	0.014772
76	C	7	X	-0.133252	-0.066272	-0.049648	-0.003364	-0.044209
77	C	7	Y	-0.044548	0.032430	-0.069571	-0.023511	0.066433
78	C	7	Z	-0.007762	0.027231	-0.057045	0.062232	-0.159329
79	C	7	S	0.130149	-0.019648	0.085567	-0.000851	0.028791
80	C	7	X	0.086286	0.101018	-0.077657	0.167394	0.063801
81	C	7	Y	-0.028270	-0.053776	-0.004122	0.108101	0.008259
82	C	7	Z	-0.002443	-0.011701	-0.007842	0.049645	-0.044269
83	C	8	S	0.033990	0.004399	0.059710	-0.080244	-0.022547
84	C	8	X	-0.033377	-0.042588	-0.083406	0.127431	0.010329
85	C	8	Y	0.053210	-0.040733	0.091690	-0.019897	0.005885
86	C	8	Z	0.014344	-0.000499	-0.001533	0.025979	-0.114669
87	C	8	S	0.028281	0.085091	0.059998	-0.210742	-0.016947
88	C	8	X	-0.048655	-0.036889	-0.022410	-0.000563	-0.012336
89	C	8	Y	0.006952	-0.011479	0.017662	0.032198	0.017783

90	C	8	Z	0.000013	-0.001410	-0.003452	0.014829	-0.019327
91	C	9	S	-0.038998	0.000318	-0.048954	0.035477	0.009924
92	C	9	X	0.072145	0.010215	0.108533	-0.073073	-0.004433
93	C	9	Y	-0.003099	-0.005235	-0.103565	0.200122	0.103613
94	C	9	Z	-0.006368	0.008495	-0.058728	0.067300	-0.073142
95	C	9	S	-0.090316	-0.031000	-0.076632	0.006061	-0.008994
96	C	9	X	0.005248	-0.028098	-0.024497	0.070712	-0.000147
97	C	9	Y	0.018680	0.004437	0.054060	-0.062935	-0.009319
98	C	9	Z	0.004417	0.004598	0.011442	-0.017227	-0.025882
99	C	10	S	0.032183	-0.017392	0.053597	-0.024893	-0.016007
100	C	10	X	-0.110920	-0.040976	-0.104541	0.074553	-0.020744
101	C	10	Y	-0.000827	0.036987	0.036793	-0.138704	-0.007776
102	C	10	Z	-0.007362	0.029169	-0.032192	-0.048887	-0.127535
103	C	10	S	-0.035462	-0.039697	0.105678	-0.037852	-0.009422
104	C	10	X	0.023243	0.010685	0.044044	-0.019678	-0.006122
105	C	10	Y	0.035870	-0.008157	-0.064322	0.111473	0.015441
106	C	10	Z	0.006462	-0.001893	-0.034256	0.032599	-0.025907
107	C	11	S	-0.038928	-0.001412	-0.056020	0.060585	0.015292
108	C	11	X	-0.047022	-0.031036	-0.013393	-0.007032	-0.012877
109	C	11	Y	0.030634	-0.062672	0.009068	0.141237	0.081398
110	C	11	Z	-0.032309	0.011957	-0.093344	0.042706	-0.148704
111	C	11	S	-0.058688	-0.020366	-0.117688	0.195236	-0.023430
112	C	11	X	0.040405	-0.041397	0.028818	-0.015868	0.002132
113	C	11	Y	0.116756	-0.003274	-0.020664	0.009447	0.012618
114	C	11	Z	0.027408	0.009608	-0.024351	0.004495	-0.039699
115	N	12	S	0.008055	0.004596	0.023265	-0.006218	0.002081
116	N	12	X	0.030175	0.056179	0.032598	0.004050	0.012502
117	N	12	Y	-0.026147	0.003386	-0.104371	-0.062772	-0.042988
118	N	12	Z	-0.140039	0.021646	-0.154217	-0.106794	-0.016873
119	N	12	S	0.001965	0.011734	0.014122	-0.029669	0.006137
120	N	12	X	0.054016	-0.015455	0.019615	-0.004579	0.003341
121	N	12	Y	-0.011803	-0.001668	-0.033656	-0.015362	0.007924
122	N	12	Z	-0.053911	0.002516	-0.068148	-0.049120	-0.010911
123	C	13	S	0.006448	-0.017257	-0.034249	-0.001166	-0.009442
124	C	13	X	-0.034271	-0.034323	-0.000586	0.015809	-0.037922
125	C	13	Y	-0.113553	0.046883	-0.034153	0.001754	0.033110
126	C	13	Z	-0.056529	0.001138	-0.149920	-0.144486	0.100834
127	C	13	S	0.043889	-0.074649	-0.087223	-0.034930	-0.035449
128	C	13	X	0.087345	-0.000656	0.078510	0.007795	0.012950
129	C	13	Y	-0.038208	0.023651	0.001848	0.007810	0.009789
130	C	13	Z	0.009759	-0.001216	-0.029104	-0.040825	0.024394
131	C	14	S	0.003887	0.003056	0.005292	-0.005410	-0.001208
132	C	14	X	0.097609	0.005934	-0.014384	-0.020282	-0.006580
133	C	14	Y	-0.002981	-0.020168	-0.015220	-0.030086	0.079424
134	C	14	Z	-0.007695	0.029725	-0.070684	-0.076201	0.221460
135	C	14	S	0.059725	0.066881	0.039341	-0.017742	0.011259

136	C	14	X	-0.009624	0.017819	0.055909	0.042947	0.003368
137	C	14	Y	-0.011120	-0.007511	0.066451	0.007794	0.043436
138	C	14	Z	-0.009199	0.008294	-0.044688	-0.024163	0.061810
139	C	15	S	0.009641	-0.004158	-0.016058	-0.000821	0.004205
140	C	15	X	0.072008	-0.006077	-0.016584	0.001638	-0.018314
141	C	15	Y	-0.031951	0.038272	0.028760	0.019285	0.054068
142	C	15	Z	0.062679	0.007205	0.024313	0.011704	0.152183
143	C	15	S	-0.039567	-0.030782	0.052418	0.045981	0.018936
144	C	15	X	-0.015824	-0.042348	-0.011188	-0.031360	0.001004
145	C	15	Y	0.003636	-0.007604	0.045443	0.016865	0.028501
146	C	15	Z	0.012211	0.008514	-0.007807	-0.003828	0.036619
147	C	16	S	-0.029506	-0.005609	0.020523	0.007251	-0.008638
148	C	16	X	-0.044004	-0.022882	-0.007212	-0.009461	-0.001709
149	C	16	Y	0.026555	0.023886	0.012996	0.000565	0.052588
150	C	16	Z	0.008868	0.003594	0.010760	0.003255	0.137217
151	C	16	S	-0.060447	-0.025508	0.041362	-0.010626	-0.013422
152	C	16	X	0.028574	-0.011211	-0.008156	-0.020417	0.001758
153	C	16	Y	-0.017181	-0.005287	0.006769	-0.005842	0.003630
154	C	16	Z	0.015259	0.003939	0.003157	0.004451	0.035879
155	C	17	S	0.031280	0.000956	-0.012995	-0.007770	0.004323
156	C	17	X	0.038567	0.010565	0.031767	0.010349	-0.031171
157	C	17	Y	-0.010610	-0.020599	0.014102	-0.005186	0.036201
158	C	17	Z	0.016645	0.018649	-0.003678	-0.007190	0.125200
159	C	17	S	0.063899	0.002052	-0.027159	-0.008570	0.011189
160	C	17	X	0.025407	-0.003096	-0.024421	-0.006617	0.011624
161	C	17	Y	-0.021616	0.003136	0.010572	0.009585	0.010398
162	C	17	Z	0.011170	0.000604	-0.008628	-0.009226	0.033494
163	C	18	S	-0.010424	0.000448	0.008934	0.004913	-0.003215
164	C	18	X	0.103479	0.002160	-0.054466	-0.020697	0.017442
165	C	18	Y	-0.018609	0.027172	-0.005674	-0.001259	0.057167
166	C	18	Z	0.017096	-0.001290	-0.018682	-0.026818	0.128442
167	C	18	S	0.054718	0.010627	0.010869	-0.008633	-0.009655
168	C	18	X	0.014755	0.014668	0.024793	0.006638	-0.010805
169	C	18	Y	0.013730	0.002391	-0.004867	0.001910	0.010226
170	C	18	Z	-0.003711	0.001948	0.001442	-0.004330	0.028206
171	C	19	S	0.018987	-0.009634	-0.014769	-0.007853	0.004238
172	C	19	X	-0.073814	-0.022752	0.045837	0.019378	-0.040145
173	C	19	Y	0.001154	0.013011	0.000436	-0.021584	0.053310
174	C	19	Z	-0.013350	0.006178	-0.035852	-0.040157	0.165474
175	C	19	S	-0.031632	-0.023037	-0.039780	0.010361	0.006384
176	C	19	X	0.038787	0.003737	-0.000050	0.004004	-0.012007
177	C	19	Y	0.029024	0.013089	-0.003786	-0.016235	0.015902
178	C	19	Z	-0.006616	-0.001332	-0.006779	-0.005980	0.040387
179	O	20	S	-0.064347	-0.032099	0.009767	0.001765	-0.003494
180	O	20	X	-0.178338	-0.061669	0.032453	0.010854	-0.000250
181	O	20	Y	0.017987	-0.060879	0.077515	0.077065	-0.093484

182 O 20 Z 0.079989 0.034347 0.146097 0.132508 -0.174073
 183 O 20 S -0.068482 -0.033370 0.012061 0.004764 -0.005633
 184 O 20 X -0.093746 -0.037653 0.004208 -0.004653 -0.008678
 185 O 20 Y 0.012729 -0.007625 0.036222 0.036271 -0.055848
 186 O 20 Z 0.040046 0.005313 0.073694 0.070355 -0.089428
 187 N 21 S 0.014272 0.009464 0.009053 0.027905 0.033728
 188 N 21 X -0.147261 -0.115873 -0.039406 -0.112032 -0.113085
 189 N 21 Y -0.042639 0.031422 0.032910 0.021217 -0.010428
 190 N 21 Z 0.047731 -0.019747 0.065514 0.054716 0.136979
 191 N 21 S 0.000304 -0.003243 0.020768 0.015764 0.038314
 192 N 21 X -0.067682 -0.032673 -0.022411 -0.070699 -0.064407
 193 N 21 Y -0.016935 -0.013328 0.018707 -0.008060 0.000421
 194 N 21 Z 0.033404 0.001739 0.040299 0.039297 0.067645
 195 H 22 S 0.056227 0.045511 -0.032096 0.044310 0.050967
 196 H 22 S 0.020362 0.014686 -0.016882 0.036469 0.026871
 197 H 23 S 0.000250 -0.012850 -0.087177 0.168340 0.016663
 198 H 23 S 0.007725 -0.008592 -0.049287 0.114278 0.016176
 199 H 24 S 0.063720 0.002403 0.121856 -0.123100 -0.038718
 200 H 24 S 0.043995 -0.002428 0.084516 -0.107795 -0.044373
 201 H 25 S 0.020778 -0.033238 0.014340 0.030531 -0.012946
 202 H 25 S 0.026731 -0.001912 0.002401 0.029141 0.000194
 203 H 26 S -0.025056 -0.001702 -0.108059 0.166139 0.061061
 204 H 26 S -0.009444 -0.000208 -0.067016 0.108388 0.038352
 205 H 27 S 0.077611 0.035528 0.100774 -0.120014 -0.015563
 206 H 27 S 0.028483 0.031540 0.069553 -0.095801 -0.006019
 207 H 28 S -0.056995 0.029554 0.007506 0.029032 0.002956
 208 H 28 S 0.002807 0.012569 0.021333 0.004028 0.008716
 209 H 29 S -0.024947 -0.012519 0.005788 0.005402 -0.005854
 210 H 29 S -0.008930 -0.007129 -0.001545 -0.003029 -0.004207
 211 H 30 S -0.004649 -0.000128 -0.031346 -0.009889 0.020215
 212 H 30 S -0.001817 -0.001189 -0.019285 -0.004573 0.014915
 213 H 31 S -0.067371 0.009615 0.035379 0.018750 -0.014378
 214 H 31 S -0.031765 0.009231 0.026794 0.011087 -0.008602
 215 H 32 S 0.002399 0.001700 0.007615 -0.004695 -0.007478
 216 H 32 S -0.015127 -0.002677 0.009850 0.004987 -0.004914
 217 H 33 S 0.030390 0.069324 0.005271 -0.000037 -0.009201
 218 H 33 S -0.002662 0.024039 0.007653 0.000793 -0.003420
 219 H 34 S 0.010665 0.073316 -0.014224 0.023712 -0.047392
 220 H 34 S 0.004423 0.030343 0.014459 0.019891 -0.015504
 221 H 35 S 0.004935 -0.059141 -0.028901 -0.054423 -0.019823
 222 H 35 S 0.012406 -0.021618 0.003535 -0.017682 -0.002463

46 47 48 49 50
 -0.6167 -0.6138 -0.6100 -0.6014 -0.5894
 A A A A A

1 CO 1 S -0.020499 0.004826 0.003032 -0.023797 -0.015408

2	CO	1	X	0.014588	-0.000066	0.001120	-0.024515	-0.015623
3	CO	1	Y	-0.014524	-0.011024	-0.001298	-0.028092	0.031934
4	CO	1	Z	-0.010489	0.002045	0.006785	-0.000327	0.005226
5	CO	1	XX	0.054170	0.047475	0.046265	0.115193	-0.074104
6	CO	1	YY	-0.093967	-0.055229	-0.036315	-0.114077	0.140461
7	CO	1	ZZ	0.039797	0.007755	-0.009950	-0.001117	-0.066357
8	CO	1	XY	-0.038367	0.003031	-0.054627	0.099295	0.022900
9	CO	1	XZ	0.027842	-0.034946	-0.044892	0.058774	0.094785
10	CO	1	YZ	0.060238	0.004053	0.012809	-0.083856	-0.080446
11	CO	1	XX	0.023371	0.020244	0.020390	0.045630	-0.030034
12	CO	1	YY	-0.040042	-0.022976	-0.015404	-0.046101	0.057739
13	CO	1	ZZ	0.016671	0.002732	-0.004986	0.000471	-0.027704
14	CO	1	XY	-0.016183	0.000561	-0.022962	0.038299	0.007095
15	CO	1	XZ	0.012363	-0.014478	-0.017822	0.024012	0.038290
16	CO	1	YZ	0.026824	0.001416	0.004993	-0.032879	-0.033061
17	CO	1	S	0.063654	-0.015628	-0.013176	0.073494	0.052954
18	CO	1	X	-0.007019	0.007388	0.005137	0.025793	0.008188
19	CO	1	Y	0.009236	0.007887	-0.000037	0.021707	-0.015777
20	CO	1	Z	0.008094	-0.007703	-0.012978	0.001535	-0.002649
21	CO	1	S	-0.017932	0.000752	0.009073	0.010313	-0.001100
22	CO	1	X	0.005827	-0.002814	0.002571	-0.002879	-0.002453
23	CO	1	Y	-0.008431	0.000863	0.002387	0.005503	-0.003688
24	CO	1	Z	0.005843	0.000204	-0.008262	0.009998	0.005581
25	CO	1	S	-0.015263	0.004424	0.001059	-0.019322	-0.011661
26	CO	1	X	-0.001957	-0.001308	-0.000362	0.003100	0.002039
27	CO	1	Y	0.003343	0.002788	0.000100	0.005502	-0.007633
28	CO	1	Z	0.002114	-0.000032	-0.000930	0.001134	-0.000145
29	CO	1	XX	0.008021	0.004902	0.003445	0.028797	-0.021671
30	CO	1	YY	-0.015439	-0.011090	-0.006491	-0.024963	0.031733
31	CO	1	ZZ	0.007417	0.006188	0.003046	-0.003834	-0.010062
32	CO	1	XY	-0.004097	0.002787	-0.004950	0.023556	0.007236
33	CO	1	XZ	0.000522	-0.006655	-0.010601	-0.002614	0.014319
34	CO	1	YZ	0.008126	0.003615	0.002809	-0.014544	-0.018339
35	C	2	S	-0.010218	-0.013774	-0.032927	-0.013617	-0.000330
36	C	2	X	-0.052349	-0.056958	-0.162455	0.069777	-0.044469
37	C	2	Y	0.006873	-0.061335	-0.179392	0.039288	-0.240790
38	C	2	Z	-0.027459	-0.013813	-0.013899	-0.130509	-0.087997
39	C	2	S	0.053597	0.003920	-0.057988	-0.110759	-0.311576
40	C	2	X	-0.006906	0.015035	0.074459	0.006336	0.192033
41	C	2	Y	0.002763	0.013326	0.040707	0.013828	0.117252
42	C	2	Z	-0.006440	0.004479	0.021947	-0.028473	0.034829
43	C	3	S	0.009076	0.009434	0.026856	-0.010489	0.022821
44	C	3	X	0.063209	0.067565	0.179063	-0.009655	0.032184
45	C	3	Y	-0.004671	0.041455	0.116007	0.031208	0.242306
46	C	3	Z	-0.026631	0.015762	0.072093	-0.117355	0.070445
47	C	3	S	-0.015341	0.007320	0.072800	0.033677	0.229045

48	C	3	X	-0.008923	-0.011920	-0.057013	-0.002605	-0.066493
49	C	3	Y	0.003545	0.001514	-0.001561	0.038112	0.016170
50	C	3	Z	-0.004961	0.000241	0.004146	-0.020843	-0.000594
51	C	4	S	-0.023555	-0.024492	-0.059788	0.014750	-0.010548
52	C	4	X	-0.025213	-0.045806	-0.137338	0.007259	-0.082900
53	C	4	Y	-0.011690	-0.064204	-0.180773	0.050914	-0.175335
54	C	4	Z	-0.043111	-0.024161	-0.030507	-0.111885	-0.028808
55	C	4	S	-0.061155	-0.021260	-0.077010	0.006336	-0.054452
56	C	4	X	0.030289	-0.000974	-0.030785	0.010464	-0.090594
57	C	4	Y	0.000511	0.022161	0.028799	-0.020518	0.002720
58	C	4	Z	-0.008656	0.006500	0.016250	-0.036950	0.006058
59	C	5	S	0.015892	0.000748	0.011654	-0.029552	0.038677
60	C	5	X	0.010386	0.010139	0.027808	0.034669	-0.024496
61	C	5	Y	0.014744	-0.000682	-0.015523	0.027248	0.104670
62	C	5	Z	-0.045679	-0.003273	0.033295	-0.110008	0.089379
63	C	5	S	-0.062268	-0.146166	-0.203881	0.060674	0.229401
64	C	5	X	0.032990	-0.014133	-0.054304	0.020210	-0.083275
65	C	5	Y	-0.068354	-0.086181	-0.148204	0.064354	0.062988
66	C	5	Z	-0.033898	-0.029905	-0.040803	-0.025074	0.033597
67	C	6	S	-0.022234	0.000942	-0.007177	0.025352	-0.037439
68	C	6	X	0.017374	0.029572	0.036935	0.087405	-0.103587
69	C	6	Y	-0.014654	-0.010358	-0.045722	0.094663	-0.148791
70	C	6	Z	-0.040681	0.003211	0.029977	-0.100432	-0.073469
71	C	6	S	-0.113166	-0.011903	0.025482	0.073776	-0.086219
72	C	6	X	0.068181	0.121092	0.207418	0.100919	-0.282993
73	C	6	Y	-0.145748	-0.143299	-0.181959	0.125434	0.206689
74	C	6	Z	-0.059419	-0.042332	-0.041069	0.007921	0.060424
75	C	7	S	0.019267	-0.002771	0.004359	-0.035014	0.045044
76	C	7	X	0.039436	0.022976	0.077853	-0.068996	0.041107
77	C	7	Y	-0.017245	-0.057707	-0.118908	-0.021242	0.261357
78	C	7	Z	-0.041343	-0.009012	0.016962	-0.186352	0.017356
79	C	7	S	0.087497	-0.004166	-0.038355	-0.171915	0.177181
80	C	7	X	-0.082419	-0.008194	0.044966	0.139972	0.149154
81	C	7	Y	0.050029	0.030977	-0.004115	0.045420	-0.367270
82	C	7	Z	0.004633	0.010801	0.012103	-0.042459	-0.120859
83	C	8	S	-0.002519	0.011054	0.023249	-0.007320	0.015674
84	C	8	X	-0.008541	0.100357	0.230812	0.170195	0.021730
85	C	8	Y	0.019108	0.052235	0.086561	0.104095	-0.245310
86	C	8	Z	-0.014828	0.019981	0.051957	-0.078025	-0.122380
87	C	8	S	-0.082488	-0.023299	0.041825	0.006892	0.382456
88	C	8	X	0.035672	-0.024213	-0.084106	-0.071240	-0.096535
89	C	8	Y	0.027189	-0.009873	-0.049492	-0.024539	-0.076046
90	C	8	Z	0.002484	-0.001407	-0.007440	-0.027554	-0.033032
91	C	9	S	0.005428	-0.015265	-0.022690	-0.015939	0.018826
92	C	9	X	0.011576	-0.072413	-0.186847	-0.136132	-0.060255
93	C	9	Y	-0.009591	-0.046158	-0.108113	-0.020697	0.197527

94	C	9	Z	-0.013904	-0.006399	-0.012872	-0.062197	-0.000526
95	C	9	S	0.065545	-0.015458	-0.083925	-0.050079	-0.137346
96	C	9	X	0.002321	0.011441	0.013287	0.003663	-0.049406
97	C	9	Y	-0.017526	0.014180	0.048588	0.025416	0.008009
98	C	9	Z	-0.006266	0.004358	0.016313	-0.009737	-0.012443
99	C	10	S	0.007553	0.034284	0.057614	0.024058	-0.047193
100	C	10	X	0.010901	0.088484	0.228025	0.156792	-0.017747
101	C	10	Y	-0.020364	0.013343	0.047540	0.023685	-0.075317
102	C	10	Z	-0.010660	0.003312	-0.001736	-0.017830	-0.075992
103	C	10	S	0.005523	0.039687	0.101326	0.089005	-0.081909
104	C	10	X	-0.035454	-0.028498	-0.011923	-0.012006	0.008153
105	C	10	Y	-0.014496	0.014436	0.021186	-0.007396	0.043254
106	C	10	Z	-0.006736	0.008268	0.006609	-0.004504	-0.000851
107	C	11	S	0.014821	-0.008401	-0.005268	-0.045356	0.054060
108	C	11	X	-0.025103	0.000761	-0.002866	0.026915	-0.032440
109	C	11	Y	0.002990	0.005980	-0.007149	0.028362	0.075041
110	C	11	Z	0.009746	0.010117	-0.001044	0.056940	-0.018270
111	C	11	S	0.145368	0.145933	0.233554	-0.027898	-0.179532
112	C	11	X	0.106891	0.127331	0.136254	0.026032	-0.152331
113	C	11	Y	-0.043428	-0.008742	-0.043103	-0.047614	0.087051
114	C	11	Z	-0.006488	-0.006643	-0.020694	-0.013605	0.011332
115	N	12	S	-0.005435	0.029078	0.021062	0.060061	-0.064867
116	N	12	X	0.071459	0.012323	0.044039	0.008019	-0.069004
117	N	12	Y	-0.084644	-0.028953	0.000008	-0.066740	0.096169
118	N	12	Z	0.036423	-0.008730	-0.044933	0.231851	0.066197
119	N	12	S	-0.028242	0.046730	0.056316	0.095812	-0.094905
120	N	12	X	0.012888	0.012045	-0.002026	-0.008258	-0.021303
121	N	12	Y	-0.034496	-0.010089	-0.001676	-0.026237	0.062312
122	N	12	Z	0.019258	-0.000855	-0.020863	0.117431	0.032826
123	C	13	S	0.059240	0.026690	-0.005246	-0.014143	0.017703
124	C	13	X	-0.118516	-0.046773	0.012110	0.000732	0.022560
125	C	13	Y	-0.010333	-0.010693	0.054194	0.134493	-0.020621
126	C	13	Z	-0.035647	-0.009880	-0.014649	0.064441	0.079276
127	C	13	S	0.184714	0.106198	-0.030920	0.025168	0.031605
128	C	13	X	0.008896	0.002322	-0.015135	-0.049579	-0.041116
129	C	13	Y	-0.030161	-0.027271	0.020413	0.013742	-0.016641
130	C	13	Z	0.000923	0.003495	-0.018106	0.015340	0.020062
131	C	14	S	-0.071741	0.035648	-0.012530	-0.013571	0.003795
132	C	14	X	0.147070	-0.082783	0.012408	-0.054346	0.004367
133	C	14	Y	-0.063466	0.174762	-0.051748	-0.067923	0.015771
134	C	14	Z	-0.019654	-0.049412	0.113406	-0.077090	-0.032525
135	C	14	S	-0.032201	0.210382	-0.084360	-0.083750	-0.023886
136	C	14	X	-0.071279	-0.148276	0.045635	-0.017294	-0.028913
137	C	14	Y	-0.129178	0.004525	0.008206	-0.021719	-0.023666
138	C	14	Z	0.023857	-0.004931	0.039559	-0.021537	-0.003544
139	C	15	S	0.078340	-0.022474	0.011706	0.004704	-0.005430

140	C	15	X	-0.114197	-0.107912	0.052076	0.066298	-0.009779
141	C	15	Y	-0.070559	-0.118494	0.092792	-0.000236	-0.035201
142	C	15	Z	-0.016835	0.062688	0.034837	-0.116246	-0.025756
143	C	15	S	0.035347	0.065422	-0.027453	-0.013796	-0.038097
144	C	15	X	-0.010527	-0.096210	0.028018	0.006178	0.028170
145	C	15	Y	-0.113145	-0.042460	0.024556	0.008076	-0.010775
146	C	15	Z	0.031983	0.015612	0.007360	-0.040380	-0.005364
147	C	16	S	-0.077302	0.013766	-0.008662	-0.001895	0.006316
148	C	16	X	0.231642	-0.019684	-0.024336	-0.053677	0.017013
149	C	16	Y	-0.082559	0.208332	-0.049391	-0.063196	-0.014000
150	C	16	Z	0.013862	-0.056900	0.095206	-0.133229	-0.065085
151	C	16	S	-0.223273	-0.042377	0.010988	0.025781	0.040877
152	C	16	X	-0.018620	-0.139175	0.050098	0.009042	0.004527
153	C	16	Y	-0.072777	-0.061626	0.030883	0.000758	0.005894
154	C	16	Z	0.018407	0.019043	0.014112	-0.041650	-0.023221
155	C	17	S	0.043403	-0.036648	0.012614	-0.003729	-0.001701
156	C	17	X	-0.310331	-0.069440	0.036028	0.068451	-0.000032
157	C	17	Y	-0.027567	-0.304616	0.137030	-0.038621	-0.033633
158	C	17	Z	-0.049476	0.135933	0.027558	-0.129947	-0.066122
159	C	17	S	0.130008	-0.135337	0.049903	-0.016194	-0.019336
160	C	17	X	0.138046	0.001047	-0.007740	-0.025216	-0.004088
161	C	17	Y	0.014034	0.033212	-0.008231	-0.022287	-0.007956
162	C	17	Z	-0.004083	-0.006629	0.022189	-0.033612	-0.019108
163	C	18	S	-0.041351	0.004871	0.001781	0.007090	-0.001888
164	C	18	X	0.343186	-0.027577	-0.003796	-0.038727	-0.000467
165	C	18	Y	-0.039925	0.333789	-0.088502	-0.058713	-0.016643
166	C	18	Z	0.005610	-0.112063	0.114924	-0.120697	-0.067494
167	C	18	S	-0.066247	0.009929	0.015653	0.046003	-0.013209
168	C	18	X	-0.091561	0.050558	-0.009287	0.028558	-0.006297
169	C	18	Y	0.046316	-0.058493	0.030135	-0.012613	-0.013157
170	C	18	Z	-0.034642	0.031323	0.007759	-0.027737	-0.014708
171	C	19	S	0.070293	-0.013156	-0.004935	-0.015774	0.006795
172	C	19	X	-0.283271	-0.029039	0.001076	0.050123	0.015094
173	C	19	Y	-0.079596	-0.233051	0.123620	-0.028526	-0.029022
174	C	19	Z	-0.040088	0.108078	0.041563	-0.112892	-0.046701
175	C	19	S	0.142927	-0.153278	0.030944	-0.035832	0.016606
176	C	19	X	0.032333	-0.069565	0.031306	0.028926	-0.011089
177	C	19	Y	-0.008619	0.150535	-0.042470	-0.008396	-0.004246
178	C	19	Z	-0.004853	-0.058493	0.040415	-0.032566	-0.017766
179	O	20	S	-0.031845	0.030564	-0.017138	-0.031023	0.009345
180	O	20	X	0.111637	-0.060199	-0.001448	-0.079858	0.017977
181	O	20	Y	-0.010740	0.028116	-0.077233	0.044622	0.054251
182	O	20	Z	0.075668	-0.038961	-0.087263	0.126893	0.064540
183	O	20	S	-0.070563	0.063631	-0.024598	-0.044549	0.009808
184	O	20	X	0.057513	-0.027667	-0.000615	-0.053640	0.010141
185	O	20	Y	-0.002489	0.018442	-0.035031	0.028951	0.024921

186	O	20	Z	0.037770	-0.020165	-0.050691	0.067808	0.037562
187	N	21	S	-0.021402	-0.013066	-0.029521	0.029790	-0.009771
188	N	21	X	0.024747	-0.000768	-0.039925	-0.047226	-0.166375
189	N	21	Y	-0.013164	-0.005003	-0.003028	-0.002762	-0.044074
190	N	21	Z	-0.025853	-0.018175	-0.034740	0.077574	0.035492
191	N	21	S	-0.032902	-0.034139	-0.078723	0.040811	-0.060960
192	N	21	X	0.012525	0.004894	-0.014800	-0.015915	-0.099973
193	N	21	Y	-0.004443	-0.000028	-0.007392	-0.000333	-0.045796
194	N	21	Z	-0.017041	-0.011406	-0.022670	0.039206	0.024255
195	H	22	S	-0.036194	-0.064170	-0.183649	0.042950	-0.160942
196	H	22	S	-0.019129	-0.038974	-0.121489	0.031663	-0.171415
197	H	23	S	0.049407	0.037780	0.098670	-0.014690	-0.041115
198	H	23	S	0.028752	0.023871	0.068369	-0.001455	-0.014484
199	H	24	S	0.004313	0.036994	0.098225	-0.004110	0.137242
200	H	24	S	0.004352	0.035072	0.084532	-0.021220	0.096922
201	H	25	S	-0.002862	0.086904	0.186218	0.140971	-0.105370
202	H	25	S	-0.016856	0.054855	0.130965	0.109906	-0.029863
203	H	26	S	-0.007412	-0.037169	-0.079446	-0.027633	0.162781
204	H	26	S	-0.002467	-0.024119	-0.055942	-0.015798	0.093364
205	H	27	S	-0.012609	-0.043200	-0.115818	-0.085952	-0.055941
206	H	27	S	-0.016628	-0.047255	-0.081848	-0.050991	-0.033160
207	H	28	S	0.040875	-0.016127	0.036814	0.083243	-0.034908
208	H	28	S	0.005403	-0.016479	0.002005	0.025215	-0.012215
209	H	29	S	-0.010033	-0.175034	0.068913	0.019945	-0.008752
210	H	29	S	-0.022441	-0.142543	0.057247	0.019818	-0.003775
211	H	30	S	0.245753	0.121674	-0.056198	-0.048175	0.005387
212	H	30	S	0.170507	0.079048	-0.038052	-0.036845	0.001611
213	H	31	S	-0.237451	0.181706	-0.058599	0.028139	0.006896
214	H	31	S	-0.158766	0.124009	-0.039874	0.020531	0.003160
215	H	32	S	-0.037607	-0.220485	0.083496	0.013450	-0.007076
216	H	32	S	-0.033027	-0.179901	0.070117	0.011247	-0.009746
217	H	33	S	0.007689	-0.030766	0.021589	0.033033	-0.015023
218	H	33	S	0.004813	-0.024783	0.015669	0.009543	-0.009689
219	H	34	S	-0.001725	0.006955	0.028511	-0.033671	0.017763
220	H	34	S	0.004254	-0.000113	0.000755	-0.010015	0.007179
221	H	35	S	0.010116	0.002953	-0.010708	-0.004212	-0.002840
222	H	35	S	0.002118	0.002097	-0.004696	0.007615	0.015588

51	52	53	54	55
-0.5830	-0.5670	-0.5522	-0.5309	-0.5093

A	A	A	A	A
---	---	---	---	---

1	CO	1	S	-0.014449	-0.010182	-0.007697	-0.019388	0.014136
2	CO	1	X	-0.008075	0.007405	-0.026935	-0.003265	0.001152
3	CO	1	Y	-0.028733	-0.049857	0.085721	-0.015882	-0.005291
4	CO	1	Z	0.008168	0.005096	0.019139	0.014746	-0.004933
5	CO	1	XX	0.109087	0.123487	-0.160555	0.047232	-0.004413

6 CO 1 YY -0.112401 -0.177053 0.255457 -0.052481 0.018598
7 CO 1 ZZ 0.003315 0.053566 -0.094901 0.005249 -0.014185
8 CO 1 XY 0.070059 0.038785 -0.026428 0.033873 -0.006191
9 CO 1 XZ -0.036396 -0.090855 0.146165 0.021273 0.001591
10 CO 1 YZ -0.017784 0.052900 -0.054465 0.038712 0.040612
11 CO 1 XX 0.043342 0.048097 -0.063076 0.018276 -0.001713
12 CO 1 YY -0.045210 -0.070884 0.102066 -0.020426 0.006621
13 CO 1 ZZ 0.001868 0.022787 -0.038990 0.002150 -0.004908
14 CO 1 XY 0.026884 0.016386 -0.011837 0.014509 -0.002747
15 CO 1 XZ -0.014791 -0.036922 0.058039 0.009937 0.000841
16 CO 1 YZ -0.005950 0.022713 -0.022994 0.015335 0.015834
17 CO 1 S 0.039040 0.026855 0.032606 0.058500 -0.047581
18 CO 1 X 0.001055 0.001974 0.015475 0.000030 0.012552
19 CO 1 Y 0.026124 0.020603 -0.067601 -0.002480 0.010916
20 CO 1 Z -0.011560 -0.017514 -0.011848 -0.022040 0.007972
21 CO 1 S 0.007749 0.003548 -0.004420 0.003423 -0.008240
22 CO 1 X -0.004841 -0.004472 -0.001383 -0.001983 -0.003153
23 CO 1 Y -0.001569 -0.002297 -0.007336 -0.000030 0.001017
24 CO 1 Z -0.000856 -0.002496 0.002008 -0.002499 0.005174
25 CO 1 S -0.014032 -0.010044 -0.003646 -0.015600 0.010369
26 CO 1 X 0.000870 -0.001241 0.003876 0.001066 -0.001325
27 CO 1 Y 0.004558 0.010393 -0.015906 0.004765 -0.000296
28 CO 1 Z -0.000116 0.000088 -0.002999 -0.001910 0.000288
29 CO 1 XX 0.023379 0.043990 -0.049348 0.009741 0.001797
30 CO 1 YY -0.023680 -0.051858 0.065147 -0.014071 -0.004548
31 CO 1 ZZ 0.000301 0.007868 -0.015799 0.004330 0.002751
32 CO 1 XY 0.016207 0.007327 -0.006598 -0.009601 0.002912
33 CO 1 XZ -0.013045 -0.022751 0.035537 -0.011396 -0.000404
34 CO 1 YZ -0.006027 0.011246 -0.012340 0.013547 0.003913
35 C 2 S 0.008754 -0.004595 0.001263 -0.004582 -0.000975
36 C 2 X -0.274796 0.047321 -0.039946 0.006132 0.010618
37 C 2 Y 0.091582 -0.046941 0.052332 -0.050314 0.040829
38 C 2 Z -0.035713 -0.092709 -0.108526 0.170553 -0.160563
39 C 2 S 0.331408 -0.185325 0.030088 -0.008180 -0.029807
40 C 2 X -0.087631 0.081677 -0.005536 0.004796 0.016024
41 C 2 Y -0.044271 0.055979 -0.004048 -0.009139 0.018411
42 C 2 Z -0.029067 -0.009911 -0.041057 0.052800 -0.054798
43 C 3 S 0.013249 0.009577 -0.010601 -0.001204 0.001488
44 C 3 X 0.230127 -0.040509 0.065522 0.000347 -0.002589
45 C 3 Y -0.070983 0.106579 0.033237 -0.010216 0.030199
46 C 3 Z -0.056687 -0.127123 -0.178025 0.061123 -0.112222
47 C 3 S -0.133912 0.161737 -0.059437 0.006857 0.023454
48 C 3 X -0.016893 -0.042764 0.009334 0.003244 -0.011487
49 C 3 Y -0.021103 0.021122 0.015571 -0.007407 0.010961
50 C 3 Z -0.016807 -0.035017 -0.048966 0.017913 -0.037258
51 C 4 S -0.036311 -0.011891 0.016288 0.002513 -0.005382

52	C	4	X	-0.182072	0.054057	-0.062924	-0.000772	0.012107
53	C	4	Y	0.017199	0.022570	0.064550	0.027779	-0.008543
54	C	4	Z	-0.045622	-0.199006	-0.186067	-0.090814	0.021679
55	C	4	S	-0.063194	-0.122395	0.058877	0.026019	-0.032901
56	C	4	X	0.046764	-0.028264	0.010330	-0.014935	0.000439
57	C	4	Y	0.012893	-0.052870	0.037330	0.008827	-0.016097
58	C	4	Z	-0.007396	-0.080591	-0.049407	-0.025865	-0.002128
59	C	5	S	0.046413	0.021722	-0.007429	0.001450	0.001406
60	C	5	X	0.133921	-0.042569	0.067489	0.019563	-0.020086
61	C	5	Y	-0.044538	0.139784	-0.011715	0.075743	-0.045039
62	C	5	Z	-0.033736	-0.131617	-0.112835	-0.173608	0.135673
63	C	5	S	-0.162721	0.293228	-0.060839	-0.002183	0.049141
64	C	5	X	0.003804	0.076917	-0.044619	-0.008639	0.010622
65	C	5	Y	-0.186003	0.189352	-0.045564	0.051701	0.001350
66	C	5	Z	-0.070769	-0.002115	-0.074592	-0.060884	0.065196
67	C	6	S	-0.043204	-0.021887	0.008578	-0.013006	-0.005219
68	C	6	X	-0.206516	0.024049	-0.038545	0.020752	0.015904
69	C	6	Y	-0.013306	-0.096698	0.054693	0.026550	-0.042645
70	C	6	Z	-0.032543	-0.014040	0.005103	-0.131292	0.123215
71	C	6	S	-0.091808	-0.042874	-0.004514	-0.056423	0.010942
72	C	6	X	0.158413	-0.244943	0.085273	0.015453	-0.048240
73	C	6	Y	-0.321801	0.261207	-0.068531	0.038350	0.015224
74	C	6	Z	-0.107647	0.084757	-0.019223	-0.040075	0.053687
75	C	7	S	0.043547	0.010064	-0.001621	0.003391	0.003638
76	C	7	X	0.279345	-0.023782	0.031807	-0.011293	-0.007464
77	C	7	Y	-0.034541	0.117514	-0.057644	-0.043906	0.024657
78	C	7	Z	-0.067847	0.057381	-0.010748	0.205378	-0.089682
79	C	7	S	0.168915	0.072573	-0.034688	-0.016108	0.019334
80	C	7	X	-0.287030	0.095083	-0.005253	0.003828	0.011260
81	C	7	Y	0.247763	-0.181276	0.024097	-0.037748	-0.021710
82	C	7	Z	0.045973	-0.040576	0.006498	0.074811	-0.044497
83	C	8	S	-0.001615	-0.003879	0.001741	-0.002991	-0.000201
84	C	8	X	-0.204627	0.017631	-0.009556	0.004108	0.001504
85	C	8	Y	0.058009	-0.152882	0.019382	-0.077673	0.016156
86	C	8	Z	-0.024382	0.073077	0.143606	0.235196	-0.070947
87	C	8	S	-0.303613	0.153104	-0.006743	0.023456	0.015970
88	C	8	X	0.157280	-0.031110	-0.000487	-0.007460	-0.000759
89	C	8	Y	0.136995	-0.047614	-0.020495	-0.033611	-0.009017
90	C	8	Z	0.027272	0.022691	0.040335	0.070601	-0.028025
91	C	9	S	0.019165	-0.008552	0.009644	-0.006481	-0.002833
92	C	9	X	0.210190	0.004368	-0.008819	0.008451	0.002843
93	C	9	Y	-0.042097	0.098570	-0.132746	-0.016838	0.009743
94	C	9	Z	-0.033673	0.194255	0.172442	0.157410	-0.004399
95	C	9	S	0.233453	-0.106697	0.017240	-0.046850	-0.040226
96	C	9	X	-0.009224	0.009375	-0.000032	0.013659	0.022296
97	C	9	Y	-0.068651	-0.007908	0.004579	0.007324	0.012037

98	C	9	Z	-0.021145	0.042642	0.058535	0.052307	0.002867
99	C	10	S	-0.011403	0.007238	-0.019613	0.008102	0.009226
100	C	10	X	-0.145572	-0.003182	0.022311	0.000142	-0.000146
101	C	10	Y	-0.015480	-0.201476	0.051857	-0.035444	-0.033423
102	C	10	Z	0.011604	0.139270	0.227761	-0.035657	0.058032
103	C	10	S	-0.082215	0.042062	-0.013425	0.083268	0.002129
104	C	10	X	-0.048391	0.063855	-0.000456	0.029745	0.037968
105	C	10	Y	-0.076403	-0.004312	-0.008115	-0.011822	0.023883
106	C	10	Z	-0.021688	0.048945	0.069800	-0.008688	0.023554
107	C	11	S	0.028770	-0.008181	0.032756	-0.003432	0.000724
108	C	11	X	0.166782	0.016343	-0.019674	-0.002804	-0.006589
109	C	11	Y	-0.053990	0.105437	-0.141071	0.088283	-0.010563
110	C	11	Z	-0.002311	0.200209	0.054571	-0.176513	0.083843
111	C	11	S	0.257371	-0.221055	0.093589	-0.006610	-0.014627
112	C	11	X	0.093332	-0.223678	0.082186	-0.010562	-0.051517
113	C	11	Y	-0.076593	-0.006539	-0.022823	-0.031194	0.022032
114	C	11	Z	-0.015929	0.079147	0.028938	-0.076455	0.049967
115	N	12	S	0.002167	0.048155	-0.095345	0.028882	-0.006280
116	N	12	X	-0.090034	-0.003016	-0.011656	0.019218	0.012989
117	N	12	Y	-0.152236	-0.223686	0.296996	-0.112457	-0.004470
118	N	12	Z	0.059164	-0.037538	-0.084601	-0.084446	-0.146347
119	N	12	S	-0.026627	0.030049	-0.131543	0.042193	-0.020850
120	N	12	X	-0.038587	-0.022557	0.004488	-0.005726	0.008371
121	N	12	Y	-0.076859	-0.152046	0.190064	-0.063903	-0.020789
122	N	12	Z	0.035607	-0.021577	-0.050625	-0.058591	-0.091514
123	C	13	S	-0.009796	-0.015921	0.045536	-0.022848	0.006587
124	C	13	X	0.051027	0.009270	0.047510	-0.041216	0.008259
125	C	13	Y	0.045851	0.040420	-0.099029	0.061677	-0.021619
126	C	13	Z	0.030299	-0.182670	0.012171	0.127204	-0.035455
127	C	13	S	0.019697	-0.007773	0.007207	-0.078809	0.008528
128	C	13	X	-0.010077	-0.024225	0.011005	0.020593	0.004779
129	C	13	Y	0.008456	0.012631	-0.040178	0.050937	-0.005058
130	C	13	Z	0.016092	-0.063978	0.004742	0.054445	-0.009549
131	C	14	S	-0.015632	-0.022816	0.025332	-0.004179	0.000845
132	C	14	X	-0.085648	-0.054938	0.060240	-0.030438	-0.006600
133	C	14	Y	-0.020058	-0.060779	0.028083	0.086343	0.053475
134	C	14	Z	0.003411	-0.045805	-0.031840	0.239465	0.123308
135	C	14	S	-0.039764	-0.068886	0.032987	0.028917	0.007744
136	C	14	X	0.005181	0.033583	-0.020087	0.030467	-0.010129
137	C	14	Y	-0.031766	-0.037702	0.057304	0.052659	0.029531
138	C	14	Z	0.007933	-0.007688	-0.034895	0.092275	0.057015
139	C	15	S	-0.003823	0.009924	-0.008318	0.001579	-0.001209
140	C	15	X	0.039296	0.030250	-0.026224	0.004583	0.011670
141	C	15	Y	0.015861	0.048292	-0.020611	0.007228	-0.090983
142	C	15	Z	-0.021209	0.023497	0.037462	0.009461	-0.233901
143	C	15	S	-0.022364	0.035386	0.009995	0.016699	0.001865

144	C	15	X	-0.034233	-0.062120	0.056520	-0.010115	0.014230
145	C	15	Y	-0.003540	0.007375	0.025435	0.009280	-0.039512
146	C	15	Z	-0.003715	0.008411	0.005808	-0.005312	-0.096291
147	C	16	S	-0.003237	-0.011803	0.012979	-0.003414	0.003805
148	C	16	X	-0.053584	-0.048801	0.031889	0.009285	0.033674
149	C	16	Y	-0.009532	0.032431	0.014676	-0.079532	-0.125495
150	C	16	Z	-0.030016	0.110459	0.020882	-0.205937	-0.324193
151	C	16	S	-0.018613	-0.077485	0.069837	-0.011306	0.014043
152	C	16	X	-0.008747	-0.020231	0.018015	0.004923	0.006029
153	C	16	Y	-0.000987	-0.008696	0.016094	-0.032750	-0.041698
154	C	16	Z	-0.010372	0.044772	0.004214	-0.080145	-0.129783
155	C	17	S	-0.003305	-0.000079	0.000364	-0.000016	-0.002034
156	C	17	X	0.046236	0.011239	-0.014240	0.021836	0.001155
157	C	17	Y	-0.013389	0.046449	0.005608	-0.094333	-0.027819
158	C	17	Z	-0.020320	0.123144	-0.001505	-0.233900	-0.075557
159	C	17	S	-0.007820	0.029342	-0.021424	0.002985	-0.014273
160	C	17	X	-0.012619	0.005368	-0.004160	0.007313	-0.002842
161	C	17	Y	-0.005672	0.017650	-0.005290	-0.028558	-0.005503
162	C	17	Z	-0.006144	0.033414	0.000810	-0.073842	-0.020240
163	C	18	S	-0.000872	0.001218	-0.000889	0.000053	-0.000419
164	C	18	X	-0.056072	-0.025344	0.012904	0.007277	-0.017357
165	C	18	Y	-0.006035	0.032351	-0.007943	-0.041206	0.089258
166	C	18	Z	-0.025008	0.089202	-0.015418	-0.109629	0.227385
167	C	18	S	0.008615	-0.000423	-0.026085	-0.000274	-0.003022
168	C	18	X	0.008279	-0.000112	-0.012697	0.006353	-0.006640
169	C	18	Y	-0.005239	0.023596	-0.018982	-0.014886	0.026388
170	C	18	Z	-0.004432	0.021156	0.001382	-0.038651	0.075830
171	C	19	S	-0.002614	-0.008726	0.008644	-0.001268	0.000966
172	C	19	X	0.058802	0.010786	-0.004912	-0.006302	-0.029739
173	C	19	Y	-0.007980	0.009633	-0.004394	0.032475	0.130236
174	C	19	Z	-0.003538	0.028825	-0.031398	0.090963	0.339024
175	C	19	S	0.020384	0.031094	-0.022774	0.006725	-0.005178
176	C	19	X	0.019226	0.026914	-0.051719	0.000773	-0.017816
177	C	19	Y	-0.004656	-0.012881	0.000850	0.004254	0.053155
178	C	19	Z	0.001695	0.021430	-0.015473	0.029590	0.131299
179	O	20	S	-0.025200	-0.028800	0.032645	-0.012782	0.007595
180	O	20	X	-0.079475	-0.064117	0.068470	-0.022730	0.011965
181	O	20	Y	-0.009887	-0.047373	0.051331	-0.006709	0.070300
182	O	20	Z	0.012175	-0.036685	0.025047	0.007590	0.135199
183	O	20	S	-0.028570	-0.037242	0.047519	-0.016501	0.009008
184	O	20	X	-0.053104	-0.046957	0.048307	-0.018798	0.012046
185	O	20	Y	0.001255	-0.019954	0.017560	-0.008112	0.043008
186	O	20	Z	0.004514	-0.023413	0.018188	0.002307	0.078651
187	N	21	S	-0.035121	-0.037145	0.061429	-0.001815	-0.008581
188	N	21	X	-0.079536	0.055413	-0.165662	-0.017492	0.030219
189	N	21	Y	-0.059932	-0.050755	0.017112	-0.027702	0.010673

190	N	21	Z	-0.017584	-0.025077	0.156463	0.053197	-0.044188
191	N	21	S	-0.093263	-0.023895	0.072927	-0.008452	-0.014871
192	N	21	X	-0.050591	0.053168	-0.119638	-0.002558	0.023370
193	N	21	Y	-0.038516	-0.011124	-0.008386	0.006336	-0.004369
194	N	21	Z	-0.016957	-0.033538	0.106483	0.014285	-0.018708
195	H	22	S	-0.138257	-0.012507	-0.014984	0.001475	0.003450
196	H	22	S	-0.055096	-0.037977	-0.005029	-0.002238	-0.001992
197	H	23	S	0.201443	-0.051905	0.046886	-0.001211	-0.004683
198	H	23	S	0.121948	-0.024860	0.030182	-0.003494	0.000343
199	H	24	S	-0.048746	0.041537	-0.011257	0.004651	-0.000312
200	H	24	S	-0.026374	0.008465	-0.012351	0.001536	-0.002392
201	H	25	S	-0.126201	-0.051349	0.021865	-0.004548	-0.000567
202	H	25	S	-0.146799	-0.018371	0.015052	0.001988	0.002937
203	H	26	S	-0.043234	0.118508	-0.064096	0.020152	0.006095
204	H	26	S	-0.014210	0.076548	-0.051717	0.007322	0.001815
205	H	27	S	0.115394	-0.041949	0.023793	-0.009942	0.000004
206	H	27	S	0.081106	-0.006442	0.009125	-0.000794	0.006428
207	H	28	S	0.049407	0.084958	-0.101452	0.017077	-0.014308
208	H	28	S	0.031071	0.025540	-0.045758	0.012996	-0.010993
209	H	29	S	0.007050	0.010846	-0.007029	-0.000014	0.001260
210	H	29	S	0.009491	0.004189	-0.007610	0.002217	0.001526
211	H	30	S	-0.034853	-0.016619	0.010335	-0.001730	0.002790
212	H	30	S	-0.024166	-0.007374	0.004276	-0.000034	0.001620
213	H	31	S	0.038201	0.011763	-0.009705	0.002083	-0.000672
214	H	31	S	0.023964	0.003894	-0.004067	0.003590	0.000189
215	H	32	S	0.004728	0.003978	0.000700	-0.000604	-0.000314
216	H	32	S	0.003085	0.012580	-0.003591	0.002851	-0.001693
217	H	33	S	0.025036	0.029880	-0.038975	0.008454	0.004845
218	H	33	S	0.005702	0.012022	-0.017291	0.004177	-0.000530
219	H	34	S	0.011667	-0.037963	-0.033251	-0.050390	0.033619
220	H	34	S	-0.003867	-0.016759	-0.017386	-0.028981	0.031440
221	H	35	S	0.008760	0.055328	-0.055990	0.022318	-0.003791
222	H	35	S	-0.001348	0.034227	-0.023997	0.021045	-0.006638

56	57	58	59	60
-0.5037	-0.4869	-0.4524	-0.3464	-0.3267
A	A	A	A	A

1	CO	1	S	-0.015536	-0.006667	-0.005789	0.032259	-0.142960
2	CO	1	X	-0.015747	-0.005353	-0.008988	0.008091	-0.025029
3	CO	1	Y	0.006982	0.003636	0.025458	-0.025784	0.063982
4	CO	1	Z	-0.004414	-0.002862	0.017037	0.043204	-0.088924
5	CO	1	XX	0.007825	-0.009380	-0.009796	-0.010977	0.087844
6	CO	1	YY	0.020597	0.010663	0.029151	0.009687	-0.041168
7	CO	1	ZZ	-0.028422	-0.001283	-0.019354	0.001289	-0.046675
8	CO	1	XY	0.049384	-0.006988	-0.004480	-0.006880	0.006497
9	CO	1	XZ	0.056145	0.001098	0.021526	0.034867	-0.126637

10	CO	1	YZ	-0.050065	-0.011533	-0.002230	0.058578	0.027413
11	CO	1	XX	0.002220	-0.003817	-0.002507	-0.003034	0.027593
12	CO	1	YY	0.008773	0.003730	0.009697	0.004142	-0.014336
13	CO	1	ZZ	-0.010993	0.000087	-0.007190	-0.001108	-0.013257
14	CO	1	XY	0.018317	-0.004018	-0.002062	-0.001353	0.000606
15	CO	1	XZ	0.020200	0.000186	0.007084	0.013672	-0.040809
16	CO	1	YZ	-0.018091	-0.004706	-0.001339	0.020932	0.007642
17	CO	1	S	0.053802	0.030656	0.020066	-0.113940	0.512862
18	CO	1	X	0.001269	0.032073	0.028883	0.000652	0.097578
19	CO	1	Y	0.001315	-0.006188	-0.052841	0.061316	-0.212826
20	CO	1	Z	0.011850	0.003098	-0.034827	-0.125977	0.214377
21	CO	1	S	0.003220	0.006252	-0.007198	-0.122244	0.595446
22	CO	1	X	-0.005796	-0.003829	-0.000063	-0.021424	0.065626
23	CO	1	Y	0.003979	-0.003309	-0.010772	0.025915	-0.116877
24	CO	1	Z	0.017141	0.001674	-0.005341	-0.029964	0.076516
25	CO	1	S	-0.011197	-0.004062	-0.003837	0.028634	-0.126787
26	CO	1	X	0.004576	-0.001398	0.000206	-0.002579	0.002075
27	CO	1	Y	-0.000943	-0.001409	-0.003140	0.002863	-0.001352
28	CO	1	Z	0.001184	0.000002	-0.002003	-0.002497	0.008445
29	CO	1	XX	-0.007807	0.007183	-0.010563	-0.008311	0.017638
30	CO	1	YY	0.010843	-0.003170	0.008967	-0.009831	-0.014399
31	CO	1	ZZ	-0.003035	-0.004014	0.001596	0.018142	-0.003240
32	CO	1	XY	-0.004912	0.009323	-0.003274	-0.013522	0.003155
33	CO	1	XZ	0.010268	-0.005236	0.006360	-0.010446	-0.036161
34	CO	1	YZ	-0.011120	0.001758	0.005823	0.002366	-0.014150
35	C	2	S	0.001662	-0.002728	0.000194	-0.004488	-0.003438
36	C	2	X	-0.015462	0.001778	-0.008789	0.004202	0.001970
37	C	2	Y	-0.047447	-0.002642	-0.071345	-0.018742	-0.004175
38	C	2	Z	0.188787	0.017402	0.273297	0.064216	0.027717
39	C	2	S	0.022797	-0.026381	-0.016043	0.007779	-0.016850
40	C	2	X	-0.013423	0.010179	0.000834	0.003972	0.000614
41	C	2	Y	-0.020989	0.018445	-0.030504	0.001565	-0.013684
42	C	2	Z	0.066818	0.013433	0.115558	0.034306	0.016757
43	C	3	S	-0.004013	-0.001535	-0.002803	-0.001334	0.011269
44	C	3	X	0.009452	0.011138	-0.002160	0.001320	-0.016829
45	C	3	Y	-0.034056	0.066371	-0.055980	0.000989	-0.017119
46	C	3	Z	0.133357	-0.246259	0.213768	0.000457	0.009496
47	C	3	S	-0.031521	0.021539	0.002866	0.024306	-0.001371
48	C	3	X	0.013907	-0.004973	-0.004166	0.001267	-0.002128
49	C	3	Y	-0.010831	0.037823	-0.022652	-0.014982	-0.011462
50	C	3	Z	0.045172	-0.081945	0.098162	0.005040	0.011353
51	C	4	S	0.011126	-0.001210	0.005932	0.000810	-0.025744
52	C	4	X	-0.024708	0.013911	-0.004293	0.002311	0.025256
53	C	4	Y	0.011758	0.095893	0.038567	0.024709	0.020660
54	C	4	Z	-0.031283	-0.303103	-0.127792	-0.074801	-0.034451
55	C	4	S	0.061801	-0.068326	-0.003967	0.057552	0.015397

56	C	4	X	-0.004881	0.032769	0.003412	-0.046520	-0.000960
57	C	4	Y	0.022130	0.023829	0.001979	0.014844	0.052150
58	C	4	Z	0.001904	-0.135096	-0.058847	-0.059158	-0.018017
59	C	5	S	-0.006038	-0.001309	0.001561	0.001119	-0.000989
60	C	5	X	0.035197	0.005733	0.026138	0.004382	-0.030119
61	C	5	Y	0.053482	0.007558	0.100856	0.004490	-0.029250
62	C	5	Z	-0.165502	-0.029141	-0.275679	0.019932	-0.025333
63	C	5	S	-0.040683	0.006748	0.039338	-0.008505	0.047873
64	C	5	X	-0.029608	0.077678	0.040849	-0.045084	-0.118257
65	C	5	Y	0.010139	-0.007324	0.089153	0.075087	-0.024830
66	C	5	Z	-0.078535	-0.017429	-0.127567	0.039209	-0.024836
67	C	6	S	0.006925	0.003856	0.000200	-0.016356	-0.019113
68	C	6	X	-0.024784	-0.000386	-0.007069	0.026588	0.009173
69	C	6	Y	0.061691	-0.094577	-0.009638	-0.041280	0.003708
70	C	6	Z	-0.159461	0.309656	0.019666	0.092439	0.036955
71	C	6	S	-0.021857	0.009426	0.035557	-0.182061	0.019487
72	C	6	X	0.042940	-0.120117	-0.067176	0.044546	0.066685
73	C	6	Y	0.000386	-0.099745	0.044143	0.010879	0.060671
74	C	6	Z	-0.065067	0.129772	0.029612	0.071708	0.064180
75	C	7	S	-0.004637	-0.000246	-0.006370	0.004750	0.006330
76	C	7	X	0.011563	-0.005423	0.009725	-0.006812	-0.013764
77	C	7	Y	-0.028726	-0.080968	0.009243	-0.002719	-0.002626
78	C	7	Z	0.094209	0.297586	-0.007378	0.002950	-0.022395
79	C	7	S	-0.021864	0.102096	-0.000219	-0.017378	-0.068482
80	C	7	X	-0.004845	-0.044446	0.014699	-0.015168	0.041273
81	C	7	Y	0.007940	-0.078621	-0.018498	-0.024080	0.012269
82	C	7	Z	0.043046	0.089349	-0.010657	0.004812	-0.020412
83	C	8	S	0.000402	0.005033	0.002213	-0.005990	-0.005630
84	C	8	X	-0.002274	-0.005216	0.000068	0.010712	0.002067
85	C	8	Y	-0.015704	-0.001474	0.078974	0.037844	0.021116
86	C	8	Z	0.082615	0.005280	-0.299785	-0.163981	-0.058811
87	C	8	S	0.000256	0.002571	0.014204	0.045982	0.005398
88	C	8	X	0.000133	0.021645	0.002988	-0.008525	-0.014989
89	C	8	Y	0.004756	-0.010299	0.027564	0.014854	0.001337
90	C	8	Z	0.031739	0.001705	-0.128236	-0.106889	-0.040159
91	C	9	S	0.005435	0.002669	0.000948	-0.004153	0.001762
92	C	9	X	-0.006273	-0.004498	-0.001943	0.001643	-0.004720
93	C	9	Y	-0.018422	0.065418	0.060777	0.010409	-0.008758
94	C	9	Z	0.007266	-0.259581	-0.217571	-0.003979	0.025960
95	C	9	S	0.051203	0.015111	-0.013419	-0.033803	-0.059090
96	C	9	X	-0.030167	0.017305	0.007223	-0.017748	0.016181
97	C	9	Y	-0.011418	0.011130	0.025445	0.049319	0.017262
98	C	9	Z	-0.000842	-0.097612	-0.098709	0.010599	0.022916
99	C	10	S	-0.015650	0.000655	0.004229	0.013036	-0.002256
100	C	10	X	0.001671	-0.027861	0.001180	0.035202	0.009281
101	C	10	Y	0.049850	0.098364	-0.040145	-0.099991	-0.018145

102	C	10	Z	-0.057739	-0.301198	0.151220	0.149688	0.053668
103	C	10	S	-0.016355	-0.075192	-0.026752	0.175304	0.048771
104	C	10	X	-0.042490	-0.014806	0.021425	0.058189	0.062627
105	C	10	Y	-0.030056	0.088957	0.005305	-0.157459	-0.001939
106	C	10	Z	-0.027494	-0.113171	0.069812	0.079680	0.040412
107	C	11	S	0.002625	-0.001754	0.004224	-0.008951	-0.012358
108	C	11	X	0.005171	-0.010237	0.017902	0.017482	-0.021855
109	C	11	Y	0.000218	-0.004217	-0.089323	0.031582	0.021269
110	C	11	Z	-0.096144	-0.028654	0.308122	-0.025776	-0.051490
111	C	11	S	-0.001595	-0.007851	-0.037184	-0.125022	-0.008824
112	C	11	X	0.058185	-0.018095	-0.059581	0.046321	-0.051611
113	C	11	Y	-0.018983	0.098701	-0.002772	-0.123072	-0.027116
114	C	11	Z	-0.054719	0.014067	0.162215	-0.080703	-0.044244
115	N	12	S	-0.007141	-0.009033	-0.023890	0.021488	-0.055466
116	N	12	X	-0.024676	-0.007260	0.000579	0.049419	0.000139
117	N	12	Y	0.049604	0.022085	0.052926	-0.099805	0.057059
118	N	12	Z	0.195853	0.015249	-0.093905	-0.314531	-0.124552
119	N	12	S	0.004833	-0.002896	-0.059713	0.055183	-0.133843
120	N	12	X	-0.006817	0.001991	0.017653	0.030243	-0.009048
121	N	12	Y	0.055294	-0.003357	0.017128	-0.057177	0.001710
122	N	12	Z	0.119080	0.008538	-0.059208	-0.258515	-0.080334
123	C	13	S	-0.001373	-0.003264	0.028391	0.003042	-0.006953
124	C	13	X	-0.000217	0.004041	0.044966	-0.057081	0.030101
125	C	13	Y	0.007762	-0.015998	-0.052689	0.147503	0.038971
126	C	13	Z	0.028295	0.019774	-0.145204	0.427663	0.081877
127	C	13	S	-0.000103	-0.054714	0.135098	0.073084	-0.229382
128	C	13	X	-0.011945	0.041899	-0.037812	-0.064425	0.154337
129	C	13	Y	0.000255	0.008350	-0.069174	0.123123	0.089935
130	C	13	Z	0.007112	0.005275	-0.067265	0.306046	0.050597
131	C	14	S	-0.002586	0.005483	0.000239	0.001474	-0.007513
132	C	14	X	0.019853	0.008478	-0.007466	-0.004183	0.005794
133	C	14	Y	-0.081068	0.000467	0.025541	0.029305	0.047118
134	C	14	Z	-0.236611	-0.016115	0.071710	0.083914	0.027123
135	C	14	S	-0.022976	0.045840	-0.062142	0.054418	-0.062990
136	C	14	X	0.016637	0.042802	-0.080021	-0.067388	0.231998
137	C	14	Y	-0.044800	0.009837	0.000466	-0.037783	0.202457
138	C	14	Z	-0.099261	-0.006476	0.035116	0.070333	-0.012682
139	C	15	S	0.001561	-0.002575	0.002838	-0.017485	0.059137
140	C	15	X	0.028026	-0.000398	-0.003706	-0.010350	0.122595
141	C	15	Y	-0.121111	-0.010765	0.031641	-0.076518	-0.116698
142	C	15	Z	-0.281624	-0.007803	0.075676	-0.253670	-0.014894
143	C	15	S	0.016948	-0.009620	0.004084	-0.125421	0.363639
144	C	15	X	0.009118	0.000422	0.012068	0.032374	0.028374
145	C	15	Y	-0.046365	-0.002630	0.007246	-0.100377	0.053585
146	C	15	Z	-0.105847	-0.005195	0.036682	-0.152368	-0.081648
147	C	16	S	0.001302	0.001335	-0.000497	0.009852	-0.032647

148	C	16	X	0.004131	0.001384	0.002136	0.011835	-0.036025
149	C	16	Y	-0.012124	0.004382	-0.019976	0.008712	0.008787
150	C	16	Z	-0.038967	0.006116	-0.046881	0.022917	-0.004247
151	C	16	S	-0.000779	0.006047	0.004531	0.078117	-0.160594
152	C	16	X	-0.010331	0.004233	-0.002166	-0.005757	0.013339
153	C	16	Y	-0.003294	0.008147	-0.012146	0.047228	-0.068400
154	C	16	Z	-0.008297	0.001848	-0.023113	0.002788	0.035112
155	C	17	S	0.000639	0.000621	-0.000208	-0.005310	0.027376
156	C	17	X	-0.017994	-0.000614	0.007808	-0.028557	0.029872
157	C	17	Y	0.091590	0.005483	-0.036595	0.103928	-0.002573
158	C	17	Z	0.241942	0.015245	-0.096995	0.243309	0.072928
159	C	17	S	-0.001328	0.000138	-0.005300	-0.065597	0.183526
160	C	17	X	-0.005952	0.000050	0.002192	-0.043728	0.065604
161	C	17	Y	0.041896	0.001048	-0.017042	0.067866	0.011219
162	C	17	Z	0.086135	0.005825	-0.041614	0.158635	0.049328
163	C	18	S	0.000138	-0.000398	-0.000445	-0.001388	0.000711
164	C	18	X	-0.024138	-0.001268	0.000432	0.003520	0.000584
165	C	18	Y	0.117214	0.003151	-0.007921	-0.022253	-0.003672
166	C	18	Z	0.294348	0.007323	-0.017201	-0.052859	-0.022280
167	C	18	S	-0.010561	-0.008434	0.000976	0.036502	-0.103236
168	C	18	X	-0.010483	-0.003610	-0.002638	0.023516	-0.036869
169	C	18	Y	0.046018	0.001433	-0.007309	-0.027912	0.026422
170	C	18	Z	0.103747	0.002778	-0.007025	-0.040668	-0.032546
171	C	19	S	0.001420	0.002096	0.000677	-0.002052	0.019577
172	C	19	X	-0.004684	0.002929	-0.006398	0.013451	0.030977
173	C	19	Y	0.029410	-0.003264	0.033671	-0.078836	-0.030320
174	C	19	Z	0.091047	-0.007337	0.080038	-0.224359	-0.042913
175	C	19	S	0.017229	0.021828	-0.026103	-0.043704	0.153450
176	C	19	X	-0.000087	-0.001249	-0.013445	0.019168	-0.006496
177	C	19	Y	0.008823	-0.013539	0.032020	-0.015718	-0.110504
178	C	19	Z	0.046936	0.001493	0.030081	-0.146476	0.001007
179	O	20	S	-0.013666	-0.001051	0.004899	0.041095	-0.187590
180	O	20	X	-0.014211	-0.000905	0.004243	0.027272	-0.084807
181	O	20	Y	0.081847	0.002659	-0.001883	0.043753	0.024399
182	O	20	Z	0.161983	0.003298	-0.015093	0.093341	-0.006729
183	O	20	S	-0.024512	-0.002276	0.014351	0.084160	-0.430169
184	O	20	X	-0.003967	-0.000950	0.011839	0.029093	-0.052262
185	O	20	Y	0.045572	0.003444	-0.002852	0.039405	0.002514
186	O	20	Z	0.096434	0.002389	-0.011498	0.061570	0.002912
187	N	21	S	0.024159	0.006457	0.021309	0.011152	-0.155534
188	N	21	X	-0.069769	-0.007863	-0.046880	-0.002697	0.122816
189	N	21	Y	-0.011862	0.001601	-0.009770	-0.010884	0.028747
190	N	21	Z	0.074120	0.009322	0.076246	0.022213	-0.111965
191	N	21	S	0.030105	0.025867	0.061232	0.012962	-0.436368
192	N	21	X	-0.052626	0.004243	-0.022179	0.020982	0.107857
193	N	21	Y	-0.004631	-0.000701	0.007756	0.005312	-0.025342

194	N	21	Z	0.045607	-0.008947	0.032728	0.003554	-0.105507
195	H	22	S	-0.005858	0.000824	-0.001437	0.002340	0.005797
196	H	22	S	-0.000384	-0.007180	-0.001293	-0.002054	0.010607
197	H	23	S	0.009414	0.002381	0.002518	0.000060	-0.006293
198	H	23	S	0.003247	0.004789	0.003145	-0.004098	-0.009345
199	H	24	S	0.000873	0.000626	0.006253	0.003131	-0.017748
200	H	24	S	0.001874	-0.005395	-0.006062	0.004814	0.016620
201	H	25	S	0.001916	-0.001171	-0.002156	0.002651	0.004698
202	H	25	S	-0.002555	-0.007842	-0.002691	0.008392	0.013953
203	H	26	S	-0.011948	-0.006249	-0.000259	0.014214	0.000269
204	H	26	S	-0.007957	0.002276	0.002887	-0.005489	-0.006339
205	H	27	S	0.001135	0.002877	0.008383	-0.004338	-0.005640
206	H	27	S	0.000288	-0.010520	0.010359	0.052025	0.012472
207	H	28	S	0.004623	-0.011767	-0.015415	-0.005771	-0.022012
208	H	28	S	0.002691	0.008374	-0.020666	-0.043519	-0.048215
209	H	29	S	-0.002659	-0.002036	0.001680	0.007066	-0.034604
210	H	29	S	-0.004380	0.002315	-0.003388	0.017049	-0.043554
211	H	30	S	0.000261	-0.000156	-0.000521	0.003944	-0.015161
212	H	30	S	0.002078	0.000406	-0.001769	-0.001242	-0.012423
213	H	31	S	0.001914	0.000287	-0.000156	-0.002405	0.007039
214	H	31	S	-0.000341	0.000345	-0.001962	0.005213	-0.007842
215	H	32	S	-0.003975	-0.000459	0.002149	0.003223	-0.014566
216	H	32	S	-0.000440	0.004440	-0.007378	-0.013382	0.013469
217	H	33	S	0.013833	-0.000312	-0.008923	0.000485	0.064017
218	H	33	S	0.006544	-0.001426	-0.005702	-0.018284	0.194890
219	H	34	S	-0.038158	-0.009794	-0.065970	-0.020720	0.065708
220	H	34	S	-0.023580	-0.010308	-0.058574	-0.011831	0.116330
221	H	35	S	-0.004712	-0.006756	0.001853	0.018610	0.006967
222	H	35	S	0.010861	-0.008627	0.009784	0.021217	0.030837

61	62	63	64	65
-0.2837	-0.2657	-0.2599	-0.2514	-0.2394
A	A	A	A	A

1	CO	1	S	0.011740	0.005248	0.012418	-0.002248	0.009760
2	CO	1	X	-0.006445	0.030528	0.048811	-0.063803	0.030497
3	CO	1	Y	-0.025903	0.003442	0.022155	-0.012797	-0.013873
4	CO	1	Z	-0.029617	0.038062	0.066043	-0.081812	-0.032404
5	CO	1	XX	-0.026014	0.004850	0.023670	-0.008002	-0.009158
6	CO	1	YY	0.011525	0.002666	-0.030983	0.018445	0.016339
7	CO	1	ZZ	0.014489	-0.007516	0.007312	-0.010442	-0.007181
8	CO	1	XY	-0.000069	0.010911	0.005099	0.006386	0.011974
9	CO	1	XZ	-0.005886	-0.005793	-0.016944	0.005917	0.053172
10	CO	1	YZ	-0.014150	0.004004	-0.002150	0.017654	0.000644
11	CO	1	XX	-0.009836	0.001647	0.008356	-0.003241	-0.001239
12	CO	1	YY	0.004375	0.002114	-0.008650	0.005263	0.003812
13	CO	1	ZZ	0.005461	-0.003762	0.000294	-0.002022	-0.002573

14 CO 1 XY -0.001134 0.005607 0.004994 0.002373 0.006034
15 CO 1 XZ -0.001159 -0.004942 -0.003952 0.004006 0.012447
16 CO 1 YZ -0.003751 0.003148 -0.000420 0.006419 0.000163
17 CO 1 S -0.039504 -0.034495 -0.095283 0.014180 0.000978
18 CO 1 X 0.016231 -0.111934 -0.173404 0.114715 -0.027439
19 CO 1 Y 0.068965 0.028142 -0.016955 -0.009124 0.059011
20 CO 1 Z 0.083734 -0.130975 -0.214079 0.283331 0.066229
21 CO 1 S -0.000321 0.051900 0.260702 -0.070227 -0.518814
22 CO 1 X 0.019933 -0.125811 -0.157488 0.390120 -0.422125
23 CO 1 Y 0.114446 -0.035966 -0.104581 0.164940 -0.094885
24 CO 1 Z 0.027464 -0.080605 -0.266092 0.233746 0.510637
25 CO 1 S 0.009546 -0.002110 -0.010984 0.003167 0.031867
26 CO 1 X -0.000252 0.001948 -0.001055 0.006559 -0.000838
27 CO 1 Y 0.001422 -0.002173 -0.002558 0.003833 0.000897
28 CO 1 Z 0.001871 0.000827 -0.000493 0.002600 0.001093
29 CO 1 XX 0.026645 -0.013160 -0.020775 0.001412 -0.047702
30 CO 1 YY -0.018832 0.011807 0.031783 -0.014555 0.022873
31 CO 1 ZZ -0.007812 0.001352 -0.011007 0.013144 0.024829
32 CO 1 XY 0.016645 -0.014683 -0.022227 -0.014988 -0.019614
33 CO 1 XZ -0.010288 0.028226 -0.005036 0.000773 0.037621
34 CO 1 YZ -0.008207 -0.011080 -0.006825 -0.015142 -0.000014
35 C 2 S -0.000445 0.001695 0.005681 0.000385 0.006615
36 C 2 X -0.007789 -0.001513 -0.006574 -0.001772 0.005332
37 C 2 Y -0.086697 0.002217 -0.000278 -0.002480 -0.007306
38 C 2 Z 0.329054 -0.008185 0.007206 0.007790 -0.017274
39 C 2 S -0.008610 -0.090414 -0.180451 0.130601 0.220931
40 C 2 X -0.006869 0.037322 0.068710 -0.060434 -0.080505
41 C 2 Y -0.072548 0.031416 0.023949 -0.092856 -0.097376
42 C 2 Z 0.264579 -0.003652 0.004016 -0.010058 -0.051653
43 C 3 S 0.002454 0.004997 0.013469 -0.010151 -0.024179
44 C 3 X 0.001988 -0.003232 -0.005245 0.017870 0.032620
45 C 3 Y 0.038435 0.010925 0.056568 0.062062 0.047282
46 C 3 Z -0.157131 -0.054854 -0.251795 -0.194233 -0.070280
47 C 3 S 0.000934 0.105400 0.191952 -0.198800 -0.289054
48 C 3 X -0.001873 -0.047121 -0.081773 0.094547 0.113291
49 C 3 Y 0.035339 0.023125 0.064758 0.012931 -0.006887
50 C 3 Z -0.109390 -0.046810 -0.240087 -0.216254 -0.078873
51 C 4 S -0.001189 -0.003505 -0.013828 0.004195 0.048441
52 C 4 X 0.019955 0.002889 0.004522 -0.017111 -0.018751
53 C 4 Y 0.081643 -0.015005 -0.050964 -0.039695 -0.059428
54 C 4 Z -0.269217 0.048211 0.186766 0.154562 0.069303
55 C 4 S -0.044052 -0.113958 -0.164496 0.316662 0.470617
56 C 4 X 0.035209 -0.002010 -0.042172 -0.081589 -0.037509
57 C 4 Y 0.078949 -0.075964 -0.156392 0.078294 0.037042
58 C 4 Z -0.270436 0.026262 0.158736 0.220625 0.106622
59 C 5 S -0.003750 0.020456 0.051347 -0.036511 -0.034126

60	C	5	X	-0.021417	-0.024373	-0.068682	0.040628	0.086720
61	C	5	Y	-0.120444	-0.017259	-0.055353	0.034031	0.070276
62	C	5	Z	0.337331	0.006288	0.045776	0.010276	0.008599
63	C	5	S	0.007841	0.199067	0.479324	-0.319814	-0.336040
64	C	5	X	0.016427	0.049160	-0.028416	-0.241846	-0.201134
65	C	5	Y	-0.146563	0.044656	0.126745	-0.013489	-0.051032
66	C	5	Z	0.329838	0.034466	0.113841	-0.017456	-0.006817
67	C	6	S	-0.000729	0.004788	0.000404	-0.019404	0.034863
68	C	6	X	-0.001125	-0.003168	-0.009503	0.003178	0.005457
69	C	6	Y	0.020628	0.011680	0.079518	0.087678	-0.030841
70	C	6	Z	-0.065344	-0.030988	-0.211323	-0.270083	-0.047521
71	C	6	S	0.112346	0.010709	-0.056493	0.028579	0.092417
72	C	6	X	-0.048884	-0.152492	-0.130342	0.434241	0.549760
73	C	6	Y	0.018539	0.116269	0.436355	0.130216	-0.116610
74	C	6	Z	-0.066570	-0.023438	-0.167721	-0.277986	-0.074420
75	C	7	S	0.004512	0.001647	0.006502	-0.005413	-0.014548
76	C	7	X	-0.005625	-0.003894	-0.013736	0.003724	0.026724
77	C	7	Y	-0.000411	-0.020352	-0.079130	-0.050156	-0.014178
78	C	7	Z	-0.021630	0.065907	0.266346	0.199509	0.103940
79	C	7	S	0.031276	0.060553	-0.011485	-0.324644	-0.382769
80	C	7	X	-0.002760	0.024166	0.145690	0.114434	0.063817
81	C	7	Y	0.009056	-0.113752	-0.187726	0.159735	0.220844
82	C	7	Z	-0.018736	0.048164	0.257258	0.262408	0.186889
83	C	8	S	-0.003166	-0.003994	-0.010969	-0.003797	0.015109
84	C	8	X	0.002356	0.002994	0.003975	0.001406	0.003645
85	C	8	Y	0.071671	0.003539	0.013514	-0.011466	0.003014
86	C	8	Z	-0.250732	-0.013613	-0.026660	0.051215	-0.064321
87	C	8	S	-0.038810	0.087813	0.141781	-0.046586	-0.018682
88	C	8	X	0.011395	-0.012757	-0.063807	-0.065915	-0.049544
89	C	8	Y	0.061908	-0.013743	0.000608	0.027825	0.042837
90	C	8	Z	-0.193137	-0.023201	-0.037953	0.063451	-0.062113
91	C	9	S	0.001674	0.005135	0.004298	-0.007573	0.002155
92	C	9	X	-0.003427	-0.007729	-0.010603	0.004525	0.000973
93	C	9	Y	-0.043211	0.009709	0.058838	0.069873	0.010446
94	C	9	Z	0.147255	-0.051812	-0.224059	-0.228399	-0.036204
95	C	9	S	0.019932	-0.025189	-0.062125	-0.073383	-0.030085
96	C	9	X	0.009102	-0.027044	-0.065443	-0.036892	-0.047904
97	C	9	Y	-0.049172	0.044596	0.104504	0.098693	0.042818
98	C	9	Z	0.096122	-0.033866	-0.201119	-0.216634	-0.027528
99	C	10	S	-0.008738	-0.010353	-0.007622	0.008056	-0.002610
100	C	10	X	0.018503	0.015907	0.021607	-0.000657	0.001479
101	C	10	Y	-0.047610	-0.017104	-0.061095	-0.045385	-0.019750
102	C	10	Z	0.206688	0.049215	0.202683	0.133983	0.093777
103	C	10	S	-0.094735	-0.016862	0.131872	0.184610	0.233072
104	C	10	X	0.016638	0.081386	0.065207	0.000730	0.001421
105	C	10	Y	-0.019601	-0.071253	-0.185689	-0.121104	-0.139802

106	C	10	Z	0.208708	0.024441	0.175585	0.122931	0.076368
107	C	11	S	0.000936	0.004506	-0.005472	-0.022829	0.031576
108	C	11	X	-0.026065	-0.005087	0.000578	0.025550	0.003403
109	C	11	Y	0.079463	-0.002218	-0.000038	-0.000182	0.005279
110	C	11	Z	-0.282699	0.000513	0.023765	0.069437	-0.084359
111	C	11	S	-0.009843	-0.205631	-0.404587	0.105054	0.478238
112	C	11	X	-0.085096	-0.103335	-0.133280	0.139901	0.178121
113	C	11	Y	0.148841	-0.000940	-0.110389	-0.210059	-0.353333
114	C	11	Z	-0.243533	0.017221	-0.004503	0.007495	-0.174265
115	N	12	S	0.002997	0.000333	0.014468	0.001886	0.014646
116	N	12	X	-0.020669	0.004544	0.014637	0.001797	-0.006905
117	N	12	Y	-0.004258	0.008405	-0.005780	-0.000873	-0.013578
118	N	12	Z	0.134533	0.010277	0.043427	-0.052093	-0.016493
119	N	12	S	0.040638	0.013589	0.000056	-0.030515	-0.008193
120	N	12	X	-0.029141	-0.002884	0.003354	0.030101	-0.084280
121	N	12	Y	0.002068	0.029264	0.071524	-0.004710	-0.030510
122	N	12	Z	0.135527	-0.037508	0.023361	-0.019141	0.010057
123	C	13	S	-0.012851	-0.019831	-0.020355	0.052208	-0.018385
124	C	13	X	-0.019674	-0.005715	-0.019268	0.003471	0.007795
125	C	13	Y	-0.006632	0.034832	0.050470	-0.031265	0.002816
126	C	13	Z	-0.058895	0.067690	0.033696	-0.103217	-0.084658
127	C	13	S	0.037306	-0.143912	0.019248	0.463501	-0.447114
128	C	13	X	-0.081457	-0.044945	-0.110997	-0.082920	0.207111
129	C	13	Y	-0.005495	0.090158	0.000230	-0.092726	0.098163
130	C	13	Z	-0.056867	0.105173	0.034536	-0.080115	-0.085701
131	C	14	S	0.003097	-0.018946	-0.027543	0.028046	-0.034608
132	C	14	X	0.006021	0.011212	-0.006519	-0.016969	0.005462
133	C	14	Y	-0.043524	-0.025608	-0.002599	0.004182	0.062912
134	C	14	Z	-0.089723	-0.132080	-0.048973	0.117904	0.020266
135	C	14	S	-0.020506	-0.156948	-0.261972	0.162046	-0.337324
136	C	14	X	-0.054972	0.173912	-0.014736	-0.366679	0.410032
137	C	14	Y	-0.105587	-0.055825	0.005968	-0.042596	0.412019
138	C	14	Z	-0.061658	-0.172671	-0.077880	0.144523	-0.036503
139	C	15	S	-0.008907	0.006521	0.010808	-0.009496	0.053312
140	C	15	X	-0.026028	0.053032	0.017404	-0.047351	0.105649
141	C	15	Y	0.044765	-0.130380	0.055281	-0.011448	-0.059323
142	C	15	Z	0.063061	-0.265538	0.197171	-0.186124	0.016963
143	C	15	S	-0.124076	0.105890	0.097407	-0.099001	0.440980
144	C	15	X	-0.010670	-0.036109	-0.017701	0.047649	0.090115
145	C	15	Y	0.022101	-0.068231	0.140899	-0.151098	0.302562
146	C	15	Z	0.070278	-0.281313	0.172052	-0.132131	-0.132196
147	C	16	S	0.005069	-0.011567	-0.017896	0.025812	-0.043403
148	C	16	X	0.000918	-0.027663	0.005479	-0.008723	0.006073
149	C	16	Y	0.005692	0.170835	-0.036803	-0.015761	0.034788
150	C	16	Z	0.025891	0.386620	-0.138402	0.063836	-0.064012
151	C	16	S	0.049279	-0.142799	-0.115128	0.221106	-0.253223

152	C	16	X	0.008336	-0.021118	0.055695	-0.120068	0.229586
153	C	16	Y	0.014457	0.135852	-0.102050	0.042995	-0.034664
154	C	16	Z	0.018291	0.453674	-0.139995	0.045098	-0.000796
155	C	17	S	-0.005047	0.007214	0.008037	-0.017987	0.028317
156	C	17	X	0.002566	0.022931	0.012414	-0.028592	0.030075
157	C	17	Y	-0.033791	-0.074309	-0.018335	0.055458	-0.015816
158	C	17	Z	-0.099295	-0.157720	-0.016992	0.079081	0.044457
159	C	17	S	-0.032097	0.122266	0.114840	-0.250229	0.353583
160	C	17	X	-0.010365	0.061489	0.041385	-0.096101	0.109506
161	C	17	Y	-0.039576	-0.058706	-0.023582	0.068167	-0.069084
162	C	17	Z	-0.084624	-0.172009	-0.006235	0.072769	0.071525
163	C	18	S	0.001492	-0.001220	-0.001644	0.005462	-0.004017
164	C	18	X	-0.001650	0.022456	-0.010257	0.009451	0.007555
165	C	18	Y	0.015824	-0.090477	0.066526	-0.067201	0.016366
166	C	18	Z	0.042743	-0.248726	0.155036	-0.140379	-0.005694
167	C	18	S	0.047195	-0.094211	-0.017824	0.138449	-0.149503
168	C	18	X	0.012287	-0.018952	-0.028828	0.088250	-0.085182
169	C	18	Y	0.010553	-0.061193	0.077820	-0.113895	0.052147
170	C	18	Z	0.044570	-0.271612	0.145083	-0.114521	-0.017873
171	C	19	S	-0.007160	0.008081	0.003785	-0.018922	0.024449
172	C	19	X	-0.013207	-0.017491	0.017514	-0.031667	0.035856
173	C	19	Y	0.026450	0.131960	-0.049949	0.036171	-0.029694
174	C	19	Z	0.062530	0.370336	-0.109307	0.034100	-0.028028
175	C	19	S	-0.037475	0.184649	0.042355	-0.332344	0.274768
176	C	19	X	0.014001	-0.016014	0.025279	-0.040425	-0.015217
177	C	19	Y	0.048668	0.076166	-0.053186	0.180895	-0.208183
178	C	19	Z	0.042411	0.445124	-0.110416	-0.031589	0.020149
179	O	20	S	0.031551	-0.067270	-0.066083	0.124178	-0.158687
180	O	20	X	-0.000977	0.032162	0.024275	-0.066177	0.109727
181	O	20	Y	-0.038351	0.092347	0.033401	-0.078747	0.102820
182	O	20	Z	-0.043260	0.078098	-0.005371	0.017045	-0.126910
183	O	20	S	0.071764	-0.193313	-0.185409	0.354174	-0.462289
184	O	20	X	-0.026015	0.035042	0.008219	-0.056061	0.137748
185	O	20	Y	-0.026964	0.100849	0.015374	-0.084967	0.129486
186	O	20	Z	-0.029213	0.063889	-0.026576	0.046251	-0.125411
187	N	21	S	-0.007682	-0.025605	-0.102805	0.016419	0.237510
188	N	21	X	0.011122	0.017211	0.037452	-0.033744	-0.033620
189	N	21	Y	-0.021285	0.002075	0.015347	-0.008564	-0.045403
190	N	21	Z	-0.024166	0.020583	0.044919	-0.029217	-0.098533
191	N	21	S	-0.042537	-0.053807	-0.342511	-0.013166	0.840878
192	N	21	X	0.031595	-0.009796	-0.000445	-0.009200	-0.048153
193	N	21	Y	-0.039651	0.004703	0.017135	-0.009506	-0.039353
194	N	21	Z	-0.014373	0.038055	0.064421	0.027611	-0.109043
195	H	22	S	0.001128	-0.000197	-0.000950	-0.004004	-0.008576
196	H	22	S	0.003638	-0.013914	-0.017300	0.033698	0.026273
197	H	23	S	-0.002029	-0.001772	-0.004274	0.004657	0.005127

198	H	23	S	-0.000487	0.009650	0.010296	-0.017366	-0.009378
199	H	24	S	-0.003192	-0.004961	-0.019744	-0.001746	0.033104
200	H	24	S	-0.007804	-0.023599	-0.038782	0.049289	-0.037663
201	H	25	S	0.002441	0.003641	0.008841	0.000708	-0.007974
202	H	25	S	0.001061	0.008919	0.031330	0.018325	-0.005331
203	H	26	S	-0.000602	0.000354	0.000095	0.001405	-0.001088
204	H	26	S	0.007014	-0.015268	-0.015116	-0.006737	-0.017091
205	H	27	S	-0.001172	-0.000415	0.006253	0.010880	0.004090
206	H	27	S	-0.003585	0.093200	0.069449	0.004177	0.007431
207	H	28	S	0.009090	0.007006	0.011256	-0.023107	0.017554
208	H	28	S	-0.017125	-0.015749	-0.029588	-0.100626	-0.007490
209	H	29	S	0.006491	-0.016278	-0.013932	0.033494	-0.037678
210	H	29	S	0.000760	0.005679	0.007300	-0.052069	0.110457
211	H	30	S	0.001882	0.000861	-0.001335	0.001470	-0.001880
212	H	30	S	-0.001669	0.009172	-0.001953	-0.003094	-0.009590
213	H	31	S	-0.001818	0.003892	0.003785	-0.008936	0.010399
214	H	31	S	0.000808	-0.013356	-0.007028	0.019968	-0.016296
215	H	32	S	0.002065	-0.008661	-0.009224	0.018564	-0.021936
216	H	32	S	-0.007142	0.009424	-0.018912	-0.030186	0.033467
217	H	33	S	-0.018724	0.081573	0.046408	-0.115168	0.163884
218	H	33	S	-0.063409	0.245444	0.149050	-0.373423	0.667295
219	H	34	S	0.085029	-0.006464	0.029197	0.050799	-0.104041
220	H	34	S	0.168285	0.055706	0.159589	0.037829	-0.395206
221	H	35	S	-0.021802	0.011842	0.036821	0.000714	-0.072943
222	H	35	S	-0.067996	0.054306	0.158546	-0.032196	-0.339481

66	67	68
-0.2320	-0.2075	-0.1981

A	A	A
---	---	---

1	CO	1	S	0.030133	0.015396	-0.028214
2	CO	1	X	0.025066	-0.012755	0.014280
3	CO	1	Y	-0.001543	-0.006342	-0.034680
4	CO	1	Z	0.019576	-0.010596	-0.009274
5	CO	1	XX	-0.015122	-0.027668	-0.017592
6	CO	1	YY	0.012372	0.017128	0.085428
7	CO	1	ZZ	0.002750	0.010539	-0.067836
8	CO	1	XY	0.003745	-0.025729	-0.002033
9	CO	1	XZ	0.001709	-0.009228	-0.026763
10	CO	1	YZ	-0.030372	0.039941	-0.038386
11	CO	1	XX	-0.006174	-0.008645	-0.010193
12	CO	1	YY	0.005308	0.005939	0.027316
13	CO	1	ZZ	0.000866	0.002705	-0.017123
14	CO	1	XY	0.000337	-0.009976	-0.000764
15	CO	1	XZ	0.002318	-0.004745	-0.007613
16	CO	1	YZ	-0.009387	0.014366	-0.007999
17	CO	1	S	-0.148047	-0.037908	0.022601

18 CO 1 X -0.020132 0.078826 0.003808
19 CO 1 Y 0.057658 0.058448 0.115704
20 CO 1 Z -0.063297 0.007230 -0.014253
21 CO 1 S 0.127282 -0.256836 1.052823
22 CO 1 X -0.224154 -0.017949 -0.388933
23 CO 1 Y -0.018610 -0.096634 1.151386
24 CO 1 Z -0.169958 0.180120 -0.151265
25 CO 1 S 0.008553 0.023247 -0.069576
26 CO 1 X -0.005424 -0.002890 -0.001463
27 CO 1 Y -0.004427 -0.002438 -0.002118
28 CO 1 Z -0.001023 0.002581 0.004683
29 CO 1 XX 0.014653 -0.001591 0.054636
30 CO 1 YY -0.009335 -0.009926 -0.046940
31 CO 1 ZZ -0.005318 0.011517 -0.007696
32 CO 1 XY 0.018556 0.022918 0.013854
33 CO 1 XZ -0.022265 0.034793 -0.030326
34 CO 1 YZ 0.004650 -0.033485 -0.023313
35 C 2 S 0.006735 0.005772 0.000372
36 C 2 X -0.006656 -0.009475 0.015540
37 C 2 Y -0.038213 -0.046761 0.010351
38 C 2 Z 0.148828 0.176001 -0.091235
39 C 2 S -0.145665 0.080709 -0.039600
40 C 2 X 0.057309 -0.054814 0.024253
41 C 2 Y 0.015772 -0.056022 0.106982
42 C 2 Z 0.187549 0.256621 -0.091251
43 C 3 S 0.011094 0.004735 0.000719
44 C 3 X -0.008068 -0.000003 0.008312
45 C 3 Y 0.001516 0.003448 -0.024347
46 C 3 Z -0.041211 -0.018715 0.085311
47 C 3 S 0.194122 -0.000466 0.163179
48 C 3 X -0.095984 0.014061 -0.090270
49 C 3 Y 0.059346 0.023452 0.075216
50 C 3 Z -0.038288 -0.043863 0.130854
51 C 4 S -0.002760 0.002022 0.028288
52 C 4 X 0.018989 0.014741 0.023043
53 C 4 Y 0.018494 0.028568 -0.067319
54 C 4 Z -0.099092 -0.132813 -0.018641
55 C 4 S -0.307207 0.069947 -0.275276
56 C 4 X 0.090407 0.021138 0.216535
57 C 4 Y -0.124128 0.056193 -0.309978
58 C 4 Z -0.180753 -0.192296 -0.109162
59 C 5 S 0.033785 0.007439 -0.031590
60 C 5 X -0.055208 -0.019594 0.011856
61 C 5 Y -0.094636 -0.072600 -0.020383
62 C 5 Z 0.171501 0.231427 -0.038301
63 C 5 S 0.392286 0.002037 -0.237764

64	C	5	X	0.195819	-0.101139	0.485602
65	C	5	Y	-0.054008	-0.173380	-0.274827
66	C	5	Z	0.234152	0.271927	-0.116650
67	C	6	S	0.014332	-0.001810	0.003561
68	C	6	X	-0.015035	-0.001826	0.015646
69	C	6	Y	0.045972	0.071256	-0.037118
70	C	6	Z	-0.119231	-0.217522	-0.003320
71	C	6	S	0.036268	-0.107932	0.035348
72	C	6	X	-0.311028	0.160394	-0.127577
73	C	6	Y	0.107894	-0.029943	-0.529125
74	C	6	Z	-0.138287	-0.305362	-0.182218
75	C	7	S	0.005140	0.001510	-0.003181
76	C	7	X	-0.002772	0.003499	0.004306
77	C	7	Y	0.030823	0.066469	-0.011015
78	C	7	Z	-0.120504	-0.238889	0.017766
79	C	7	S	0.215122	-0.021641	0.400544
80	C	7	X	-0.009610	-0.046495	-0.221849
81	C	7	Y	-0.092209	0.182577	0.002880
82	C	7	Z	-0.170495	-0.271230	0.042906
83	C	8	S	0.003899	-0.011734	-0.001748
84	C	8	X	-0.008653	0.002287	0.009980
85	C	8	Y	-0.016628	-0.078866	-0.020368
86	C	8	Z	0.102861	0.297778	0.054019
87	C	8	S	0.012657	-0.047210	-0.181223
88	C	8	X	0.017481	-0.023203	0.109305
89	C	8	Y	-0.047369	-0.044691	0.038170
90	C	8	Z	0.118997	0.409552	0.073191
91	C	9	S	-0.000109	-0.008189	0.017857
92	C	9	X	0.002555	0.009043	-0.023125
93	C	9	Y	0.000592	0.043021	0.012945
94	C	9	Z	0.008890	-0.153128	-0.086069
95	C	9	S	-0.028079	-0.003336	0.284118
96	C	9	X	0.063505	-0.070003	-0.021193
97	C	9	Y	-0.030902	0.074774	-0.082027
98	C	9	Z	-0.015090	-0.189817	-0.125375
99	C	10	S	0.007747	0.016758	-0.038179
100	C	10	X	-0.037387	0.008893	0.016522
101	C	10	Y	0.057670	-0.011955	0.001851
102	C	10	Z	-0.076656	-0.128689	0.028916
103	C	10	S	-0.112104	0.118305	-0.423188
104	C	10	X	-0.043065	-0.011148	-0.117397
105	C	10	Y	0.231259	-0.143617	0.047116
106	C	10	Z	-0.062644	-0.215431	0.090811
107	C	11	S	0.008943	-0.036972	-0.009360
108	C	11	X	-0.017279	0.059209	-0.055224
109	C	11	Y	-0.047350	-0.061468	-0.018035

110	C	11	Z	0.144941	0.322082	-0.008937
111	C	11	S	0.006590	-0.150377	0.059001
112	C	11	X	-0.134469	0.264928	0.184568
113	C	11	Y	0.163196	-0.229397	0.255727
114	C	11	Z	0.226919	0.350387	0.027562
115	N	12	S	-0.008694	0.022577	-0.136610
116	N	12	X	-0.017466	0.060118	-0.003616
117	N	12	Y	0.043461	-0.007679	0.058496
118	N	12	Z	0.125688	-0.241609	-0.047566
119	N	12	S	-0.017385	0.099503	-0.266715
120	N	12	X	-0.047226	0.095356	-0.042984
121	N	12	Y	0.049216	0.000724	0.139265
122	N	12	Z	0.130865	-0.251082	-0.043587
123	C	13	S	-0.006029	0.042597	-0.038115
124	C	13	X	0.026587	0.013355	0.052385
125	C	13	Y	-0.093706	0.079101	0.019469
126	C	13	Z	-0.269437	0.179717	0.055797
127	C	13	S	-0.189200	0.137393	-0.422279
128	C	13	X	0.025066	0.062394	0.017946
129	C	13	Y	-0.105973	0.123924	0.362314
130	C	13	Z	-0.365600	0.259103	-0.089987
131	C	14	S	-0.029330	0.002560	-0.024325
132	C	14	X	-0.040821	0.022007	-0.003274
133	C	14	Y	0.153631	-0.039785	-0.004482
134	C	14	Z	0.347811	-0.149038	-0.005341
135	C	14	S	-0.214899	-0.043685	0.354446
136	C	14	X	0.083506	0.083069	0.364595
137	C	14	Y	0.262949	0.045296	-0.416123
138	C	14	Z	0.431311	-0.258751	0.197169
139	C	15	S	0.005289	0.011148	-0.031280
140	C	15	X	0.036320	0.010813	0.019179
141	C	15	Y	-0.071923	0.023849	-0.042415
142	C	15	Z	-0.170573	0.059341	0.035066
143	C	15	S	0.056737	0.100758	-0.292879
144	C	15	X	0.003514	-0.000269	-0.412379
145	C	15	Y	0.031882	0.140815	-0.404359
146	C	15	Z	-0.261049	0.035271	0.134191
147	C	16	S	-0.020526	-0.013133	-0.000003
148	C	16	X	0.011293	0.003485	-0.007950
149	C	16	Y	-0.010091	0.043146	-0.014348
150	C	16	Z	-0.103069	0.036934	0.010553
151	C	16	S	-0.143631	-0.108622	-0.387043
152	C	16	X	0.103898	0.082022	-0.202407
153	C	16	Y	-0.039109	0.044440	-0.114659
154	C	16	Z	-0.095378	0.070115	0.049692
155	C	17	S	0.005310	0.008641	0.011960

156	C	17	X	-0.013652	0.019644	0.004533
157	C	17	Y	0.106239	-0.054230	-0.022078
158	C	17	Z	0.298427	-0.137351	-0.022879
159	C	17	S	0.127909	0.100404	0.176098
160	C	17	X	0.027974	0.044799	0.087364
161	C	17	Y	0.090855	-0.101479	0.087059
162	C	17	Z	0.348825	-0.158676	-0.075617
163	C	18	S	-0.005281	-0.004670	-0.008704
164	C	18	X	0.022264	-0.011332	-0.016139
165	C	18	Y	-0.091585	0.061480	0.011291
166	C	18	Z	-0.252677	0.139923	0.033859
167	C	18	S	-0.089934	-0.061123	-0.203977
168	C	18	X	-0.039124	-0.048275	-0.073641
169	C	18	Y	-0.087518	0.058657	0.111662
170	C	18	Z	-0.267804	0.153675	0.004411
171	C	19	S	0.005778	0.008028	0.016198
172	C	19	X	0.015292	0.005513	0.017999
173	C	19	Y	-0.016987	-0.003044	-0.009095
174	C	19	Z	-0.013268	-0.050135	-0.011932
175	C	19	S	0.145707	0.059042	0.513717
176	C	19	X	-0.015261	-0.053889	0.122045
177	C	19	Y	-0.117740	0.000768	-0.120186
178	C	19	Z	-0.055660	0.002460	0.023723
179	O	20	S	-0.052407	-0.013180	-0.052441
180	O	20	X	0.044925	0.055058	0.003898
181	O	20	Y	0.091411	0.045025	-0.082620
182	O	20	Z	0.051903	-0.077227	-0.010686
183	O	20	S	-0.175841	-0.061325	-0.151569
184	O	20	X	0.023851	0.064159	-0.030879
185	O	20	Y	0.094739	0.078424	-0.047953
186	O	20	Z	0.018868	-0.072139	0.003589
187	N	21	S	-0.036800	-0.007320	0.005878
188	N	21	X	0.011956	0.013277	0.093902
189	N	21	Y	-0.026077	-0.038393	-0.201882
190	N	21	Z	0.048006	-0.038801	0.117735
191	N	21	S	-0.138660	-0.042463	0.062095
192	N	21	X	0.022441	0.015615	0.178690
193	N	21	Y	-0.064759	-0.099267	-0.255247
194	N	21	Z	0.054891	0.003516	0.121632
195	H	22	S	-0.001284	-0.004517	-0.005016
196	H	22	S	-0.037295	0.002507	-0.043300
197	H	23	S	-0.006191	-0.003844	-0.013022
198	H	23	S	0.015419	-0.013155	0.003060
199	H	24	S	-0.008859	-0.003086	-0.005750
200	H	24	S	-0.095458	-0.036590	-0.338428
201	H	25	S	-0.001774	0.004873	0.000624

202 H 25 S -0.012525 0.008273 -0.049202
 203 H 26 S -0.009837 0.010397 -0.008279
 204 H 26 S 0.000866 0.017820 -0.001069
 205 H 27 S -0.002350 0.011427 -0.027860
 206 H 27 S -0.119698 0.109439 -0.049800
 207 H 28 S 0.000963 -0.022724 -0.033359
 208 H 28 S 0.038952 -0.139678 -0.251232
 209 H 29 S -0.009812 -0.002748 -0.025865
 210 H 29 S 0.079102 0.092296 -0.139738
 211 H 30 S 0.003128 0.001765 -0.009832
 212 H 30 S 0.011143 -0.001238 0.003302
 213 H 31 S 0.006082 0.000291 0.001146
 214 H 31 S -0.007066 -0.008457 -0.039638
 215 H 32 S -0.005228 -0.003484 -0.013565
 216 H 32 S 0.024207 -0.037951 -0.035592
 217 H 33 S 0.073124 0.044227 0.022682
 218 H 33 S 0.251595 0.267134 -0.068585
 219 H 34 S 0.061032 0.072841 0.037128
 220 H 34 S 0.252735 0.211165 0.383114
 221 H 35 S -0.018314 -0.025574 -0.041421
 222 H 35 S -0.043708 -0.133291 -0.503066

**** BETA SET ****

		1	2	3	4	5
		-4.0853	-2.6837	-2.6779	-2.6753	-1.3744
		A	A	A	A	A
1	CO 1 S	0.766868	-0.006101	0.005059	-0.001931	-0.016821
2	CO 1 X	0.001688	0.384450	0.495093	0.554931	0.029173
3	CO 1 Y	-0.007364	-0.115169	0.657138	-0.506016	0.005998
4	CO 1 Z	0.006505	0.736703	-0.155286	-0.369094	-0.006610
5	CO 1 XX	-0.000482	-0.001344	0.004244	-0.001030	0.011326
6	CO 1 YY	-0.000603	-0.000797	-0.005107	0.005307	-0.005239
7	CO 1 ZZ	0.001085	0.002141	0.000863	-0.004277	-0.006086
8	CO 1 XY	0.000294	-0.001589	0.000439	-0.001532	0.003750
9	CO 1 XZ	0.001133	0.001717	0.001549	0.003087	-0.005149
10	CO 1 YZ	-0.000625	-0.003228	0.002524	-0.001064	-0.002340
11	CO 1 XX	0.000384	-0.000601	-0.000640	0.000126	0.010213
12	CO 1 YY	-0.000226	-0.000482	0.000467	-0.000357	-0.005423
13	CO 1 ZZ	-0.000157	0.001083	0.000173	0.000231	-0.004789
14	CO 1 XY	-0.000037	-0.000229	-0.000978	-0.000697	0.004258
15	CO 1 XZ	-0.000462	0.000663	0.000384	-0.000310	-0.005355
16	CO 1 YZ	-0.000049	-0.000855	0.000751	0.000349	-0.000845
17	CO 1 S	-0.023057	-0.000335	-0.000526	-0.001889	0.028849
18	CO 1 X	0.000057	-0.000935	-0.002717	-0.005478	-0.026818
19	CO 1 Y	-0.005768	0.003684	-0.002886	0.002514	0.002970

20	CO	1	Z	0.003868	-0.003035	0.001541	0.002037	0.008995
21	CO	1	S	0.000639	0.001325	-0.000531	0.001299	0.008522
22	CO	1	X	-0.000065	0.000652	0.000525	0.000573	-0.010258
23	CO	1	Y	0.000012	0.000052	0.001261	-0.000272	-0.001728
24	CO	1	Z	-0.000299	0.001417	-0.000136	-0.000866	0.004541
25	CO	1	S	0.267916	-0.002097	0.001769	-0.000941	-0.015349
26	CO	1	X	0.000227	0.104689	0.136212	0.153395	0.003114
27	CO	1	Y	-0.001073	-0.031833	0.180234	-0.139106	-0.000530
28	CO	1	Z	0.000935	0.200115	-0.042953	-0.101504	-0.000907
29	CO	1	XX	-0.001927	-0.001617	0.001288	-0.000353	0.014823
30	CO	1	YY	-0.000169	0.001628	-0.001141	0.001479	-0.001028
31	CO	1	ZZ	0.002095	-0.000011	-0.000147	-0.001125	-0.013796
32	CO	1	XY	0.000523	-0.001371	-0.000880	-0.001209	0.005446
33	CO	1	XZ	0.003352	0.000676	0.000404	0.001858	-0.002353
34	CO	1	YZ	0.000989	-0.000653	0.000725	-0.000341	-0.007382
35	C	2	S	-0.000093	0.000002	0.000013	-0.000033	-0.000159
36	C	2	X	-0.000010	-0.000011	0.000034	0.000021	-0.000089
37	C	2	Y	0.000037	-0.000020	0.000025	-0.000002	0.000082
38	C	2	Z	0.000028	-0.000002	0.000000	0.000028	-0.000007
39	C	2	S	0.010009	0.001300	-0.002944	0.005062	-0.014631
40	C	2	X	-0.003837	-0.000718	0.000674	-0.001620	0.002953
41	C	2	Y	-0.000251	-0.001899	0.004116	-0.001315	-0.002071
42	C	2	Z	-0.000060	-0.000493	0.001146	-0.000495	-0.000073
43	C	3	S	-0.000007	0.000019	-0.000010	-0.000002	-0.000259
44	C	3	X	0.000090	0.000028	-0.000010	0.000090	-0.000116
45	C	3	Y	0.000062	0.000012	0.000000	0.000079	-0.000216
46	C	3	Z	0.000006	-0.000002	0.000000	0.000028	-0.000073
47	C	3	S	-0.008979	-0.004284	0.004775	-0.008508	0.008871
48	C	3	X	0.004126	0.001416	-0.001381	0.003350	-0.007403
49	C	3	Y	-0.000483	-0.000520	0.002436	-0.000814	0.002968
50	C	3	Z	0.000262	0.000096	0.000761	0.000156	-0.000357
51	C	4	S	-0.000153	0.000120	0.000000	0.000033	0.000118
52	C	4	X	-0.000083	-0.000123	0.000055	-0.000179	0.000371
53	C	4	Y	0.000030	-0.000024	0.000001	0.000052	0.000076
54	C	4	Z	0.000084	0.000064	-0.000003	0.000012	-0.000083
55	C	4	S	0.008959	0.008848	-0.008360	0.012515	-0.029045
56	C	4	X	0.001416	-0.001187	0.003275	-0.000151	0.006765
57	C	4	Y	0.008547	0.003039	-0.002716	0.008277	-0.009238
58	C	4	Z	0.002166	0.000320	-0.001202	0.001946	0.000060
59	C	5	S	-0.000164	-0.000141	0.000000	0.000115	0.001495
60	C	5	X	0.000373	0.000029	-0.000134	0.000119	-0.001494
61	C	5	Y	0.000145	0.000083	0.000038	0.000039	-0.000242
62	C	5	Z	0.000022	0.000000	0.000183	-0.000081	0.000013
63	C	5	S	-0.018885	-0.000126	0.002455	-0.012965	0.052158
64	C	5	X	-0.005982	-0.009474	0.009602	-0.012669	0.011208
65	C	5	Y	-0.012588	0.002158	-0.001714	-0.008449	-0.002803

66	C	5	Z	-0.004419	0.000619	0.001062	-0.002780	-0.004576
67	C	6	S	-0.000133	0.000040	-0.000143	0.000007	0.000269
68	C	6	X	-0.000010	-0.000033	0.000212	-0.000070	-0.000553
69	C	6	Y	0.000212	0.000047	0.000100	0.000070	-0.000630
70	C	6	Z	-0.000033	-0.000004	0.000064	0.000043	-0.000371
71	C	6	S	0.010798	-0.005286	-0.001263	0.001284	0.056591
72	C	6	X	-0.000033	0.012331	-0.014674	0.010418	-0.006384
73	C	6	Y	-0.016284	0.003927	-0.003773	-0.009258	0.041901
74	C	6	Z	-0.003720	0.001468	-0.001689	-0.002592	0.016210
75	C	7	S	-0.000088	0.000087	-0.000034	0.000004	-0.000105
76	C	7	X	0.000067	-0.000025	0.000005	0.000001	0.000332
77	C	7	Y	0.000032	-0.000036	-0.000021	0.000061	0.000023
78	C	7	Z	0.000071	0.000045	0.000063	0.000030	-0.000144
79	C	7	S	0.002610	-0.008605	0.008512	-0.004355	-0.025555
80	C	7	X	-0.009592	0.004173	-0.005839	-0.001312	0.022889
81	C	7	Y	0.002065	0.004655	-0.008064	0.002440	0.001091
82	C	7	Z	-0.000366	0.000926	-0.002453	0.000462	0.000176
83	C	8	S	-0.000013	-0.000005	-0.000030	-0.000005	-0.000231
84	C	8	X	0.000042	-0.000022	0.000023	-0.000019	0.000196
85	C	8	Y	0.000019	0.000013	0.000019	-0.000005	-0.000087
86	C	8	Z	-0.000003	0.000003	0.000016	-0.000027	-0.000019
87	C	8	S	-0.005900	-0.000945	0.006423	-0.001870	0.008707
88	C	8	X	0.004260	-0.001669	0.000355	0.000816	-0.009614
89	C	8	Y	0.000110	0.000453	-0.002357	-0.000460	-0.002046
90	C	8	Z	0.000419	0.000264	-0.000650	0.000103	-0.000965
91	C	9	S	-0.000057	0.000040	0.000045	0.000071	-0.000202
92	C	9	X	-0.000036	-0.000001	0.000075	-0.000053	-0.000045
93	C	9	Y	-0.000031	0.000011	0.000051	-0.000030	0.000141
94	C	9	Z	-0.000010	0.000004	0.000015	-0.000004	-0.000059
95	C	9	S	0.005716	-0.002230	-0.004235	0.002839	-0.013176
96	C	9	X	0.002074	-0.000112	0.000494	0.000700	-0.000766
97	C	9	Y	-0.002933	0.000820	0.002868	-0.000604	0.000963
98	C	9	Z	-0.001018	0.000217	0.001032	-0.000482	0.001580
99	C	10	S	0.000046	0.000110	-0.000106	-0.000047	-0.000059
100	C	10	X	-0.000015	-0.000067	-0.000042	-0.000050	0.000477
101	C	10	Y	0.000100	-0.000130	-0.000082	0.000084	-0.000397
102	C	10	Z	0.000085	0.000019	-0.000012	0.000003	0.000239
103	C	10	S	-0.014427	0.006664	0.006290	-0.004840	0.015767
104	C	10	X	-0.001710	0.000117	0.004341	-0.003820	0.008633
105	C	10	Y	0.005845	-0.001472	-0.001482	0.002238	-0.003967
106	C	10	Z	0.001980	-0.000543	-0.001439	0.001415	-0.003213
107	C	11	S	0.000204	0.000035	-0.000238	-0.000170	0.001515
108	C	11	X	-0.000087	0.000005	0.000158	0.000105	-0.000358
109	C	11	Y	0.000075	0.000001	0.000295	0.000011	-0.000470
110	C	11	Z	-0.000139	-0.000069	-0.000007	0.000039	0.000403
111	C	11	S	0.012528	0.005686	-0.015583	0.010100	-0.032805

112	C	11	X	0.000125	0.004574	-0.003203	0.010530	-0.048327
113	C	11	Y	0.012328	-0.007953	0.000439	0.005054	-0.008516
114	C	11	Z	0.002937	-0.002684	0.001500	0.000523	-0.004915
115	N	12	S	0.000146	-0.001696	0.004012	-0.003466	0.012488
116	N	12	X	0.000033	0.000168	0.000680	-0.000102	-0.003660
117	N	12	Y	-0.000184	0.001734	-0.003799	0.003091	-0.000251
118	N	12	Z	0.000063	0.000205	0.000570	-0.000918	0.000216
119	N	12	S	0.004495	-0.002264	0.001144	0.001035	-0.016881
120	N	12	X	0.002592	-0.001434	0.003202	0.004755	0.004551
121	N	12	Y	-0.008784	0.002299	0.000660	0.000452	0.004557
122	N	12	Z	0.000538	0.001539	-0.000506	-0.000159	-0.002248
123	C	13	S	0.000338	0.000096	0.000096	0.000365	0.013109
124	C	13	X	0.000093	0.000055	0.000107	0.000146	-0.000898
125	C	13	Y	0.000359	-0.000173	0.000009	-0.000270	-0.005643
126	C	13	Z	0.000015	-0.000082	0.000072	0.000045	0.002179
127	C	13	S	0.007198	-0.005403	0.000697	0.000966	0.189249
128	C	13	X	0.003045	0.001223	0.001054	0.004322	-0.095309
129	C	13	Y	-0.000588	0.004870	-0.001505	0.002433	-0.038598
130	C	13	Z	0.001084	-0.001700	0.000766	0.000503	0.001653
131	C	14	S	0.000146	0.000004	-0.000041	0.000126	0.033507
132	C	14	X	0.000041	0.000111	-0.000022	0.000242	0.003863
133	C	14	Y	0.000074	-0.000106	-0.000057	-0.000167	-0.015920
134	C	14	Z	0.000017	-0.000019	0.000025	0.000058	0.006480
135	C	14	S	0.002761	0.006586	0.005061	0.007588	0.151387
136	C	14	X	-0.005323	0.005626	0.003738	0.002651	-0.191545
137	C	14	Y	-0.001495	-0.000959	-0.006168	0.000634	-0.198128
138	C	14	Z	-0.000350	0.001143	0.002360	-0.000278	0.055004
139	C	15	S	0.000219	0.000255	-0.000133	0.000127	0.185577
140	C	15	X	-0.000263	0.000336	0.000083	0.000380	0.078663
141	C	15	Y	-0.000130	-0.000152	0.000128	0.000012	-0.064464
142	C	15	Z	0.000029	0.000011	-0.000100	-0.000053	0.031222
143	C	15	S	-0.009339	0.006178	0.003498	0.008788	-0.258849
144	C	15	X	0.007352	-0.006833	-0.012713	-0.009212	0.001280
145	C	15	Y	-0.001136	-0.003948	-0.007622	-0.003788	-0.197448
146	C	15	Z	0.001102	0.000997	0.002535	0.001554	0.082829
147	C	16	S	-0.000169	0.000076	0.000034	0.000141	0.035598
148	C	16	X	0.000051	-0.000141	-0.000194	-0.000155	0.018858
149	C	16	Y	0.000018	0.000019	-0.000016	-0.000013	0.003969
150	C	16	Z	-0.000019	0.000031	0.000013	-0.000007	0.000011
151	C	16	S	0.009075	-0.010438	-0.014095	-0.012061	-0.018332
152	C	16	X	0.003450	-0.003165	-0.006653	-0.005096	-0.032864
153	C	16	Y	0.004017	-0.002850	-0.003456	-0.003541	0.054493
154	C	16	Z	-0.001222	0.000608	0.000353	0.000586	-0.025379
155	C	17	S	0.000034	-0.000047	-0.000041	-0.000004	0.003970
156	C	17	X	-0.000015	0.000047	0.000049	0.000068	0.001818
157	C	17	Y	0.000043	-0.000036	-0.000068	-0.000078	-0.000708

158	C	17	Z	-0.000023	0.000023	0.000027	0.000035	0.000465
159	C	17	S	-0.003545	0.003267	0.002892	0.002180	-0.051867
160	C	17	X	-0.002225	0.002064	0.001358	0.001365	-0.007476
161	C	17	Y	-0.001912	0.001173	0.002977	0.001865	0.002945
162	C	17	Z	0.000569	-0.000200	-0.000849	-0.000527	-0.001405
163	C	18	S	-0.000071	0.000017	0.000053	0.000027	0.002568
164	C	18	X	0.000015	0.000006	0.000049	0.000056	0.001456
165	C	18	Y	-0.000007	0.000023	0.000034	0.000044	0.000563
166	C	18	Z	-0.000003	0.000001	0.000001	-0.000018	-0.000061
167	C	18	S	0.006353	-0.003985	-0.001066	-0.002055	0.069134
168	C	18	X	0.002077	-0.001429	0.000629	-0.000093	0.019937
169	C	18	Y	-0.000888	0.000767	0.002358	0.000736	-0.001876
170	C	18	Z	0.000498	-0.000384	-0.000985	-0.000259	0.002012
171	C	19	S	-0.000069	0.000029	0.000037	0.000132	0.005032
172	C	19	X	-0.000058	0.000010	-0.000023	-0.000038	0.000804
173	C	19	Y	0.000050	-0.000003	-0.000033	0.000007	0.000173
174	C	19	Z	-0.000022	0.000023	0.000023	0.000041	0.000123
175	C	19	S	-0.005385	0.004061	0.003691	-0.000811	-0.077918
176	C	19	X	0.002066	-0.000821	0.003918	-0.000343	0.041135
177	C	19	Y	0.002318	-0.002037	0.000237	0.000169	0.072955
178	C	19	Z	-0.000555	0.000507	0.000338	-0.000232	-0.023832
179	O	20	S	0.000362	-0.001372	-0.004446	-0.003435	0.668821
180	O	20	X	0.000426	-0.000992	-0.003601	-0.002763	-0.095529
181	O	20	Y	0.000062	-0.000153	-0.000496	-0.001096	-0.026628
182	O	20	Z	-0.000164	0.000818	0.001077	0.000379	0.017966
183	O	20	S	0.001912	0.001893	-0.000622	-0.000319	0.139433
184	O	20	X	0.002991	0.002598	0.000546	0.000704	0.017722
185	O	20	Y	0.001009	-0.000469	0.002326	-0.000125	0.015969
186	O	20	Z	-0.000185	0.000640	-0.001072	0.000125	-0.006567
187	N	21	S	0.000210	-0.001070	0.002189	0.004262	0.003678
188	N	21	X	-0.000424	0.001035	-0.001470	-0.002956	0.000370
189	N	21	Y	0.000081	-0.000088	0.000657	0.000219	0.000545
190	N	21	Z	0.000413	-0.000335	0.001608	0.002815	0.000660
191	N	21	S	0.001874	-0.002357	0.003412	-0.001544	0.001298
192	N	21	X	-0.004343	0.001458	-0.000358	-0.002804	-0.013086
193	N	21	Y	0.000598	-0.002405	0.003129	-0.002399	-0.003814
194	N	21	Z	0.002438	0.000619	0.000264	0.000014	-0.001277
195	H	22	S	-0.000021	0.000024	-0.000044	0.000004	0.000055
196	H	22	S	0.000661	0.000651	-0.001179	0.000457	0.001004
197	H	23	S	0.000017	0.000039	-0.000003	0.000038	0.000040
198	H	23	S	-0.000861	-0.000250	0.000641	-0.000692	0.003137
199	H	24	S	0.000126	0.000037	0.000030	0.000132	-0.000009
200	H	24	S	0.003504	0.000978	-0.001222	0.003220	-0.001430
201	H	25	S	-0.000034	0.000035	-0.000023	-0.000009	0.000114
202	H	25	S	-0.001155	0.000553	-0.000019	-0.000022	0.004027
203	H	26	S	0.000000	0.000024	-0.000026	-0.000020	0.000131

204	H	26	S	0.000966	-0.000196	-0.000971	-0.000028	0.001662
205	H	27	S	0.000088	-0.000015	0.000079	-0.000050	0.000294
206	H	27	S	-0.001208	-0.000193	0.001819	-0.002434	0.003708
207	H	28	S	-0.000051	-0.000168	0.000138	-0.000191	0.000386
208	H	28	S	-0.000473	-0.002286	0.001115	-0.001519	0.002316
209	H	29	S	-0.000039	0.000033	0.000068	0.000068	0.006868
210	H	29	S	0.001584	-0.000765	-0.001242	-0.001199	0.033087
211	H	30	S	-0.000061	0.000022	0.000033	0.000041	0.000678
212	H	30	S	-0.000843	0.000701	0.000728	0.000522	0.004914
213	H	31	S	-0.000049	0.000019	-0.000019	0.000028	-0.000454
214	H	31	S	0.000586	-0.000428	-0.000434	-0.000173	0.000866
215	H	32	S	-0.000061	0.000031	-0.000083	0.000006	-0.000188
216	H	32	S	-0.000435	0.000845	-0.000736	0.000178	-0.033972
217	H	33	S	0.000247	-0.000298	0.000716	-0.000054	0.165094
218	H	33	S	-0.000028	-0.000525	0.001095	-0.000139	-0.033631
219	H	34	S	-0.000303	0.000363	-0.000249	0.000004	-0.000316
220	H	34	S	-0.000676	0.000282	0.000155	-0.001400	0.000009
221	H	35	S	-0.000063	-0.000475	0.000352	-0.000336	0.000505
222	H	35	S	-0.000035	-0.001014	0.001659	-0.001468	0.001092

6	7	8	9	10
-1.2321	-1.2149	-1.1287	-1.1114	-1.0654

A	A	A	A	A
---	---	---	---	---

1	CO	1	S	-0.022927	-0.014735	0.004670	-0.009556	0.001905
2	CO	1	X	-0.005584	-0.024376	-0.007375	0.000222	0.008489
3	CO	1	Y	-0.026845	0.012400	0.001837	-0.002850	-0.002384
4	CO	1	Z	0.011420	0.018949	0.005023	0.006426	-0.004596
5	CO	1	XX	-0.005120	0.007821	-0.000226	0.000470	0.001917
6	CO	1	YY	0.011826	-0.013406	-0.002375	0.000160	0.001914
7	CO	1	ZZ	-0.006706	0.005584	0.002602	-0.000630	-0.003831
8	CO	1	XY	-0.004331	0.000185	-0.005960	-0.003769	-0.003268
9	CO	1	XZ	-0.004240	-0.016040	0.001943	-0.005198	0.005033
10	CO	1	YZ	-0.004887	0.002438	0.002463	-0.000871	-0.001815
11	CO	1	XX	-0.005156	0.007970	-0.002027	0.001678	0.000353
12	CO	1	YY	0.010428	-0.012035	-0.001987	0.000357	0.002180
13	CO	1	ZZ	-0.005273	0.004064	0.004014	-0.002035	-0.002533
14	CO	1	XY	-0.004594	-0.001551	-0.001370	-0.000970	-0.002360
15	CO	1	XZ	-0.003809	-0.012902	-0.000223	-0.004634	0.004043
16	CO	1	YZ	-0.002535	0.002813	0.001623	-0.001342	-0.001820
17	CO	1	S	0.047544	0.040554	-0.010136	0.019170	-0.003659
18	CO	1	X	-0.001147	0.045094	-0.021914	0.001996	-0.031201
19	CO	1	Y	0.021456	-0.005848	0.005809	-0.018446	0.007607
20	CO	1	Z	-0.018879	-0.034473	0.018281	0.003628	0.015940
21	CO	1	S	0.020640	0.025113	0.011580	-0.055963	0.006507
22	CO	1	X	0.012135	0.011324	-0.025828	-0.022423	0.012630
23	CO	1	Y	0.004739	0.005500	0.005772	-0.027911	0.000606

24 CO 1 Z -0.007281 -0.008033 -0.001563 0.013425 -0.004992
25 CO 1 S -0.022185 -0.010754 0.002969 -0.006421 0.001025
26 CO 1 X 0.000292 -0.002736 0.003486 0.000631 0.001387
27 CO 1 Y -0.003125 0.000258 -0.000986 0.001874 -0.000106
28 CO 1 Z 0.001103 0.000989 -0.002206 -0.000998 -0.000693
29 CO 1 XX 0.007803 0.003946 0.013155 0.002161 0.009187
30 CO 1 YY 0.001301 -0.012647 0.002187 -0.010189 0.000455
31 CO 1 ZZ -0.009105 0.008701 -0.015341 0.008029 -0.009642
32 CO 1 XY -0.004696 0.008300 -0.017135 -0.012494 -0.003766
33 CO 1 XZ -0.011935 -0.027900 0.011180 0.000688 0.004521
34 CO 1 YZ -0.008261 -0.000053 0.001722 0.008624 -0.000684
35 C 2 S 0.007037 0.013465 -0.038998 -0.174852 0.193712
36 C 2 X -0.002750 -0.005021 0.012603 0.049697 -0.023463
37 C 2 Y -0.000499 -0.002265 0.001742 0.012280 -0.050852
38 C 2 Z -0.000134 -0.000873 0.000759 0.004315 -0.014358
39 C 2 S -0.045229 0.156383 -0.061273 -0.152661 -0.143082
40 C 2 X 0.023475 -0.055099 0.023012 0.053633 0.107771
41 C 2 Y -0.021319 -0.008756 -0.012969 -0.072026 0.021301
42 C 2 Z -0.004702 -0.003494 -0.001267 -0.018209 0.008011
43 C 3 S 0.007889 0.021320 -0.027880 -0.139384 0.252385
44 C 3 X -0.003445 -0.008944 0.008014 0.038982 -0.063552
45 C 3 Y -0.000135 -0.001078 -0.004758 -0.020329 0.018483
46 C 3 Z -0.000245 -0.000942 -0.000948 -0.003769 0.001617
47 C 3 S 0.028867 -0.103042 0.006974 -0.010672 0.017579
48 C 3 X -0.016485 0.040144 -0.022489 -0.045428 -0.013583
49 C 3 Y -0.030118 -0.008060 0.007854 -0.003964 0.001316
50 C 3 Z -0.009630 -0.001854 -0.000368 -0.002494 0.000336
51 C 4 S 0.027655 0.081617 -0.025439 -0.137184 0.266935
52 C 4 X -0.011448 -0.035349 0.001780 0.007967 -0.004167
53 C 4 Y 0.003910 0.009093 -0.008699 -0.040268 0.058635
54 C 4 Z 0.000692 0.000917 -0.002782 -0.012058 0.017372
55 C 4 S 0.065246 0.123719 -0.093640 -0.137233 -0.051868
56 C 4 X -0.077113 0.008129 0.032921 0.035459 0.047072
57 C 4 Y -0.007462 0.097578 -0.011200 -0.021871 -0.001821
58 C 4 Z -0.004312 0.034718 0.002257 -0.005370 0.001226
59 C 5 S 0.094117 0.241679 -0.033719 -0.148428 0.166865
60 C 5 X -0.024763 -0.062006 -0.008613 -0.042298 0.080865
61 C 5 Y -0.010223 -0.061455 -0.022917 -0.059595 0.003639
62 C 5 Z -0.005595 -0.028996 -0.008874 -0.025103 0.008178
63 C 5 S 0.184757 -0.362937 0.006999 0.045336 -0.145046
64 C 5 X -0.111528 -0.140973 0.070311 0.097593 0.013408
65 C 5 Y 0.145698 -0.223495 -0.072610 -0.069901 -0.150174
66 C 5 Z 0.035003 -0.092722 -0.027154 -0.013410 -0.048157
67 C 6 S 0.081299 0.057487 -0.107446 -0.293588 0.000796
68 C 6 X -0.023695 0.005744 0.007719 -0.023891 0.067285
69 C 6 Y -0.005123 -0.027521 -0.009942 -0.017871 -0.054590

70	C	6	Z	-0.000668	-0.009224	-0.005064	-0.007069	-0.017566
71	C	6	S	0.094019	-0.078462	0.243549	0.463580	0.025169
72	C	6	X	-0.012651	0.382116	-0.110754	-0.152977	0.114365
73	C	6	Y	0.318684	-0.314732	-0.021242	0.065587	-0.185947
74	C	6	Z	0.102941	-0.096116	0.007611	0.020524	-0.056772
75	C	7	S	0.022954	0.018603	-0.079552	-0.287530	0.058240
76	C	7	X	-0.005208	-0.002214	0.011640	0.022746	0.044640
77	C	7	Y	-0.002253	-0.005081	0.003891	0.015386	-0.050838
78	C	7	Z	-0.000863	-0.001494	0.000837	0.003556	-0.013322
79	C	7	S	-0.198351	-0.100802	0.072830	0.117527	-0.000784
80	C	7	X	0.132141	-0.097440	0.040708	0.180711	0.098069
81	C	7	Y	-0.059430	0.145092	-0.011669	0.045441	-0.151979
82	C	7	Z	-0.016385	0.039623	-0.007540	0.014925	-0.040524
83	C	8	S	0.010808	0.002084	-0.051702	-0.177148	-0.100304
84	C	8	X	-0.002725	0.000346	0.010857	0.028311	0.046287
85	C	8	Y	-0.004117	-0.001162	0.011178	0.041477	-0.011658
86	C	8	Z	-0.001064	-0.000170	0.002704	0.010443	-0.003841
87	C	8	S	0.124555	-0.097299	-0.012431	-0.036129	0.148452
88	C	8	X	-0.037398	0.016823	-0.014815	-0.082854	-0.034619
89	C	8	Y	-0.041765	0.031144	0.001869	0.036725	-0.099061
90	C	8	Z	-0.010433	0.007426	0.001295	0.009863	-0.027219
91	C	9	S	0.015804	-0.002215	-0.050556	-0.142826	-0.188241
92	C	9	X	-0.003444	0.001114	0.000706	-0.006891	0.012429
93	C	9	Y	-0.005912	0.000594	0.016131	0.043213	0.048321
94	C	9	Z	-0.001362	0.000188	0.003614	0.010603	0.011131
95	C	9	S	-0.090910	0.090554	0.001972	-0.098108	0.002413
96	C	9	X	-0.000175	-0.021477	0.001150	-0.017370	0.011953
97	C	9	Y	0.033793	-0.022255	-0.017951	-0.000574	0.013504
98	C	9	Z	0.007443	-0.005100	-0.001973	0.000220	0.004391
99	C	10	S	0.065820	-0.018738	-0.078094	-0.144491	-0.245753
100	C	10	X	-0.002887	0.002137	-0.008922	-0.036526	-0.040815
101	C	10	Y	-0.028667	0.008592	0.020558	0.021464	0.034051
102	C	10	Z	-0.007820	0.002211	0.006875	0.006962	0.010523
103	C	10	S	0.075725	0.011305	-0.081555	-0.065175	-0.001928
104	C	10	X	0.080256	-0.091854	0.002347	0.071646	-0.015403
105	C	10	Y	-0.013640	-0.043443	0.021889	0.022549	-0.025421
106	C	10	Z	-0.004209	-0.007906	0.002986	0.002898	-0.006172
107	C	11	S	0.218027	-0.051570	-0.138028	-0.166633	-0.228356
108	C	11	X	-0.074126	0.036418	0.005739	-0.064839	-0.003646
109	C	11	Y	-0.041745	0.005141	0.007338	-0.013735	-0.040457
110	C	11	Z	-0.002935	-0.001841	-0.000883	-0.004852	-0.017193
111	C	11	S	-0.202202	0.396305	-0.101807	-0.207940	0.107284
112	C	11	X	-0.205092	0.293733	-0.109594	-0.219510	0.157898
113	C	11	Y	-0.040504	-0.115345	0.110644	0.102263	0.014304
114	C	11	Z	-0.015845	-0.041560	0.022446	0.039656	-0.004790
115	N	12	S	0.503476	-0.179982	-0.067260	0.099863	0.017984

116	N	12	X	-0.053008	0.031919	-0.049698	-0.064640	-0.100019
117	N	12	Y	0.092193	-0.037699	-0.020073	0.009681	-0.016837
118	N	12	Z	-0.024905	0.007781	-0.001412	-0.010280	-0.013158
119	N	12	S	-0.074914	0.036883	-0.018933	-0.020681	0.007113
120	N	12	X	0.041706	-0.043464	0.043653	0.030762	0.039860
121	N	12	Y	-0.055497	0.036829	0.011430	-0.047857	0.013345
122	N	12	Z	0.013307	0.006687	-0.015380	-0.007496	-0.000057
123	C	13	S	0.305355	-0.125182	0.112617	0.092516	0.161347
124	C	13	X	0.123573	-0.047563	-0.064267	0.052165	-0.004333
125	C	13	Y	-0.056328	0.022339	-0.025540	-0.016690	-0.032964
126	C	13	Z	0.028459	-0.013048	0.003449	0.010691	0.007632
127	C	13	S	0.016916	-0.060736	0.384575	0.013051	0.057395
128	C	13	X	0.074101	0.007946	-0.211009	0.003266	0.035782
129	C	13	Y	-0.025486	0.041656	-0.119014	-0.040625	-0.040545
130	C	13	Z	0.022686	-0.013011	0.013968	0.009834	0.015209
131	C	14	S	0.085063	-0.040811	0.329554	-0.063318	0.097805
132	C	14	X	0.031352	-0.013057	-0.033948	0.035474	0.040505
133	C	14	Y	0.007792	-0.002562	-0.018085	0.014841	0.018810
134	C	14	Z	0.000410	-0.000210	0.004147	-0.002642	-0.003525
135	C	14	S	-0.070836	0.056948	-0.261773	-0.080049	-0.102964
136	C	14	X	-0.009476	0.039983	-0.280995	0.010380	-0.007222
137	C	14	Y	0.137505	-0.030124	-0.183438	0.070076	0.066226
138	C	14	Z	-0.056373	0.012502	0.045766	-0.023152	-0.022823
139	C	15	S	0.019052	-0.015074	0.280048	-0.101499	-0.030684
140	C	15	X	0.001889	-0.002459	-0.049943	0.031048	0.043345
141	C	15	Y	0.016426	-0.006417	0.059090	-0.010040	0.026054
142	C	15	Z	-0.006487	0.002507	-0.028101	0.006690	-0.006921
143	C	15	S	0.098548	-0.038481	-0.146875	0.064403	0.033293
144	C	15	X	0.062267	-0.006443	0.053673	0.018183	0.053330
145	C	15	Y	0.108207	-0.022427	-0.016178	0.050601	0.069889
146	C	15	Z	-0.034119	0.010054	0.010917	-0.019337	-0.023727
147	C	16	S	0.004180	-0.005003	0.227806	-0.107956	-0.117541
148	C	16	X	0.000993	-0.000850	0.027256	-0.009181	0.003671
149	C	16	Y	0.002263	-0.001649	0.059207	-0.025892	-0.021929
150	C	16	Z	-0.000797	0.000388	-0.020911	0.009211	0.008825
151	C	16	S	0.071661	0.004192	0.046319	0.011627	0.072457
152	C	16	X	0.043397	-0.007893	0.008905	0.024207	0.038345
153	C	16	Y	-0.003917	0.011990	-0.021342	-0.003842	0.018034
154	C	16	Z	0.003718	-0.005299	0.009789	0.004393	-0.004024
155	C	17	S	0.003986	-0.003272	0.189544	-0.093507	-0.116316
156	C	17	X	0.001516	-0.001450	0.057210	-0.026222	-0.026756
157	C	17	Y	0.000288	-0.000113	0.016056	-0.006672	-0.003682
158	C	17	Z	-0.000016	-0.000057	-0.001877	0.000673	-0.000565
159	C	17	S	0.001256	-0.009651	0.015618	0.008735	-0.012338
160	C	17	X	-0.008850	-0.002994	0.014653	-0.002038	-0.014673
161	C	17	Y	-0.012017	0.003453	0.007028	-0.012608	-0.008591

162	C	17	Z	0.004575	-0.001486	-0.002103	0.004008	0.002186
163	C	18	S	0.005592	-0.004170	0.187694	-0.084582	-0.076879
164	C	18	X	0.003017	-0.001961	0.050711	-0.019168	-0.004939
165	C	18	Y	-0.000161	0.000149	-0.027545	0.014689	0.022039
166	C	18	Z	0.000306	-0.000201	0.014987	-0.007320	-0.008989
167	C	18	S	0.039680	-0.010888	0.039892	-0.002475	0.053906
168	C	18	X	0.023492	-0.003893	0.002890	-0.003822	0.029888
169	C	18	Y	-0.006837	0.001391	0.010813	-0.004871	0.001109
170	C	18	Z	0.004198	-0.001626	-0.003237	0.002115	0.002123
171	C	19	S	0.021971	-0.012240	0.241149	-0.081036	-0.000008
172	C	19	X	0.006281	-0.003396	0.017095	0.005078	0.030601
173	C	19	Y	-0.005225	0.002709	-0.058652	0.021288	0.005384
174	C	19	Z	0.002680	-0.001527	0.024342	-0.007779	0.000516
175	C	19	S	-0.092503	0.034909	-0.028421	-0.010705	-0.047309
176	C	19	X	-0.004430	0.002126	0.048960	-0.016995	0.028606
177	C	19	Y	0.010285	-0.012187	0.077291	-0.010303	0.016841
178	C	19	Z	-0.003473	0.006680	-0.026806	0.001401	-0.004808
179	O	20	S	-0.032730	0.008685	-0.109437	0.033393	0.009759
180	O	20	X	0.006667	0.002065	-0.025480	0.014896	0.010651
181	O	20	Y	0.011841	-0.004411	0.062041	-0.015730	0.008281
182	O	20	Z	-0.005303	0.002568	-0.032607	0.009076	-0.003158
183	O	20	S	-0.020994	0.002484	-0.051805	0.016274	-0.009945
184	O	20	X	-0.013830	0.000669	-0.026016	0.004686	-0.007787
185	O	20	Y	-0.010896	0.002257	-0.000797	-0.011900	-0.009121
186	O	20	Z	0.002116	-0.006592	0.002421	0.003735	0.005854
187	N	21	S	0.179813	0.551860	0.054389	0.135082	-0.095526
188	N	21	X	0.017024	0.059437	0.002445	-0.008521	0.025050
189	N	21	Y	0.008915	0.008343	-0.008777	-0.024096	0.017105
190	N	21	Z	-0.010059	-0.040478	-0.009255	-0.026743	0.025439
191	N	21	S	0.013362	0.010701	0.027913	0.031154	-0.036649
192	N	21	X	0.011291	-0.012083	-0.031925	-0.018828	-0.013806
193	N	21	Y	-0.025400	-0.016444	0.015624	0.015203	0.011960
194	N	21	Z	-0.015343	-0.020968	0.003159	0.005774	0.002008
195	H	22	S	0.000733	0.000439	-0.004575	-0.022535	0.029399
196	H	22	S	0.002350	0.009361	0.000765	0.014870	-0.039982
197	H	23	S	0.000073	0.002135	-0.002787	-0.016505	0.038978
198	H	23	S	0.001879	-0.005455	0.009503	0.013823	0.004448
199	H	24	S	0.003504	0.015000	-0.002336	-0.017153	0.045417
200	H	24	S	0.003780	0.041263	-0.000576	-0.007946	0.000830
201	H	25	S	0.000299	0.000397	-0.006293	-0.023145	-0.014174
202	H	25	S	0.016063	-0.005840	0.007760	0.025302	0.034174
203	H	26	S	0.001376	-0.000991	-0.005738	-0.017020	-0.029720
204	H	26	S	-0.004063	0.001972	0.008264	0.002663	-0.005512
205	H	27	S	0.012278	-0.005375	-0.010584	-0.018047	-0.042517
206	H	27	S	0.032582	-0.027551	0.003512	0.029667	0.002407
207	H	28	S	0.041080	-0.017200	0.018120	0.014793	0.029489

208	H	28	S	0.007703	-0.014016	0.018739	0.016254	0.013473
209	H	29	S	-0.000887	-0.000161	0.030628	-0.016497	-0.022047
210	H	29	S	-0.002690	0.005462	-0.013357	-0.004592	0.004745
211	H	30	S	-0.000184	-0.000177	0.025104	-0.013368	-0.019588
212	H	30	S	-0.003626	-0.000011	0.016227	-0.008843	-0.008516
213	H	31	S	0.000303	-0.000312	0.023411	-0.011444	-0.012523
214	H	31	S	0.009949	-0.001100	-0.000725	-0.003553	0.004765
215	H	32	S	0.003057	-0.001746	0.034463	-0.011148	0.002061
216	H	32	S	0.007359	0.004144	-0.044286	0.003538	-0.007326
217	H	33	S	-0.015432	0.004228	-0.055542	0.013995	-0.004923
218	H	33	S	0.006943	0.003704	-0.008418	-0.010493	0.001400
219	H	34	S	0.045800	0.137820	0.014375	0.042988	-0.040566
220	H	34	S	-0.014377	-0.025793	-0.005749	0.020296	-0.008231
221	H	35	S	0.041171	0.140883	0.020140	0.048004	-0.028724
222	H	35	S	-0.013223	-0.021822	0.011659	0.010520	-0.005013

11	12	13	14	15
-1.0431	-1.0173	-1.0122	-0.9920	-0.9684

A	A	A	A	A
---	---	---	---	---

1	CO	1	S	0.000862	-0.005067	0.006773	0.008667	-0.004841
2	CO	1	X	0.003228	0.008281	-0.003765	0.003011	-0.006941
3	CO	1	Y	0.009996	0.005629	-0.001779	0.005795	0.000320
4	CO	1	Z	0.002127	-0.006210	-0.003763	-0.004696	0.006970
5	CO	1	XX	0.007414	0.004510	0.001715	0.001529	-0.004917
6	CO	1	YY	-0.009807	-0.002279	-0.000693	-0.002678	-0.000854
7	CO	1	ZZ	0.002393	-0.002230	-0.001022	0.001149	0.005771
8	CO	1	XY	-0.005137	0.010531	0.003952	-0.001095	0.002376
9	CO	1	XZ	-0.001888	-0.005883	0.005317	0.004405	-0.006118
10	CO	1	YZ	0.002859	-0.003796	0.000637	0.002775	0.004795
11	CO	1	XX	0.005912	0.003163	0.001467	0.000959	-0.002752
12	CO	1	YY	-0.008780	-0.001577	-0.001184	-0.001862	-0.000556
13	CO	1	ZZ	0.002868	-0.001586	-0.000283	0.000904	0.003308
14	CO	1	XY	-0.002505	0.006724	0.002972	-0.000536	0.002328
15	CO	1	XZ	-0.002640	-0.003449	0.003655	0.003140	-0.004492
16	CO	1	YZ	0.002210	-0.001942	0.000722	0.001724	0.003755
17	CO	1	S	-0.001982	0.009144	-0.016367	-0.022762	0.015619
18	CO	1	X	-0.013786	0.001708	-0.001266	-0.004036	0.031819
19	CO	1	Y	-0.009920	-0.004160	0.017398	-0.017251	-0.003217
20	CO	1	Z	0.003324	0.002561	0.006505	0.006322	-0.018552
21	CO	1	S	0.010141	0.008392	0.023979	0.002104	-0.003869
22	CO	1	X	-0.003023	0.000690	0.003672	0.002636	-0.008688
23	CO	1	Y	0.008158	0.001803	0.013403	0.003244	-0.001668
24	CO	1	Z	-0.003411	-0.000058	-0.006447	-0.000843	0.001795
25	CO	1	S	0.000602	-0.004588	0.004600	0.006207	-0.002227
26	CO	1	X	0.001536	-0.001117	-0.000626	0.000532	-0.001850
27	CO	1	Y	-0.001062	-0.000068	-0.001672	0.000515	0.000727

28 CO 1 Z -0.000648 0.000499 0.000280 0.000292 0.001020
29 CO 1 XX 0.007250 0.001829 0.000446 0.005080 -0.006476
30 CO 1 YY -0.003984 -0.000229 0.008874 -0.006378 -0.001535
31 CO 1 ZZ -0.003266 -0.001600 -0.009320 0.001298 0.008011
32 CO 1 XY -0.011659 0.013664 0.009561 -0.001281 -0.000558
33 CO 1 XZ 0.002077 -0.005569 0.004288 0.000545 -0.005493
34 CO 1 YZ 0.001791 -0.003708 -0.005068 0.003008 0.001250
35 C 2 S 0.018611 -0.065640 -0.226398 -0.059736 0.287370
36 C 2 X -0.015740 0.010224 0.027952 0.057426 0.004140
37 C 2 Y 0.027526 -0.001265 0.006573 -0.070974 -0.058451
38 C 2 Z 0.007264 -0.000203 0.002100 -0.018258 -0.015409
39 C 2 S 0.085727 -0.005467 0.069985 0.067609 -0.155281
40 C 2 X -0.055776 -0.003181 -0.048886 -0.042850 0.133787
41 C 2 Y 0.033855 -0.018336 -0.039406 -0.025419 0.057260
42 C 2 Z 0.008021 -0.004519 -0.010963 -0.010059 0.017252
43 C 3 S -0.064842 -0.030853 -0.133446 0.217141 0.235903
44 C 3 X 0.020831 0.000146 0.005587 -0.052619 0.004867
45 C 3 Y 0.009579 -0.013604 -0.045688 -0.046728 0.079499
46 C 3 Z 0.003803 -0.003642 -0.011969 -0.016458 0.021440
47 C 3 S 0.021190 -0.017204 -0.079518 -0.013707 0.091624
48 C 3 X 0.006705 -0.001845 0.010962 0.027016 0.007477
49 C 3 Y 0.022771 -0.005920 -0.009255 -0.013762 -0.016099
50 C 3 Z 0.006572 -0.002618 -0.003560 -0.001305 -0.002243
51 C 4 S -0.112925 0.017592 0.034965 0.315961 -0.112061
52 C 4 X 0.011479 -0.015066 -0.055776 0.013848 0.113590
53 C 4 Y -0.020573 0.001348 -0.000241 0.026737 0.008291
54 C 4 Z -0.005789 -0.000049 -0.001786 0.008073 0.006589
55 C 4 S -0.018860 0.009252 0.058085 -0.063538 -0.081760
56 C 4 X 0.005981 -0.003220 0.003612 0.046690 -0.011270
57 C 4 Y -0.004539 0.002458 0.035332 -0.053990 -0.022169
58 C 4 Z -0.001217 0.002436 0.013396 -0.015837 -0.008969
59 C 5 S -0.106313 0.060539 0.197399 0.049683 -0.278780
60 C 5 X -0.026042 -0.000045 -0.004277 0.096761 -0.041296
61 C 5 Y -0.013826 0.016766 0.054307 -0.093895 -0.004950
62 C 5 Z -0.008403 0.007173 0.022068 -0.023630 -0.008800
63 C 5 S 0.001946 0.019641 -0.104535 -0.037245 0.170761
64 C 5 X 0.052636 -0.019574 -0.069591 0.080792 0.114860
65 C 5 Y 0.026053 0.001086 -0.084643 -0.074534 0.130919
66 C 5 Z 0.009859 -0.003603 -0.033704 -0.015724 0.050212
67 C 6 S -0.046602 0.069941 0.236951 -0.252127 -0.082945
68 C 6 X 0.029071 -0.022813 -0.061746 -0.036917 -0.055661
69 C 6 Y 0.043028 -0.015450 -0.043668 -0.022905 0.073799
70 C 6 Z 0.011124 -0.003824 -0.010936 -0.006709 0.025217
71 C 6 S -0.061593 0.035592 -0.029940 0.010302 -0.099900
72 C 6 X -0.086325 0.002097 0.072521 -0.007275 -0.189870
73 C 6 Y -0.045688 0.033734 -0.110588 -0.129141 0.173341

74	C	6	Z	-0.012157	0.012252	-0.035260	-0.043650	0.045409
75	C	7	S	0.125473	-0.062097	-0.168123	-0.290249	0.011678
76	C	7	X	-0.003808	-0.020876	-0.076768	0.019823	0.079009
77	C	7	Y	0.048058	-0.018909	-0.051371	0.018006	-0.046294
78	C	7	Z	0.013396	-0.005623	-0.015352	0.004896	-0.010696
79	C	7	S	0.070792	-0.024617	-0.002873	0.011910	0.062046
80	C	7	X	-0.132787	0.025506	-0.047570	-0.057512	0.107212
81	C	7	Y	0.055372	0.000187	0.047753	0.016724	-0.230115
82	C	7	Z	0.012613	-0.000362	0.011787	0.005713	-0.056470
83	C	8	S	0.212315	-0.082984	-0.217314	-0.043029	-0.177563
84	C	8	X	-0.042273	0.007193	0.012068	-0.056789	0.051535
85	C	8	Y	-0.015622	0.008805	0.025060	0.076306	-0.019401
86	C	8	Z	-0.003351	0.002091	0.006086	0.021220	-0.005615
87	C	8	S	-0.086908	0.012539	-0.033524	0.002258	0.150733
88	C	8	X	0.069918	-0.023472	-0.030031	-0.027310	-0.040224
89	C	8	Y	0.049559	-0.005579	0.007735	-0.008421	-0.104645
90	C	8	Z	0.014497	-0.001701	0.001658	-0.000826	-0.030979
91	C	9	S	0.202217	-0.051283	-0.120707	0.235654	-0.167286
92	C	9	X	0.020039	-0.015572	-0.042788	-0.060046	-0.052104
93	C	9	Y	-0.043722	0.007984	0.016359	-0.036423	0.016398
94	C	9	Z	-0.010561	0.001998	0.004322	-0.006348	0.004461
95	C	9	S	0.047579	-0.016140	-0.002380	0.002412	-0.052900
96	C	9	X	0.010875	-0.008177	-0.018493	-0.002803	0.033598
97	C	9	Y	0.000602	-0.004164	-0.018023	0.025838	-0.006729
98	C	9	Z	-0.001475	-0.000160	-0.003629	0.003899	-0.001264
99	C	10	S	0.101911	0.010688	0.040635	0.315186	0.081247
100	C	10	X	0.044280	-0.008248	-0.014651	0.033794	-0.040368
101	C	10	Y	0.029040	-0.018426	-0.048371	0.011310	-0.076300
102	C	10	Z	0.005747	-0.004662	-0.012574	0.001861	-0.018521
103	C	10	S	-0.082352	0.012827	0.011862	-0.085452	0.088558
104	C	10	X	-0.007199	0.002264	-0.031576	-0.056665	0.024691
105	C	10	Y	0.041565	-0.009215	-0.013159	0.071003	0.015024
106	C	10	Z	0.013975	-0.003906	-0.004995	0.027522	-0.000182
107	C	11	S	-0.091201	0.073596	0.198537	0.040744	0.223502
108	C	11	X	0.045063	0.011078	0.055894	-0.056202	-0.049440
109	C	11	Y	0.065156	-0.011396	-0.025007	0.113346	0.008549
110	C	11	Z	0.009763	-0.001010	-0.003416	0.032903	0.015464
111	C	11	S	-0.024720	-0.008478	0.112207	0.127048	-0.137563
112	C	11	X	0.034371	-0.046016	0.058629	0.073431	-0.123189
113	C	11	Y	0.104319	-0.025055	-0.058960	0.097551	-0.056246
114	C	11	Z	0.028266	-0.007637	-0.012888	0.026691	-0.001216
115	N	12	S	-0.125613	-0.021953	-0.090297	-0.035051	0.007861
116	N	12	X	-0.083499	0.044719	0.102264	-0.000839	0.158164
117	N	12	Y	-0.022912	0.003781	-0.011671	0.025774	0.022092
118	N	12	Z	-0.003214	0.004261	0.014888	0.007395	0.023240
119	N	12	S	-0.027455	-0.006279	-0.011731	0.002231	0.002845

120	N	12	X	0.040383	-0.022329	-0.039715	0.021524	-0.041615
121	N	12	Y	0.004243	0.004605	0.023756	-0.011957	-0.000826
122	N	12	Z	-0.002991	-0.002479	-0.001331	0.003511	0.002548
123	C	13	S	0.188259	-0.012607	-0.063468	-0.000031	-0.177786
124	C	13	X	-0.098938	-0.036214	-0.097758	-0.005983	-0.035548
125	C	13	Y	-0.025988	0.026086	0.007235	0.014911	0.027433
126	C	13	Z	-0.000642	-0.011457	-0.009933	-0.000728	-0.007635
127	C	13	S	-0.028771	0.044624	-0.105950	-0.042727	-0.123546
128	C	13	X	0.075447	-0.059674	0.004235	0.089099	-0.002858
129	C	13	Y	-0.007968	-0.024699	0.048649	0.017075	0.048479
130	C	13	Z	0.014266	0.001181	-0.013364	0.011869	-0.012603
131	C	14	S	0.280848	0.032500	0.181153	0.006959	0.062829
132	C	14	X	0.038161	-0.054050	-0.013624	-0.002964	-0.073656
133	C	14	Y	0.034415	0.111504	-0.036585	0.000493	-0.032103
134	C	14	Z	-0.008362	-0.046910	0.013177	0.000740	0.005811
135	C	14	S	-0.112808	0.012957	0.017559	0.061752	0.099098
136	C	14	X	0.085063	-0.096698	0.070542	0.042483	0.031986
137	C	14	Y	0.094150	-0.027546	0.006814	0.050609	0.010555
138	C	14	Z	-0.030459	0.000752	0.003162	-0.021499	-0.004960
139	C	15	S	-0.009040	-0.325013	0.165806	0.007675	0.091482
140	C	15	X	0.092050	0.052490	0.035427	0.000044	0.021216
141	C	15	Y	0.078913	0.037459	0.047412	0.000566	0.028088
142	C	15	Z	-0.023820	-0.008643	-0.016882	-0.000041	-0.010132
143	C	15	S	0.055720	-0.104563	-0.010911	0.042339	-0.016056
144	C	15	X	0.048192	-0.003480	0.031083	-0.008010	0.013011
145	C	15	Y	0.103986	0.016434	0.004679	0.019058	-0.014109
146	C	15	Z	-0.034791	-0.004834	-0.000641	-0.005223	0.007591
147	C	16	S	-0.252287	-0.268655	-0.063333	-0.001680	-0.074963
148	C	16	X	0.021174	-0.084801	0.063773	0.003706	0.047864
149	C	16	Y	-0.039875	-0.015723	-0.013991	-0.000911	-0.005717
150	C	16	Z	0.017002	-0.000598	0.010317	0.000674	0.005731
151	C	16	S	0.082184	0.059750	0.025962	-0.005310	-0.004727
152	C	16	X	0.049818	0.015301	0.013446	0.000097	0.000957
153	C	16	Y	0.036643	0.077212	0.015661	-0.003777	0.019454
154	C	16	Z	-0.010940	-0.029798	-0.004155	0.000262	-0.007197
155	C	17	S	-0.257445	0.062937	-0.208603	-0.011111	-0.135514
156	C	17	X	-0.053470	-0.026101	-0.021430	-0.000711	-0.011988
157	C	17	Y	0.001149	0.092119	-0.025152	-0.001705	0.010030
158	C	17	Z	-0.004470	-0.038027	0.008265	0.000570	-0.004746
159	C	17	S	-0.018810	-0.049552	-0.017251	-0.000910	-0.013658
160	C	17	X	-0.008926	-0.039896	0.018032	-0.000177	0.027969
161	C	17	Y	0.000778	-0.003393	0.006989	0.001902	0.011559
162	C	17	Z	-0.000510	-0.001132	-0.001498	0.000088	-0.002280
163	C	18	S	-0.124991	0.327132	-0.171748	-0.008039	-0.014693
164	C	18	X	0.011424	0.071956	0.001112	0.001163	0.031121
165	C	18	Y	0.054173	0.008087	0.041299	0.002763	0.036954

166	C	18	Z	-0.020188	0.003072	-0.016144	-0.000997	-0.011890
167	C	18	S	0.065793	0.068642	-0.005275	0.014861	-0.037562
168	C	18	X	0.048885	-0.007857	0.021841	0.013825	-0.010332
169	C	18	Y	0.009054	0.012815	-0.007755	-0.001707	-0.007281
170	C	18	Z	-0.000012	-0.006209	0.004995	0.000937	0.001809
171	C	19	S	0.097839	0.347391	0.006103	0.003782	0.102234
172	C	19	X	0.075632	-0.050374	0.066379	0.002893	0.010152
173	C	19	Y	-0.006461	-0.032054	-0.005178	-0.000383	-0.015910
174	C	19	Z	0.009069	0.008409	0.007521	0.000535	0.006921
175	C	19	S	-0.015237	-0.055649	0.026152	-0.026329	0.011603
176	C	19	X	0.058329	0.006349	0.013134	0.005635	-0.030291
177	C	19	Y	0.015344	0.092126	-0.009745	0.003921	0.008122
178	C	19	Z	0.000154	-0.034424	0.005109	0.001229	-0.004629
179	O	20	S	0.009046	0.108384	-0.041291	-0.000943	-0.014696
180	O	20	X	0.017755	0.084917	-0.030947	-0.004901	-0.019418
181	O	20	Y	0.031912	-0.117908	0.077554	0.000911	0.047027
182	O	20	Z	-0.013910	0.063956	-0.040724	-0.000288	-0.024797
183	O	20	S	0.005007	0.068932	-0.027987	-0.000116	0.001369
184	O	20	X	-0.005705	0.020554	-0.013745	-0.003859	-0.000620
185	O	20	Y	-0.007470	-0.012468	0.011709	-0.000401	0.008835
186	O	20	Z	0.002580	0.007154	-0.003488	-0.000512	-0.006956
187	N	21	S	0.066406	-0.032063	-0.092606	-0.031080	0.098317
188	N	21	X	-0.014507	0.007727	0.030344	0.034211	-0.070260
189	N	21	Y	-0.023506	0.017568	0.054392	-0.016313	-0.061732
190	N	21	Z	-0.021494	0.014537	0.042715	0.009763	-0.062395
191	N	21	S	0.049824	-0.022523	-0.061257	-0.005359	0.080786
192	N	21	X	-0.001625	0.002049	-0.010768	0.004112	0.006312
193	N	21	Y	0.003447	-0.004880	-0.002454	0.013475	0.000964
194	N	21	Z	-0.000523	-0.000755	-0.002282	0.002160	-0.003809
195	H	22	S	0.005109	-0.013224	-0.046187	-0.014406	0.061107
196	H	22	S	0.006633	0.007115	0.024079	0.023241	-0.061286
197	H	23	S	-0.011187	-0.005374	-0.024057	0.043877	0.050365
198	H	23	S	0.001368	0.000889	0.000045	-0.011454	-0.018733
199	H	24	S	-0.020340	0.003137	0.006080	0.073632	-0.027175
200	H	24	S	-0.000500	0.000735	0.009378	-0.023518	-0.002295
201	H	25	S	0.035859	-0.016303	-0.044437	-0.010913	-0.034471
202	H	25	S	-0.037671	0.010303	0.012088	0.017247	0.038722
203	H	26	S	0.033044	-0.009073	-0.022006	0.047756	-0.035662
204	H	26	S	-0.005889	0.003684	0.006981	-0.012453	0.012846
205	H	27	S	0.018245	0.002630	0.005859	0.074130	0.020547
206	H	27	S	-0.003565	0.002577	-0.014367	-0.035970	-0.004652
207	H	28	S	0.044119	0.008772	-0.010477	0.007008	-0.038687
208	H	28	S	0.011468	0.014403	-0.017622	0.006390	-0.013110
209	H	29	S	-0.050912	-0.058576	-0.014720	-0.000324	-0.020521
210	H	29	S	0.013994	0.038962	0.005053	-0.000222	0.009767
211	H	30	S	-0.046416	0.011195	-0.041354	-0.002438	-0.032159

212	H	30	S	-0.003003	-0.012096	0.010300	0.001250	0.015960
213	H	31	S	-0.021766	0.062121	-0.033018	-0.001669	-0.003098
214	H	31	S	0.009405	-0.014792	0.011309	0.005813	0.001725
215	H	32	S	0.023158	0.073444	0.001996	0.000965	0.022223
216	H	32	S	-0.009860	-0.045799	0.001110	0.003220	-0.004201
217	H	33	S	-0.019124	0.080659	-0.049681	-0.000355	-0.028822
218	H	33	S	-0.000283	0.002990	-0.002846	0.002949	-0.005800
219	H	34	S	0.027088	-0.014051	-0.043393	-0.023070	0.064013
220	H	34	S	-0.000513	-0.003074	-0.019438	-0.000083	0.014118
221	H	35	S	0.026649	-0.016678	-0.047981	0.006539	0.048322
222	H	35	S	0.005002	-0.004240	-0.009834	0.008928	0.014932

	16	17	18	19	20
	-0.9293	-0.9058	-0.8791	-0.8733	-0.8601
	A	A	A	A	A

1	CO	1	S	0.012672	-0.011020	-0.023961	-0.021198	0.010084
2	CO	1	X	-0.001657	0.018804	0.011799	-0.005982	-0.008652
3	CO	1	Y	0.024124	0.000140	-0.004274	-0.017458	0.001737
4	CO	1	Z	-0.002481	0.001110	-0.000531	0.007716	0.012354
5	CO	1	XX	0.005428	0.028058	0.001918	-0.004278	-0.014303
6	CO	1	YY	-0.018128	-0.016565	0.005232	0.010233	-0.002264
7	CO	1	ZZ	0.012700	-0.011493	-0.007150	-0.005955	0.016568
8	CO	1	XY	0.006187	-0.018105	0.013779	0.010803	-0.014855
9	CO	1	XZ	-0.005233	0.002125	-0.015566	-0.016133	0.007962
10	CO	1	YZ	0.004313	0.002910	-0.008286	-0.018803	0.011847
11	CO	1	XX	0.003334	0.018073	0.001492	-0.002157	-0.008968
12	CO	1	YY	-0.012733	-0.011992	0.002910	0.005989	-0.001893
13	CO	1	ZZ	0.009399	-0.006082	-0.004402	-0.003832	0.010861
14	CO	1	XY	0.003234	-0.009077	0.009019	0.005861	-0.010758
15	CO	1	XZ	-0.003235	-0.000722	-0.009328	-0.008946	0.004515
16	CO	1	YZ	0.002869	0.001632	-0.003612	-0.010156	0.006504
17	CO	1	S	-0.034729	0.028507	0.059457	0.051143	-0.022245
18	CO	1	X	0.005405	-0.033044	0.006461	0.007328	0.003873
19	CO	1	Y	-0.031910	0.010762	0.031064	0.030281	-0.010087
20	CO	1	Z	0.001094	0.002024	-0.010827	-0.009617	-0.010690
21	CO	1	S	0.015554	-0.003507	0.011102	0.000810	0.006501
22	CO	1	X	-0.002318	0.009751	-0.007595	-0.001133	0.012878
23	CO	1	Y	0.006794	0.003035	0.003128	-0.001974	0.004061
24	CO	1	Z	-0.002244	-0.003429	0.000576	0.001640	-0.007705
25	CO	1	S	0.008572	-0.008509	-0.018672	-0.017879	0.008141
26	CO	1	X	0.000870	0.001091	-0.000939	-0.000863	-0.000246
27	CO	1	Y	-0.000552	-0.002250	-0.001642	-0.001077	0.000098
28	CO	1	Z	-0.000320	-0.000055	0.001165	0.000005	-0.000865
29	CO	1	XX	0.005076	0.014236	-0.008602	-0.003365	-0.004230
30	CO	1	YY	-0.010251	-0.003307	0.014332	0.007288	-0.004748
31	CO	1	ZZ	0.005175	-0.010929	-0.005730	-0.003923	0.008979

32 CO 1 XY 0.003728 -0.019899 0.002791 0.012323 -0.004543
33 CO 1 XZ -0.004069 0.008662 -0.002850 -0.005652 -0.002525
34 CO 1 YZ 0.000187 0.003583 -0.006599 -0.010968 0.002822
35 C 2 S 0.075507 0.034558 -0.117388 0.147689 -0.195021
36 C 2 X -0.003432 -0.002503 0.049764 0.070488 0.030818
37 C 2 Y -0.024121 -0.015322 -0.046871 -0.095643 -0.097284
38 C 2 Z -0.006487 -0.004108 -0.011801 -0.024059 -0.026232
39 C 2 S -0.094781 -0.033858 0.183334 -0.039287 0.139674
40 C 2 X 0.065253 0.029168 -0.098497 0.056788 -0.085148
41 C 2 Y 0.010281 0.020369 -0.039033 -0.021296 -0.097948
42 C 2 Z 0.004480 0.006351 -0.013809 -0.002977 -0.028301
43 C 3 S 0.030957 0.007548 0.160876 0.138087 0.195542
44 C 3 X 0.010793 0.005888 -0.007737 0.049127 -0.016188
45 C 3 Y 0.039026 0.024070 -0.069888 0.110423 -0.083757
46 C 3 Z 0.011355 0.007100 -0.020834 0.032790 -0.025351
47 C 3 S 0.026385 0.017980 -0.084374 -0.127880 -0.123203
48 C 3 X -0.008115 -0.003482 0.083803 0.098136 0.096654
49 C 3 Y -0.009413 0.001869 -0.029714 -0.036992 -0.070636
50 C 3 Z -0.002672 0.000691 -0.004609 -0.007026 -0.015100
51 C 4 S -0.100757 -0.060264 0.103896 -0.243227 0.048786
52 C 4 X 0.024718 0.006072 0.105031 0.037090 0.157500
53 C 4 Y 0.009707 0.010042 -0.008698 0.061263 0.024321
54 C 4 Z 0.003764 0.003519 0.001541 0.020193 0.011885
55 C 4 S -0.042115 -0.035467 0.041161 0.255122 0.030204
56 C 4 X -0.013159 0.002817 0.030418 -0.054031 0.002442
57 C 4 Y -0.001166 0.000694 0.003023 0.151868 -0.002153
58 C 4 Z -0.000674 -0.000176 0.003054 0.045741 -0.000401
59 C 5 S -0.046214 -0.001634 -0.139114 0.104815 -0.189330
60 C 5 X -0.030690 -0.017865 -0.001149 -0.158908 0.010157
61 C 5 Y 0.046701 0.033384 -0.004775 0.136583 0.107530
62 C 5 Z 0.009889 0.009583 -0.001082 0.031805 0.020702
63 C 5 S 0.118416 0.007666 -0.063828 0.001436 0.107298
64 C 5 X 0.044401 0.045222 0.034833 -0.167006 0.059647
65 C 5 Y 0.081397 0.012207 -0.036868 0.101740 0.099354
66 C 5 Z 0.026164 0.005284 -0.010544 0.017912 0.026666
67 C 6 S 0.109158 0.064187 0.027699 0.085745 0.214670
68 C 6 X 0.009233 0.022485 -0.118604 -0.042422 -0.008258
69 C 6 Y 0.026815 0.001871 0.061575 -0.161319 0.088743
70 C 6 Z 0.005295 -0.000940 0.024246 -0.050066 0.021407
71 C 6 S 0.029530 -0.050769 -0.109622 -0.092161 0.010105
72 C 6 X -0.153779 -0.100419 0.061270 0.007699 -0.106096
73 C 6 Y 0.134617 -0.026153 -0.119600 0.150331 0.099661
74 C 6 Z 0.041649 -0.007641 -0.041109 0.052356 0.036729
75 C 7 S 0.004527 -0.003297 -0.087516 -0.210580 -0.051306
76 C 7 X -0.011789 -0.011481 -0.063184 0.032638 -0.176177
77 C 7 Y -0.083020 -0.055137 0.078651 -0.075201 -0.033885

78	C	7	Z	-0.023066	-0.015257	0.021378	-0.020964	-0.013091
79	C	7	S	0.009047	0.062697	0.033026	-0.063545	-0.030729
80	C	7	X	0.088733	-0.008337	-0.139066	0.117935	-0.016815
81	C	7	Y	-0.132700	-0.083998	0.120312	-0.099116	0.038806
82	C	7	Z	-0.034922	-0.023706	0.034648	-0.028215	0.009056
83	C	8	S	-0.222656	-0.125157	0.161181	-0.051203	-0.018820
84	C	8	X	0.018854	-0.002713	-0.028458	-0.078386	-0.074511
85	C	8	Y	-0.016132	-0.001939	0.028461	0.126871	0.023638
86	C	8	Z	-0.005031	-0.000762	0.008114	0.035137	0.005652
87	C	8	S	0.103991	0.056266	-0.112863	0.206351	0.024804
88	C	8	X	-0.063388	-0.025843	0.062703	-0.100323	-0.035573
89	C	8	Y	-0.071353	-0.041772	0.069010	-0.057624	0.016524
90	C	8	Z	-0.020593	-0.010890	0.017130	-0.015049	0.003528
91	C	9	S	-0.088106	-0.002747	0.010573	0.278082	0.051483
92	C	9	X	-0.095857	-0.062976	0.115462	-0.012399	0.031987
93	C	9	Y	-0.005055	-0.006297	-0.000053	0.029137	-0.011325
94	C	9	Z	-0.000485	-0.000421	-0.002353	0.010509	-0.004821
95	C	9	S	-0.027623	-0.012253	-0.014467	-0.169367	-0.091089
96	C	9	X	0.000127	0.004387	0.009892	-0.016887	-0.020573
97	C	9	Y	-0.013173	0.005895	0.016814	0.156267	0.048253
98	C	9	Z	-0.001015	0.000531	0.004720	0.041709	0.015267
99	C	10	S	0.178653	0.109962	-0.204575	-0.026870	-0.106304
100	C	10	X	-0.012745	0.007738	0.031638	0.067965	0.063605
101	C	10	Y	-0.034067	0.006464	-0.037632	0.135410	0.014896
102	C	10	Z	-0.011043	0.001010	-0.010652	0.036231	-0.002500
103	C	10	S	-0.042945	-0.040437	0.115623	0.183245	0.057168
104	C	10	X	-0.021226	-0.024968	0.070989	0.078805	0.072814
105	C	10	Y	0.033719	0.036946	-0.058131	-0.030243	-0.040170
106	C	10	Z	0.005363	0.013028	-0.021588	-0.010532	-0.018359
107	C	11	S	0.051567	-0.025159	0.134354	-0.127454	-0.025979
108	C	11	X	0.086347	0.056187	0.043358	0.019446	0.156362
109	C	11	Y	0.111663	0.064900	-0.128197	-0.110656	-0.026794
110	C	11	Z	0.015167	0.010108	-0.022050	-0.030524	-0.028806
111	C	11	S	-0.105076	-0.020147	0.031522	-0.099197	-0.161015
112	C	11	X	-0.110692	0.020182	0.067364	-0.030655	-0.106044
113	C	11	Y	0.040529	0.063995	-0.103674	-0.051782	-0.015467
114	C	11	Z	0.017820	0.018977	-0.025622	-0.022650	-0.008259
115	N	12	S	-0.188176	-0.057857	0.007984	0.062334	-0.033840
116	N	12	X	-0.095654	-0.100795	0.152708	-0.000748	-0.130929
117	N	12	Y	0.023574	-0.026557	-0.058588	-0.076063	-0.015379
118	N	12	Z	-0.011723	-0.002049	0.020043	-0.011172	-0.036043
119	N	12	S	-0.083674	-0.066732	0.022298	0.015304	-0.030791
120	N	12	X	-0.015799	0.023946	-0.013212	-0.000995	-0.017810
121	N	12	Y	-0.004225	-0.000389	0.026871	-0.006376	-0.010726
122	N	12	Z	-0.004281	-0.000311	0.003134	-0.003216	-0.008652
123	C	13	S	0.277986	0.053277	-0.052778	-0.043116	0.121243

124	C	13	X	-0.106623	0.015347	-0.146489	0.006499	0.056218
125	C	13	Y	0.043149	-0.061136	-0.041028	-0.050096	0.006076
126	C	13	Z	-0.020184	0.021981	-0.005546	0.004542	-0.008478
127	C	13	S	0.042803	-0.041539	-0.109292	0.063019	0.143136
128	C	13	X	-0.016516	0.081873	0.004705	-0.066632	-0.088231
129	C	13	Y	0.030119	-0.029136	0.041232	-0.030501	-0.037793
130	C	13	Z	-0.010050	0.021604	-0.016997	0.000954	-0.004624
131	C	14	S	0.066702	-0.031765	0.194328	0.019594	-0.151761
132	C	14	X	0.112437	0.120301	0.038949	-0.018591	0.045305
133	C	14	Y	0.119275	-0.112371	-0.010936	-0.006173	0.048941
134	C	14	Z	-0.031089	0.051431	0.006909	-0.002119	-0.016856
135	C	14	S	-0.049701	-0.147487	-0.053361	-0.052310	-0.036765
136	C	14	X	0.068777	0.092189	0.146707	-0.057375	-0.141855
137	C	14	Y	-0.115959	0.139408	-0.005410	-0.035047	-0.075397
138	C	14	Z	0.046659	-0.044110	0.017065	0.008499	0.021446
139	C	15	S	-0.173119	0.053482	-0.094928	-0.014124	0.038740
140	C	15	X	-0.074664	0.225087	0.051532	-0.029874	-0.017385
141	C	15	Y	-0.013696	0.051418	0.145077	0.021971	-0.152374
142	C	15	Z	0.004130	-0.011265	-0.052803	-0.010660	0.056927
143	C	15	S	-0.007085	0.059150	0.054556	-0.025424	-0.113431
144	C	15	X	-0.098340	0.061903	-0.059037	0.013250	0.051791
145	C	15	Y	-0.044160	0.104647	-0.000584	-0.011845	-0.024718
146	C	15	Z	0.014038	-0.037810	-0.004930	0.005026	0.011417
147	C	16	S	0.154468	-0.212223	-0.038754	0.021610	0.047649
148	C	16	X	-0.086704	-0.074121	-0.136493	-0.001242	0.088700
149	C	16	Y	-0.000728	0.027400	0.039275	0.003540	-0.048897
150	C	16	Z	-0.005671	-0.018392	-0.026398	-0.001420	0.025972
151	C	16	S	-0.060974	0.168725	0.028793	0.000005	0.001185
152	C	16	X	-0.040438	0.023491	-0.043405	0.002769	0.034582
153	C	16	Y	-0.043815	0.110073	0.049469	-0.006605	-0.032657
154	C	16	Z	0.011805	-0.041722	-0.022741	0.003262	0.016500
155	C	17	S	0.163325	0.203018	0.205437	-0.014972	-0.115815
156	C	17	X	0.021908	-0.055564	-0.008858	0.011071	-0.002490
157	C	17	Y	-0.068727	0.096063	-0.034441	-0.013684	0.026071
158	C	17	Z	0.028484	-0.042566	0.012434	0.006225	-0.010211
159	C	17	S	0.001314	-0.065528	-0.101757	-0.001095	0.084739
160	C	17	X	-0.052388	-0.089029	-0.100876	0.008650	0.061946
161	C	17	Y	-0.010777	-0.015909	-0.024034	-0.003988	0.015611
162	C	17	Z	0.000978	-0.000294	0.001294	0.001894	-0.001947
163	C	18	S	-0.130798	0.191943	-0.113965	-0.027695	0.105338
164	C	18	X	-0.051415	-0.081526	-0.062729	0.011887	0.023959
165	C	18	Y	-0.051937	-0.083743	-0.096525	0.005193	0.069026
166	C	18	Z	0.016131	0.025858	0.032327	-0.001200	-0.024838
167	C	18	S	0.115478	-0.054506	0.040851	-0.013969	-0.009176
168	C	18	X	0.077315	-0.067846	0.039076	-0.006685	-0.031101
169	C	18	Y	0.001621	0.020218	-0.030810	-0.009266	0.039190

170	C	18	Z	0.004693	-0.013554	0.015354	0.003596	-0.017150
171	C	19	S	-0.120985	-0.215719	-0.139817	0.018473	0.071614
172	C	19	X	0.086594	-0.083587	0.109211	0.010743	-0.086677
173	C	19	Y	0.024465	-0.007844	-0.031996	-0.007395	0.049196
174	C	19	Z	-0.001223	-0.004449	0.021285	0.003202	-0.026494
175	C	19	S	0.023317	0.085414	0.083520	0.007529	-0.031685
176	C	19	X	0.120895	-0.051256	0.031927	-0.013718	0.008691
177	C	19	Y	-0.000988	-0.117728	-0.064412	0.009743	0.045156
178	C	19	Z	0.012750	0.040646	0.026996	-0.005782	-0.018550
179	O	20	S	0.019273	0.038909	0.046484	-0.001348	-0.035505
180	O	20	X	0.049069	0.024157	0.142536	0.035863	-0.131805
181	O	20	Y	-0.169563	0.296665	-0.036913	-0.044545	0.053518
182	O	20	Z	0.091904	-0.160178	0.023430	0.024495	-0.033374
183	O	20	S	0.010975	0.037832	0.044692	-0.009101	-0.033166
184	O	20	X	0.023301	-0.002607	0.060313	0.011196	-0.049413
185	O	20	Y	-0.028945	0.060637	-0.004302	-0.009454	0.012385
186	O	20	Z	0.016158	-0.032358	0.002693	0.005675	-0.008487
187	N	21	S	0.028213	0.007487	0.016255	-0.003035	0.044354
188	N	21	X	-0.024325	-0.013810	-0.058722	-0.049161	-0.131083
189	N	21	Y	-0.012169	0.002446	-0.031470	0.178722	-0.078811
190	N	21	Z	-0.022268	-0.001611	-0.033480	0.029409	-0.124508
191	N	21	S	0.037149	0.031191	0.001977	-0.015525	0.044717
192	N	21	X	0.004842	-0.006458	-0.018588	-0.002687	-0.024111
193	N	21	Y	-0.002473	0.007922	-0.005783	0.016339	-0.020235
194	N	21	Z	-0.002511	0.000020	-0.008455	0.005130	-0.026311
195	H	22	S	0.013616	0.004876	-0.031356	0.042790	-0.075030
196	H	22	S	-0.023489	-0.016590	0.034174	-0.010380	0.043896
197	H	23	S	0.006672	0.000845	0.054351	0.041146	0.067084
198	H	23	S	-0.002338	-0.000913	-0.030644	-0.037075	-0.039188
199	H	24	S	-0.031111	-0.021684	0.041746	-0.104688	0.014939
200	H	24	S	0.003914	0.000009	-0.001962	0.044099	-0.002940
201	H	25	S	-0.057795	-0.036505	0.045089	-0.012021	-0.025457
202	H	25	S	0.038243	0.016521	-0.034352	0.039422	0.001753
203	H	26	S	-0.022070	-0.000755	-0.000547	0.093628	0.011229
204	H	26	S	0.009999	-0.001789	-0.008804	-0.054144	-0.015584
205	H	27	S	0.053410	0.031249	-0.086135	-0.010065	-0.053115
206	H	27	S	-0.004709	-0.016726	0.024981	0.020661	0.033818
207	H	28	S	0.108637	-0.008479	-0.034614	-0.037849	0.043061
208	H	28	S	-0.009727	0.018489	-0.024510	0.000704	0.006146
209	H	29	S	0.051205	-0.076664	-0.022271	0.006023	0.032817
210	H	29	S	-0.016006	0.034937	0.015384	-0.003807	-0.009310
211	H	30	S	0.046752	0.062474	0.070936	-0.006023	-0.040592
212	H	30	S	-0.023886	-0.033945	-0.035016	0.001864	0.018655
213	H	31	S	-0.035072	0.057846	-0.039418	-0.010403	0.042244
214	H	31	S	0.019866	-0.026203	0.018744	-0.000540	-0.020812
215	H	32	S	-0.021302	-0.071599	-0.053731	0.002628	0.041694

216	H	32	S	-0.002776	0.050074	0.018504	-0.009589	-0.016395
217	H	33	S	0.103965	-0.182401	0.015630	0.023931	-0.024534
218	H	33	S	0.010199	-0.005128	0.001977	-0.000499	0.001106
219	H	34	S	0.022779	0.005980	0.031376	0.025623	0.097463
220	H	34	S	0.002344	-0.001269	-0.000769	0.001036	0.009244
221	H	35	S	0.009415	-0.002187	0.014240	-0.114190	0.037454
222	H	35	S	0.000743	0.000208	0.007406	-0.020498	0.005211

21	22	23	24	25
-0.8399	-0.8208	-0.8064	-0.7946	-0.7821
A	A	A	A	A

1	CO	1	S	0.010760	-0.046435	-0.000676	-0.027719	0.006760
2	CO	1	X	-0.009738	0.043743	0.009397	0.023420	0.017900
3	CO	1	Y	0.004000	-0.005911	-0.000398	0.014688	0.047545
4	CO	1	Z	0.000528	-0.004086	0.009998	-0.006716	-0.011357
5	CO	1	XX	0.019545	0.040931	-0.017603	0.066439	0.050498
6	CO	1	YY	-0.020728	-0.005754	-0.015133	-0.038016	-0.059747
7	CO	1	ZZ	0.001184	-0.035177	0.032736	-0.028423	0.009249
8	CO	1	XY	0.004095	-0.009267	0.036980	-0.002364	0.019724
9	CO	1	XZ	0.004822	-0.016435	-0.023152	-0.032841	-0.015391
10	CO	1	YZ	0.007459	-0.011937	-0.014397	-0.028564	0.020512
11	CO	1	XX	0.014515	0.024983	-0.008455	0.041378	0.031246
12	CO	1	YY	-0.013953	-0.003991	-0.010687	-0.025335	-0.035771
13	CO	1	ZZ	-0.000562	-0.020992	0.019141	-0.016044	0.004525
14	CO	1	XY	0.005116	-0.001888	0.020624	0.000852	0.013486
15	CO	1	XZ	0.001919	-0.010757	-0.013130	-0.020298	-0.010596
16	CO	1	YZ	0.003530	-0.005527	-0.007163	-0.014902	0.010681
17	CO	1	S	-0.019687	0.118647	0.004189	0.068459	-0.014872
18	CO	1	X	0.003234	-0.023416	0.003841	-0.017424	0.014140
19	CO	1	Y	0.001763	0.025119	0.017472	-0.003210	-0.028214
20	CO	1	Z	0.003715	-0.011204	-0.034863	0.002025	0.007836
21	CO	1	S	-0.003477	0.005570	0.013473	-0.021565	-0.006083
22	CO	1	X	-0.000710	0.009036	0.004635	0.000237	-0.003091
23	CO	1	Y	0.004835	0.004768	0.010492	-0.005739	-0.004760
24	CO	1	Z	-0.001850	-0.004378	-0.008872	0.008440	0.001230
25	CO	1	S	0.010497	-0.036092	0.000899	-0.022474	0.007196
26	CO	1	X	-0.000825	-0.003485	-0.000347	-0.000725	-0.004751
27	CO	1	Y	-0.000950	-0.001696	-0.001620	-0.003010	-0.003245
28	CO	1	Z	-0.000098	0.001895	0.001231	0.000526	0.000506
29	CO	1	XX	0.005965	0.009413	-0.025383	0.017995	0.005224
30	CO	1	YY	-0.004149	0.001298	-0.001131	-0.007843	-0.006222
31	CO	1	ZZ	-0.001816	-0.010712	0.026514	-0.010152	0.000998
32	CO	1	XY	0.003836	-0.018980	0.007675	-0.005368	0.003286
33	CO	1	XZ	0.004557	-0.005418	-0.008012	-0.003517	-0.000031
34	CO	1	YZ	0.004396	0.002037	-0.015722	-0.007068	0.011265
35	C	2	S	0.076289	-0.031377	-0.097318	-0.028788	-0.053428

36	C	2	X	0.057760	-0.053334	-0.054204	0.090056	-0.005697
37	C	2	Y	0.002793	0.010103	0.038594	-0.029402	-0.064529
38	C	2	Z	0.002219	0.001763	0.006284	-0.005541	-0.017607
39	C	2	S	0.036554	-0.068410	-0.007431	0.064518	-0.118403
40	C	2	X	-0.008701	0.026869	-0.031171	-0.025829	0.023289
41	C	2	Y	0.014326	0.022386	0.000228	-0.039046	-0.038333
42	C	2	Z	0.004385	0.006393	0.000168	-0.011164	-0.009383
43	C	3	S	0.038479	-0.050156	-0.014412	0.134891	0.046111
44	C	3	X	0.038192	-0.035488	-0.051641	0.081446	-0.011704
45	C	3	Y	0.033506	-0.017531	-0.080116	-0.020227	0.015551
46	C	3	Z	0.010856	-0.005623	-0.029110	-0.002083	0.005593
47	C	3	S	-0.025808	0.075045	-0.031935	-0.041127	-0.006399
48	C	3	X	0.033081	-0.049295	0.027083	0.056718	-0.007486
49	C	3	Y	0.008147	0.009880	0.001936	-0.030186	0.002160
50	C	3	Z	0.002940	0.000809	0.001165	-0.006496	0.000467
51	C	4	S	-0.043354	0.035622	0.086016	-0.051026	-0.071363
52	C	4	X	-0.012706	-0.003668	0.048174	0.060307	0.015426
53	C	4	Y	-0.012192	0.007335	0.040745	-0.036998	0.072967
54	C	4	Z	-0.003296	0.003625	-0.004007	-0.004593	0.028832
55	C	4	S	0.092411	-0.117635	0.128070	0.047686	-0.081262
56	C	4	X	-0.002075	0.004685	-0.008774	-0.006232	0.021061
57	C	4	Y	0.049830	-0.065606	-0.001457	0.006031	-0.006801
58	C	4	Z	0.015512	-0.019910	-0.001293	0.002656	-0.000108
59	C	5	S	0.074763	-0.045498	0.018503	0.038453	0.012991
60	C	5	X	-0.082436	0.065104	0.010120	-0.163280	0.029114
61	C	5	Y	-0.042916	0.022144	0.091052	-0.080867	0.106148
62	C	5	Z	-0.012521	0.017804	-0.049104	-0.017482	0.055256
63	C	5	S	-0.061047	0.060268	0.213953	0.119872	0.118153
64	C	5	X	-0.062624	0.092070	-0.077545	-0.004501	0.069162
65	C	5	Y	-0.025396	0.031262	0.174911	0.084802	0.027590
66	C	5	Z	-0.010363	0.017114	0.032581	0.030674	0.016462
67	C	6	S	-0.073825	0.019924	-0.075426	-0.011554	0.065310
68	C	6	X	-0.121579	0.087027	0.068168	-0.090280	0.080813
69	C	6	Y	-0.050372	0.017405	-0.053454	0.049047	-0.077917
70	C	6	Z	-0.014368	0.010338	-0.041398	0.011058	-0.026237
71	C	6	S	-0.013599	-0.042828	-0.226055	0.044589	0.119096
72	C	6	X	0.069333	-0.114416	-0.050213	-0.030596	-0.081255
73	C	6	Y	-0.008490	-0.005986	0.208041	0.166490	0.106814
74	C	6	Z	-0.002678	-0.003434	0.069236	0.050810	0.031477
75	C	7	S	-0.095834	0.072355	0.067342	-0.036734	-0.041004
76	C	7	X	0.070747	-0.021936	0.023887	-0.050021	-0.042227
77	C	7	Y	0.089137	-0.065295	0.049426	0.124026	-0.050915
78	C	7	Z	0.025575	-0.017026	0.006797	0.032642	-0.016388
79	C	7	S	0.011357	0.049602	-0.079522	-0.048185	0.050661
80	C	7	X	-0.035171	0.005074	0.008251	0.021005	0.112313
81	C	7	Y	0.058612	-0.095369	-0.072790	0.065945	-0.020144

82	C	7	Z	0.014895	-0.025250	-0.024026	0.018766	-0.003866
83	C	8	S	0.148490	-0.096834	0.066503	0.090852	0.065377
84	C	8	X	0.031063	-0.020102	0.058521	0.029106	-0.018805
85	C	8	Y	0.032825	-0.017489	-0.046952	-0.062247	0.079948
86	C	8	Z	0.009268	-0.004515	-0.014166	-0.017640	0.020746
87	C	8	S	-0.083217	0.107620	0.064137	-0.115867	0.071046
88	C	8	X	0.062197	-0.042807	0.052726	0.046631	-0.044093
89	C	8	Y	0.049922	-0.046348	-0.016076	0.033514	0.034781
90	C	8	Z	0.012661	-0.012100	-0.003926	0.008736	0.007092
91	C	9	S	-0.036234	0.050007	-0.094787	-0.162150	0.035339
92	C	9	X	0.091051	-0.064814	-0.004718	0.033671	0.088265
93	C	9	Y	0.010327	0.005415	-0.010139	-0.080132	0.050830
94	C	9	Z	0.000077	0.004198	-0.003760	-0.025256	0.009688
95	C	9	S	0.068411	-0.061246	0.071892	0.058720	-0.019701
96	C	9	X	-0.001140	-0.005529	-0.005056	0.017603	-0.052388
97	C	9	Y	-0.029058	0.043811	-0.034666	-0.084607	0.019810
98	C	9	Z	-0.004593	0.010221	-0.009074	-0.023162	0.011123
99	C	10	S	-0.082748	0.042883	0.079393	0.045187	-0.071848
100	C	10	X	-0.034332	0.018554	-0.079868	0.004648	-0.076676
101	C	10	Y	-0.059773	0.063716	-0.022604	-0.117421	-0.006144
102	C	10	Z	-0.018044	0.020809	-0.004770	-0.038599	-0.007330
103	C	10	S	0.056270	-0.003582	0.037686	0.001033	0.021765
104	C	10	X	0.012718	0.008795	-0.042356	-0.016673	0.011052
105	C	10	Y	-0.064236	0.024830	-0.029207	-0.011188	-0.075231
106	C	10	Z	-0.025871	0.010155	-0.005718	-0.002471	-0.030870
107	C	11	S	0.121003	-0.082677	-0.036089	0.030692	-0.016273
108	C	11	X	-0.034732	-0.014857	-0.101243	0.131667	-0.110741
109	C	11	Y	-0.043956	-0.011049	0.067910	0.146971	-0.006593
110	C	11	Z	-0.012695	0.009248	0.009411	0.013708	-0.023283
111	C	11	S	-0.008276	-0.066515	-0.110909	-0.109351	-0.224507
112	C	11	X	-0.006203	0.000844	-0.042654	-0.094909	-0.061513
113	C	11	Y	-0.103751	0.064835	-0.067221	-0.035028	-0.030999
114	C	11	Z	-0.025255	0.019489	-0.025442	-0.012054	-0.007555
115	N	12	S	-0.101334	0.086657	-0.019420	-0.061132	-0.073832
116	N	12	X	0.139987	-0.008306	0.023623	-0.228382	0.041556
117	N	12	Y	0.063697	-0.067962	0.046782	-0.007115	0.226666
118	N	12	Z	-0.000813	0.015865	-0.013709	-0.030072	-0.036945
119	N	12	S	-0.049719	0.072777	-0.037592	-0.109970	-0.075231
120	N	12	X	-0.013522	0.012194	-0.024041	-0.019242	0.005176
121	N	12	Y	0.031087	-0.000192	0.027408	-0.000502	0.079251
122	N	12	Z	-0.004272	-0.000167	0.002960	-0.003355	-0.015487
123	C	13	S	0.131247	-0.112457	-0.011595	0.037913	0.067222
124	C	13	X	-0.133835	0.034157	0.020220	0.138288	0.127824
125	C	13	Y	0.163624	-0.045627	0.059321	-0.071946	0.279269
126	C	13	Z	-0.062141	0.011701	-0.016246	0.030438	-0.063159
127	C	13	S	0.035925	-0.067097	-0.088432	0.018572	-0.134222

128	C	13	X	-0.020231	-0.012098	0.015039	0.001341	0.088405
129	C	13	Y	0.027455	-0.006864	0.026247	-0.046251	0.016260
130	C	13	Z	-0.014156	0.001755	-0.003578	0.011401	0.002291
131	C	14	S	-0.093132	-0.047707	-0.001324	-0.066382	-0.065821
132	C	14	X	0.093666	-0.073356	-0.039411	-0.025388	-0.155070
133	C	14	Y	0.167469	0.091344	-0.014187	-0.075230	-0.061379
134	C	14	Z	-0.053638	-0.050830	0.001429	0.019857	0.011073
135	C	14	S	0.009498	-0.049097	0.044061	-0.101930	-0.041499
136	C	14	X	-0.032306	0.029259	0.046408	-0.000475	0.107301
137	C	14	Y	-0.079289	0.045379	0.018902	0.074004	0.152965
138	C	14	Z	0.030937	-0.014495	-0.005246	-0.027347	-0.042833
139	C	15	S	-0.045048	-0.147843	0.008700	-0.013648	0.055665
140	C	15	X	0.103970	0.061739	0.002145	-0.088455	-0.071099
141	C	15	Y	-0.197132	-0.033207	0.023634	0.066360	0.077193
142	C	15	Z	0.076057	-0.005009	-0.012159	-0.045346	-0.049346
143	C	15	S	-0.119583	0.114504	0.032800	0.132733	0.221432
144	C	15	X	-0.007251	-0.068542	-0.024571	0.004898	-0.047863
145	C	15	Y	-0.005458	0.055508	-0.005071	0.049280	0.077753
146	C	15	Z	-0.002239	-0.028752	0.004000	-0.022226	-0.039867
147	C	16	S	0.061899	0.159056	-0.012980	0.089612	-0.038821
148	C	16	X	-0.030498	-0.154043	-0.010053	0.014374	0.029089
149	C	16	Y	-0.077230	-0.046794	0.020465	0.025369	0.126133
150	C	16	Z	0.025505	0.000243	-0.009486	-0.012052	-0.050639
151	C	16	S	0.055117	-0.028820	-0.011211	-0.032043	-0.033509
152	C	16	X	0.010561	-0.030330	-0.020954	-0.002314	-0.032439
153	C	16	Y	-0.001804	-0.055145	0.010693	-0.049040	-0.002057
154	C	16	Z	0.002055	0.015943	-0.008313	0.017498	-0.002011
155	C	17	S	0.043814	0.033666	0.013060	-0.105348	-0.007190
156	C	17	X	-0.035526	0.044708	0.006593	0.087653	0.074317
157	C	17	Y	-0.036494	-0.175484	-0.004047	-0.024325	0.031739
158	C	17	Z	0.010899	0.070503	0.001872	0.015540	-0.007480
159	C	17	S	-0.006168	-0.042523	-0.028278	0.049232	-0.021439
160	C	17	X	-0.042979	-0.019741	-0.012110	0.060804	-0.004188
161	C	17	Y	-0.014849	-0.029079	0.004300	0.024216	0.029587
162	C	17	Z	0.002191	0.010662	-0.001676	-0.004079	-0.011736
163	C	18	S	0.005559	-0.191661	-0.023374	0.012763	-0.040376
164	C	18	X	-0.024614	0.089835	0.006824	0.078009	0.049750
165	C	18	Y	0.026778	0.055947	-0.013315	0.057656	-0.055486
166	C	18	Z	-0.012248	-0.015223	0.005699	-0.016780	0.025533
167	C	18	S	0.173217	0.071649	-0.003541	-0.108320	-0.034893
168	C	18	X	0.067885	0.069413	0.011822	-0.031164	0.034584
169	C	18	Y	0.016449	-0.049167	-0.009596	0.014121	-0.001409
170	C	18	Z	-0.000774	0.025062	0.004136	-0.008375	0.002869
171	C	19	S	0.063497	0.220469	0.000732	0.031112	-0.027621
172	C	19	X	0.020282	0.067967	0.014147	-0.091310	0.006209
173	C	19	Y	0.096772	0.060641	-0.012417	-0.019777	-0.072568

174	C	19	Z	-0.034545	-0.019630	0.006049	-0.002062	0.028942
175	C	19	S	-0.079472	-0.030342	0.000442	0.024391	-0.048746
176	C	19	X	0.114864	0.010818	-0.005242	-0.059251	-0.011103
177	C	19	Y	0.083729	0.063961	-0.008336	-0.036614	-0.046776
178	C	19	Z	-0.022674	-0.025354	0.003337	0.008277	0.016615
179	O	20	S	0.021640	0.110699	0.015573	0.048871	0.064740
180	O	20	X	-0.108706	0.236981	0.037750	0.266033	0.192584
181	O	20	Y	0.233735	0.229591	0.019953	0.006474	0.042999
182	O	20	Z	-0.145372	-0.161475	-0.014739	-0.026808	-0.057719
183	O	20	S	0.036163	0.114042	0.030076	0.034184	0.089828
184	O	20	X	-0.049058	0.089131	0.024207	0.101834	0.080786
185	O	20	Y	0.061315	0.058576	0.012014	-0.002137	0.011997
186	O	20	Z	-0.037823	-0.049580	-0.012139	-0.008467	-0.020538
187	N	21	S	-0.012383	0.001760	-0.002879	0.018068	0.010033
188	N	21	X	0.059074	-0.047084	-0.243390	0.080500	-0.008579
189	N	21	Y	0.103567	-0.081947	0.345676	0.167537	-0.163705
190	N	21	Z	0.073548	-0.015612	-0.255531	0.168808	0.023250
191	N	21	S	-0.016109	0.018462	-0.006543	0.036545	0.023693
192	N	21	X	0.010647	-0.002086	-0.028469	0.033695	-0.007706
193	N	21	Y	0.029200	-0.013366	0.057412	0.047175	-0.032687
194	N	21	Z	0.018036	-0.008985	-0.073899	0.052062	0.009953
195	H	22	S	0.044590	-0.026432	-0.039985	0.013310	-0.037751
196	H	22	S	0.004419	-0.017182	0.005792	0.020385	0.010194
197	H	23	S	0.019625	-0.026317	-0.011009	0.081729	0.010080
198	H	23	S	-0.007025	0.011506	-0.011711	-0.011593	0.005264
199	H	24	S	-0.012128	0.010121	0.009173	-0.001542	-0.061983
200	H	24	S	0.014652	-0.022610	-0.013860	0.000351	-0.011681
201	H	25	S	0.066359	-0.044415	0.029386	0.028279	0.035797
202	H	25	S	-0.021760	0.013183	-0.022194	-0.012597	0.008674
203	H	26	S	-0.011669	0.021462	-0.037576	-0.093102	0.031465
204	H	26	S	0.007156	-0.013492	0.004414	0.021342	-0.002160
205	H	27	S	-0.023013	0.019583	0.059407	-0.012453	0.015681
206	H	27	S	0.024056	-0.002565	-0.002274	-0.010832	0.040577
207	H	28	S	0.137165	-0.059909	0.030462	-0.027769	0.177430
208	H	28	S	0.009697	0.003544	0.007636	0.010909	0.053228
209	H	29	S	0.057065	0.086389	-0.015087	0.018191	-0.089325
210	H	29	S	0.006523	-0.013851	0.001428	-0.023390	-0.026523
211	H	30	S	0.031278	0.023595	0.002993	-0.069279	-0.039339
212	H	30	S	-0.015845	-0.006398	-0.001478	0.013314	-0.003063
213	H	31	S	0.014461	-0.079521	-0.013878	-0.004889	-0.048268
214	H	31	S	0.007400	0.024111	0.006459	-0.007591	0.009912
215	H	32	S	0.068992	0.109907	-0.003640	-0.002482	-0.040056
216	H	32	S	-0.024563	-0.014812	0.004752	0.018128	0.028709
217	H	33	S	-0.139511	-0.177297	-0.018383	-0.043365	-0.064536
218	H	33	S	-0.011641	-0.008182	0.004938	-0.001205	-0.006222
219	H	34	S	-0.039608	0.006703	0.269427	-0.078021	-0.041607

220 H 34 S -0.011643 0.003016 0.028021 -0.001792 -0.000771
221 H 35 S -0.054302 0.040059 -0.251167 -0.086660 0.098634
222 H 35 S -0.002256 0.006077 -0.041644 -0.008807 0.018875

26 27 28 29 30
-0.7599 -0.7536 -0.7487 -0.7253 -0.7193
A A A A A

1 CO 1 S -0.036800 0.044990 -0.013432 0.012093 0.026974
2 CO 1 X 0.041178 0.028728 0.005629 -0.003103 -0.010988
3 CO 1 Y 0.007409 0.012397 0.004176 0.002908 0.015330
4 CO 1 Z -0.007905 -0.015031 -0.002965 0.002467 -0.016424
5 CO 1 XX 0.023007 -0.014041 0.003080 -0.009720 0.004335
6 CO 1 YY -0.006920 -0.007172 0.000585 -0.000555 -0.037608
7 CO 1 ZZ -0.016087 0.021213 -0.003665 0.010275 0.033273
8 CO 1 XY 0.037673 -0.003482 -0.012814 -0.021819 0.011107
9 CO 1 XZ -0.031856 0.050993 -0.002635 0.022085 -0.036306
10 CO 1 YZ -0.026447 0.022136 0.019520 0.018867 0.000716
11 CO 1 XX 0.016375 -0.009330 -0.000770 -0.007032 0.002915
12 CO 1 YY -0.005949 -0.004207 0.001934 -0.000040 -0.023489
13 CO 1 ZZ -0.010425 0.013537 -0.001164 0.007071 0.020574
14 CO 1 XY 0.023434 -0.002898 -0.006620 -0.014382 0.004906
15 CO 1 XZ -0.017781 0.027741 -0.002731 0.012434 -0.022457
16 CO 1 YZ -0.012374 0.009199 0.011601 0.009776 0.000327
17 CO 1 S 0.094501 -0.118528 0.035109 -0.037557 -0.070053
18 CO 1 X 0.005972 -0.038011 -0.018694 -0.000933 0.001940
19 CO 1 Y 0.025333 -0.019740 0.001606 -0.007307 -0.008465
20 CO 1 Z -0.015442 -0.000711 0.006316 0.012179 0.024702
21 CO 1 S -0.006758 0.002076 -0.002214 -0.006655 -0.013697
22 CO 1 X 0.010872 0.003458 0.000063 -0.005342 -0.003450
23 CO 1 Y -0.001839 0.002279 -0.006713 -0.006667 0.001590
24 CO 1 Z -0.005064 -0.005369 0.001629 -0.000546 0.010559
25 CO 1 S -0.029000 0.037100 -0.012013 0.006587 0.022006
26 CO 1 X -0.005529 0.001140 0.001762 0.000064 0.003944
27 CO 1 Y -0.003830 -0.000062 -0.000269 -0.001188 -0.001146
28 CO 1 Z 0.002659 0.000261 0.000281 -0.000712 -0.000202
29 CO 1 XX -0.017784 -0.017088 0.011602 0.004535 0.000373
30 CO 1 YY 0.014480 -0.002665 -0.000489 0.000427 -0.002900
31 CO 1 ZZ 0.003304 0.019754 -0.011113 -0.004961 0.002528
32 CO 1 XY 0.008834 -0.015406 -0.011656 0.003858 0.001771
33 CO 1 XZ -0.010716 0.018249 0.002020 0.005722 0.002262
34 CO 1 YZ -0.010476 0.005855 0.000686 0.003842 0.002089
35 C 2 S 0.119882 0.159702 -0.069421 0.045283 0.008540
36 C 2 X -0.018138 0.103250 -0.004490 0.084926 -0.037430
37 C 2 Y 0.088724 -0.025119 -0.072999 0.176998 0.014713
38 C 2 Z 0.023237 -0.008389 -0.018462 0.048455 0.001771
39 C 2 S 0.108686 -0.001914 -0.199765 -0.052445 0.132626

40	C	2	X	-0.026569	0.018786	0.021959	-0.002200	-0.027070
41	C	2	Y	0.044177	-0.067742	0.040524	0.077507	-0.042774
42	C	2	Z	0.010692	-0.017494	0.010662	0.020875	-0.011788
43	C	3	S	-0.144319	-0.102367	0.047911	-0.051639	-0.009301
44	C	3	X	-0.048681	0.001416	-0.048163	0.061045	0.015029
45	C	3	Y	0.022051	0.165267	0.028280	-0.110936	-0.023538
46	C	3	Z	0.002965	0.039602	0.009159	-0.029890	-0.007996
47	C	3	S	0.009144	-0.062377	0.072814	0.017433	-0.077640
48	C	3	X	-0.025733	-0.012343	-0.018934	-0.004056	0.015044
49	C	3	Y	0.023827	-0.007793	0.066806	0.070400	-0.040457
50	C	3	Z	0.004705	-0.001913	0.020685	0.018127	-0.011692
51	C	4	S	0.114989	0.004204	-0.075847	0.073787	0.012403
52	C	4	X	-0.063605	-0.201861	-0.019058	0.085272	0.040243
53	C	4	Y	-0.063731	0.030311	0.169252	-0.128885	-0.078104
54	C	4	Z	-0.026801	-0.022819	0.059731	-0.034624	-0.027392
55	C	4	S	0.043762	0.244660	-0.093521	-0.107584	-0.026433
56	C	4	X	-0.005699	-0.108586	0.059897	0.128993	0.006948
57	C	4	Y	-0.001953	0.052774	-0.028516	0.003086	0.027574
58	C	4	Z	-0.001033	0.001290	-0.008663	0.011137	0.009953
59	C	5	S	-0.051143	0.070515	0.078613	-0.023291	-0.044660
60	C	5	X	0.091406	0.171251	0.084108	-0.034145	-0.065215
61	C	5	Y	-0.032891	-0.022192	0.154974	0.166543	-0.053230
62	C	5	Z	-0.016867	-0.074595	0.077331	0.057297	-0.033972
63	C	5	S	-0.218658	-0.057342	0.229490	0.049368	-0.201230
64	C	5	X	-0.041338	-0.276355	0.066798	0.092405	0.046435
65	C	5	Y	-0.100201	0.070369	0.035627	-0.183222	-0.099375
66	C	5	Z	-0.036618	0.003800	0.026451	-0.059160	-0.037260
67	C	6	S	-0.005429	0.013604	-0.006207	0.155517	0.012625
68	C	6	X	-0.103038	-0.080568	0.074040	-0.167256	0.021543
69	C	6	Y	0.035875	0.045256	-0.161250	-0.135102	0.064233
70	C	6	Z	0.014319	-0.018147	-0.032400	-0.047038	0.008300
71	C	6	S	-0.099761	0.037498	-0.117566	0.390319	0.073624
72	C	6	X	0.155285	0.347757	-0.043477	-0.201507	0.018653
73	C	6	Y	-0.237468	0.141155	0.092434	-0.080467	-0.183256
74	C	6	Z	-0.075612	0.045430	0.021133	-0.023104	-0.055184
75	C	7	S	-0.023412	-0.172774	-0.092320	-0.093820	0.059318
76	C	7	X	0.101054	0.011643	0.008141	0.129619	-0.012227
77	C	7	Y	-0.039318	-0.034494	0.014909	0.075035	-0.062250
78	C	7	Z	-0.007838	-0.018152	0.007538	0.018659	-0.020409
79	C	7	S	0.016301	-0.228784	0.017853	0.043205	0.118151
80	C	7	X	-0.134637	0.164903	0.070845	-0.050951	-0.085078
81	C	7	Y	0.088605	0.181667	-0.094760	-0.053965	0.100215
82	C	7	Z	0.025011	0.044274	-0.022368	-0.016178	0.024698
83	C	8	S	-0.072980	0.022021	0.171754	0.060877	-0.067705
84	C	8	X	0.001241	-0.065228	0.076084	0.220608	-0.050801
85	C	8	Y	0.040994	0.118406	0.081279	0.049959	0.014699

86	C	8	Z	0.011769	0.028617	0.024713	0.013444	0.001812
87	C	8	S	-0.117538	-0.154297	0.093340	-0.034937	-0.111719
88	C	8	X	0.038394	-0.031318	0.004983	0.081079	0.014518
89	C	8	Y	0.016415	0.031617	-0.002426	-0.027560	0.055358
90	C	8	Z	0.003420	0.011288	-0.000793	-0.007224	0.015867
91	C	9	S	0.090001	0.025662	-0.114859	-0.055840	0.080331
92	C	9	X	-0.028265	0.125000	0.110384	-0.076213	0.010618
93	C	9	Y	0.051477	-0.027634	-0.004550	0.110338	0.070397
94	C	9	Z	0.014901	-0.015559	0.000795	0.031550	0.016359
95	C	9	S	0.051080	-0.006843	-0.028405	0.007367	0.035713
96	C	9	X	0.019712	0.037486	0.014064	0.077207	-0.020042
97	C	9	Y	0.008533	-0.014385	-0.007919	-0.025646	0.000484
98	C	9	Z	0.003668	-0.008252	-0.003553	-0.007842	-0.002112
99	C	10	S	-0.054493	-0.092456	0.073427	0.079773	-0.080286
100	C	10	X	0.052237	0.097089	-0.133232	-0.122890	-0.000540
101	C	10	Y	0.043644	-0.164422	-0.119673	0.104856	0.025367
102	C	10	Z	0.008294	-0.065903	-0.012358	0.032613	-0.001450
103	C	10	S	-0.017818	0.096424	0.121832	-0.096741	-0.081452
104	C	10	X	-0.005001	0.001713	-0.015708	0.053022	0.005058
105	C	10	Y	0.016831	-0.019058	-0.023301	0.127937	-0.000989
106	C	10	Z	0.000262	-0.003726	-0.002351	0.031277	0.002540
107	C	11	S	0.074809	0.133340	0.029203	-0.011997	0.015896
108	C	11	X	0.060787	0.108604	-0.108414	0.126008	-0.041912
109	C	11	Y	-0.106276	0.107523	0.105778	-0.065047	-0.043918
110	C	11	Z	-0.027543	-0.012344	0.071826	-0.050601	-0.027055
111	C	11	S	0.281568	0.180515	-0.071230	-0.030410	0.058940
112	C	11	X	0.131946	0.050203	0.018930	-0.218414	0.065581
113	C	11	Y	-0.029347	-0.134531	-0.090024	0.158332	0.037340
114	C	11	Z	-0.005773	-0.053958	-0.006920	0.048328	0.001322
115	N	12	S	-0.046629	-0.042587	-0.017182	-0.043132	-0.045085
116	N	12	X	0.109089	-0.160012	0.011024	-0.128549	0.033191
117	N	12	Y	-0.063990	0.077262	-0.019783	-0.021624	0.161681
118	N	12	Z	-0.005789	-0.041508	0.094165	-0.045296	-0.000303
119	N	12	S	-0.044842	-0.063197	-0.041026	-0.114079	-0.069847
120	N	12	X	-0.004853	-0.022876	-0.017233	-0.002863	0.021409
121	N	12	Y	0.016537	0.019317	0.005493	-0.046593	0.049776
122	N	12	Z	-0.006829	0.000797	0.040386	-0.027995	0.003692
123	C	13	S	0.104541	0.005195	-0.031161	0.017921	0.007991
124	C	13	X	-0.152079	0.131334	-0.105367	0.090495	0.076765
125	C	13	Y	0.034496	-0.061509	-0.134354	-0.042754	0.110201
126	C	13	Z	-0.043453	0.022027	0.080425	0.010364	0.027794
127	C	13	S	0.109012	-0.034102	-0.097042	0.107042	-0.252784
128	C	13	X	-0.013278	0.009224	0.079157	-0.041579	0.191510
129	C	13	Y	-0.015876	-0.000231	0.028176	-0.077986	-0.016180
130	C	13	Z	-0.003318	-0.001108	0.016344	0.029570	0.036173
131	C	14	S	-0.020305	-0.017516	0.067220	-0.033785	0.020556

132	C	14	X	0.155381	-0.050183	0.145846	-0.019415	0.001801
133	C	14	Y	-0.013618	-0.038921	-0.035594	-0.043933	-0.178981
134	C	14	Z	0.008170	0.004625	0.045969	0.016767	0.153333
135	C	14	S	-0.061924	0.014452	0.169899	-0.072996	0.209365
136	C	14	X	-0.069704	0.048328	0.057159	-0.083991	0.151300
137	C	14	Y	-0.016428	0.005844	0.025682	-0.020282	0.251293
138	C	14	Z	-0.000499	0.002380	-0.011851	-0.006095	-0.056965
139	C	15	S	0.007090	-0.021775	-0.028585	-0.009212	0.042388
140	C	15	X	-0.148718	0.053406	0.016450	0.049243	0.113485
141	C	15	Y	0.007466	0.031847	0.050637	0.030551	0.251395
142	C	15	Z	-0.044437	-0.009985	-0.001834	0.010401	0.084112
143	C	15	S	0.010356	0.039966	0.022259	-0.021752	0.350655
144	C	15	X	0.075520	-0.055713	0.003593	0.000587	-0.080434
145	C	15	Y	-0.006590	-0.011875	-0.036256	0.000991	0.014598
146	C	15	Z	0.003182	0.002276	0.023986	0.004717	0.014406
147	C	16	S	0.127929	-0.012457	0.091535	-0.017656	0.029055
148	C	16	X	0.122277	-0.078478	-0.018135	-0.071157	-0.143817
149	C	16	Y	-0.018441	0.014464	-0.131884	0.036405	-0.091826
150	C	16	Z	0.007515	-0.012249	0.055171	-0.013385	0.087655
151	C	16	S	0.074794	-0.070308	-0.014579	-0.019011	-0.119763
152	C	16	X	0.009281	-0.025012	-0.010109	0.000725	-0.098680
153	C	16	Y	-0.025143	-0.006247	-0.018926	0.001752	-0.017191
154	C	16	Z	0.008127	-0.001195	0.004716	0.001314	0.015932
155	C	17	S	-0.169753	0.032488	-0.080259	0.025144	-0.026888
156	C	17	X	0.081355	0.018821	-0.035730	0.040314	-0.077498
157	C	17	Y	0.076443	-0.060673	-0.034351	-0.050280	-0.146164
158	C	17	Z	-0.026289	0.024903	0.012669	0.025085	0.076570
159	C	17	S	0.052986	-0.004514	0.014018	-0.002750	-0.048443
160	C	17	X	0.040934	0.005783	0.024921	0.006474	0.003650
161	C	17	Y	0.057206	-0.009906	0.005573	-0.017214	0.010522
162	C	17	Z	-0.018587	0.004645	0.001564	0.007133	-0.003837
163	C	18	S	0.173359	-0.064272	0.095725	-0.044128	0.015870
164	C	18	X	-0.037846	0.066665	-0.055734	0.086031	-0.018680
165	C	18	Y	0.073018	0.005445	0.115966	0.006469	0.179626
166	C	18	Z	-0.033168	0.002734	-0.047587	0.005340	-0.053549
167	C	18	S	-0.020699	-0.029951	-0.026522	0.003249	-0.056607
168	C	18	X	-0.010752	-0.001904	-0.034420	0.002795	-0.004645
169	C	18	Y	0.067635	-0.013513	0.010604	-0.011743	-0.020177
170	C	18	Z	-0.028568	0.005323	-0.008158	0.005382	0.013017
171	C	19	S	-0.130378	0.065736	-0.037877	0.047033	0.004395
172	C	19	X	-0.128951	-0.009661	-0.083959	-0.044633	-0.122658
173	C	19	Y	-0.000549	-0.006853	0.050878	-0.005196	0.079419
174	C	19	Z	-0.013833	-0.000169	-0.020956	-0.001016	-0.008862
175	C	19	S	-0.059090	0.048154	0.022079	-0.016688	-0.057585
176	C	19	X	0.021092	-0.018248	-0.036842	-0.012659	-0.104854
177	C	19	Y	-0.008938	-0.016637	-0.001003	0.024339	-0.008790

178	C	19	Z	0.005813	0.003302	0.001689	-0.009232	-0.004116
179	O	20	S	0.039278	0.013895	-0.016519	-0.005560	-0.018095
180	O	20	X	0.326142	-0.036959	0.081475	-0.073894	0.034144
181	O	20	Y	-0.021668	0.010656	-0.032563	0.011845	0.112611
182	O	20	Z	-0.060580	-0.003314	0.048035	0.044083	0.335212
183	O	20	S	0.021412	0.031753	-0.048099	-0.005856	-0.033554
184	O	20	X	0.147746	0.001385	0.037586	-0.031206	0.032293
185	O	20	Y	-0.013096	0.012768	-0.012780	0.014422	0.067442
186	O	20	Z	-0.029289	-0.004227	0.019850	0.017820	0.144375
187	N	21	S	-0.028478	-0.062595	-0.000932	-0.034011	0.015205
188	N	21	X	-0.078059	0.016632	-0.070782	-0.060837	0.044143
189	N	21	Y	-0.013387	-0.021411	-0.160546	-0.148615	0.074983
190	N	21	Z	-0.085165	-0.264739	-0.018347	-0.065060	0.023486
191	N	21	S	-0.062766	-0.101456	0.012548	-0.076923	0.034744
192	N	21	X	-0.016468	0.027174	-0.041737	-0.066690	0.005166
193	N	21	Y	-0.019041	-0.042819	-0.046374	-0.035484	0.040444
194	N	21	Z	-0.037216	-0.105972	-0.007634	-0.024430	0.019614
195	H	22	S	0.065013	0.096005	-0.046239	0.117830	-0.009806
196	H	22	S	0.000152	0.037544	-0.009653	0.022345	0.008334
197	H	23	S	-0.079808	-0.070509	-0.007286	0.031376	0.008562
198	H	23	S	-0.001182	-0.002933	0.009705	0.028226	-0.003770
199	H	24	S	0.078121	-0.026247	-0.128231	0.120345	0.057667
200	H	24	S	0.013241	0.003694	-0.052613	0.045908	0.037296
201	H	25	S	-0.013767	0.020816	0.120428	0.139988	-0.047604
202	H	25	S	-0.010094	0.027300	0.016723	0.024499	-0.024800
203	H	26	S	0.060018	-0.009425	-0.051816	0.040042	0.070611
204	H	26	S	0.004422	0.008334	-0.004073	0.033408	0.014241
205	H	27	S	-0.035412	-0.132021	0.059667	0.128601	-0.022541
206	H	27	S	-0.003890	-0.050224	-0.008917	0.044984	0.008840
207	H	28	S	0.072032	-0.046651	-0.093271	-0.011509	0.061904
208	H	28	S	0.006448	-0.014064	-0.019345	0.034907	0.073841
209	H	29	S	0.050948	-0.007359	0.121377	-0.023175	0.098929
210	H	29	S	-0.013937	0.000908	0.029597	-0.004907	0.032757
211	H	30	S	-0.118734	0.016842	-0.008918	0.001984	0.061074
212	H	30	S	-0.004007	0.004813	0.011445	-0.001039	0.031515
213	H	31	S	0.105839	-0.049518	0.098167	-0.052817	0.077864
214	H	31	S	0.000871	-0.005676	0.012257	-0.012819	0.040816
215	H	32	S	-0.057099	0.021145	0.002370	0.014036	0.039430
216	H	32	S	0.000180	0.009623	0.002160	-0.012277	0.036459
217	H	33	S	-0.052573	0.004195	0.023847	0.021861	0.048152
218	H	33	S	0.002270	0.004368	0.005782	-0.001508	0.018385
219	H	34	S	0.060764	0.127289	-0.005400	0.011972	-0.008987
220	H	34	S	0.003883	0.006033	0.000257	-0.003587	0.004354
221	H	35	S	-0.011055	0.004312	0.080799	0.087290	-0.032630
222	H	35	S	-0.008775	-0.015078	0.012538	0.032409	0.001755

			31	32	33	34	35
			-0.7133	-0.7036	-0.6988	-0.6899	-0.6876
			A	A	A	A	A
1	CO 1 S		-0.021545	-0.031408	-0.024945	-0.000350	-0.012675
2	CO 1 X		-0.011732	-0.049782	0.019320	0.014965	-0.017764
3	CO 1 Y		-0.025207	0.019977	-0.001736	0.011843	0.002880
4	CO 1 Z		-0.006675	0.040227	-0.007645	-0.011385	0.018585
5	CO 1 XX		-0.013545	0.040414	0.001708	0.039883	-0.007170
6	CO 1 YY		0.014219	-0.060944	0.008307	-0.035538	-0.008936
7	CO 1 ZZ		-0.000675	0.020530	-0.010015	-0.004346	0.016106
8	CO 1 XY		-0.035752	-0.028812	0.007383	-0.009978	-0.006352
9	CO 1 XZ		-0.051567	-0.074558	-0.042432	-0.011259	-0.044859
10	CO 1 YZ		-0.009029	-0.009111	-0.033322	0.012245	-0.033843
11	CO 1 XX		-0.009737	0.022067	0.003165	0.025131	-0.004698
12	CO 1 YY		0.007751	-0.035682	0.002804	-0.021492	-0.006359
13	CO 1 ZZ		0.001985	0.013615	-0.005968	-0.003639	0.011057
14	CO 1 XY		-0.023749	-0.017838	0.002677	-0.004227	-0.006336
15	CO 1 XZ		-0.031680	-0.041863	-0.023258	-0.008073	-0.023933
16	CO 1 YZ		-0.002090	-0.002175	-0.015070	0.007058	-0.017450
17	CO 1 S		0.057193	0.080843	0.066036	0.012429	0.027724
18	CO 1 X		0.010256	0.015786	0.010763	-0.010419	-0.008523
19	CO 1 Y		0.018146	-0.016479	0.004033	-0.016290	0.000200
20	CO 1 Z		0.008261	-0.020272	-0.009459	0.002621	-0.006838
21	CO 1 S		-0.005343	0.000182	0.002306	0.013659	0.005388
22	CO 1 X		-0.004329	-0.005318	0.012556	0.005334	-0.002491
23	CO 1 Y		0.002614	-0.005852	0.005987	0.012546	0.003050
24	CO 1 Z		0.012347	0.005529	-0.003701	-0.003804	0.001827
25	CO 1 S		-0.017267	-0.028488	-0.020198	0.002756	-0.012954
26	CO 1 X		-0.001028	0.003034	-0.005258	-0.002767	0.001533
27	CO 1 Y		0.002398	-0.002477	-0.001229	0.000199	-0.001698
28	CO 1 Z		0.001424	-0.002538	0.002350	0.001315	-0.001751
29	CO 1 XX		0.002588	0.030628	-0.013986	0.010746	0.000276
30	CO 1 YY		0.000208	-0.023400	0.004935	-0.016284	-0.000538
31	CO 1 ZZ		-0.002796	-0.007227	0.009050	0.005539	0.000261
32	CO 1 XY		0.000751	0.000860	0.005108	-0.005453	0.001911
33	CO 1 XZ		-0.015700	-0.017874	-0.021263	-0.011614	-0.008299
34	CO 1 YZ		-0.002329	-0.007694	-0.009531	0.003657	-0.003438
35	C 2 S		0.014621	0.058259	0.019882	0.025626	0.007336
36	C 2 X		-0.010788	-0.168866	0.115285	0.025378	0.085760
37	C 2 Y		-0.009820	0.057695	0.018077	0.045896	0.025767
38	C 2 Z		0.001747	0.018313	0.007760	0.012827	0.007027
39	C 2 S		0.028857	0.332181	-0.216577	0.013976	-0.183523
40	C 2 X		-0.028408	-0.167636	0.087924	0.018431	0.056989
41	C 2 Y		0.013989	-0.010448	0.004620	-0.098800	0.082901
42	C 2 Z		0.003607	-0.005115	0.003941	-0.026665	0.025164
43	C 3 S		-0.021182	-0.095822	-0.011322	-0.028453	-0.005976

44	C	3	X	-0.054619	-0.232708	0.058422	0.075914	-0.030977
45	C	3	Y	0.022249	-0.043956	0.025750	-0.030828	0.016304
46	C	3	Z	0.008871	-0.007631	0.009724	-0.007536	0.007038
47	C	3	S	0.009107	-0.057570	0.062744	-0.091170	0.108132
48	C	3	X	0.004351	0.022999	-0.029577	-0.014211	-0.003102
49	C	3	Y	0.015362	-0.023361	0.022275	-0.041689	0.046639
50	C	3	Z	0.004585	-0.005846	0.005415	-0.012142	0.012785
51	C	4	S	0.019653	0.104024	0.009195	0.008684	0.025358
52	C	4	X	-0.022381	0.111622	-0.066786	0.033483	-0.059777
53	C	4	Y	0.046950	0.033320	-0.003908	-0.132773	0.109229
54	C	4	Z	0.024484	0.054925	-0.002123	-0.043745	0.046212
55	C	4	S	0.035780	-0.013151	0.036896	-0.098863	0.140248
56	C	4	X	-0.005725	0.000466	-0.027551	0.022320	-0.042751
57	C	4	Y	-0.011670	-0.035656	-0.034743	-0.009506	-0.022436
58	C	4	Z	-0.000284	0.001954	-0.013834	-0.002926	-0.006335
59	C	5	S	0.002766	-0.081238	0.034671	-0.024026	0.052581
60	C	5	X	0.043076	-0.036967	0.072137	-0.055445	0.107677
61	C	5	Y	0.001388	0.014840	0.042882	0.021068	0.066902
62	C	5	Z	0.033079	0.107938	0.023045	-0.005259	0.063156
63	C	5	S	0.024442	-0.056372	0.304425	0.048332	0.309720
64	C	5	X	-0.020589	0.089940	-0.077661	0.083221	-0.157173
65	C	5	Y	0.027451	0.017521	0.146264	-0.009102	0.158113
66	C	5	Z	0.009684	0.020168	0.048992	0.001327	0.050234
67	C	6	S	-0.025829	-0.042883	0.025793	0.062598	-0.042535
68	C	6	X	-0.019262	-0.077187	-0.016297	0.067645	-0.081383
69	C	6	Y	-0.014102	-0.021532	-0.033632	0.008799	-0.083695
70	C	6	Z	0.026529	0.019131	-0.009594	0.002787	-0.044532
71	C	6	S	-0.124731	-0.146124	0.087056	0.290181	-0.200854
72	C	6	X	0.093940	0.150055	-0.095803	-0.057126	-0.073569
73	C	6	Y	0.004794	-0.082575	0.351767	0.090287	0.305002
74	C	6	Z	0.010910	-0.019254	0.108281	0.023098	0.095735
75	C	7	S	-0.030299	-0.038401	-0.049927	-0.001569	-0.044367
76	C	7	X	0.022228	0.173161	-0.037434	-0.020311	0.016278
77	C	7	Y	0.001343	-0.108133	0.073094	-0.097191	0.176377
78	C	7	Z	0.012577	-0.015781	0.019103	-0.026536	0.038706
79	C	7	S	-0.076290	-0.153981	-0.143139	0.064644	-0.264541
80	C	7	X	-0.024720	-0.233070	0.222521	0.093788	0.119593
81	C	7	Y	0.033113	0.214417	-0.149979	0.113754	-0.290062
82	C	7	Z	0.010903	0.059659	-0.040492	0.033941	-0.083945
83	C	8	S	0.015616	-0.027160	0.025696	-0.020790	0.020751
84	C	8	X	-0.002775	0.010021	0.001257	-0.000229	-0.034606
85	C	8	Y	0.009534	0.123390	-0.046938	0.099736	-0.164868
86	C	8	Z	0.008446	0.035983	-0.012921	0.027988	-0.052277
87	C	8	S	-0.023694	-0.270740	0.196557	-0.154219	0.353184
88	C	8	X	0.010671	0.125525	-0.066726	0.002009	-0.033485
89	C	8	Y	0.003539	0.052130	-0.084763	0.055489	-0.178008

90	C	8	Z	0.001668	0.013351	-0.022383	0.015326	-0.049708
91	C	9	S	-0.016704	0.043892	-0.038462	0.024868	-0.029571
92	C	9	X	0.014291	0.063940	-0.031159	0.071287	-0.113660
93	C	9	Y	-0.038165	0.030875	-0.077932	0.091492	-0.199174
94	C	9	Z	-0.003711	0.002191	-0.021114	0.026204	-0.066181
95	C	9	S	0.037607	0.125253	-0.107374	-0.013127	-0.047094
96	C	9	X	-0.000942	0.073743	0.001575	0.030375	-0.003905
97	C	9	Y	-0.010610	-0.033788	0.038188	-0.017748	0.060217
98	C	9	Z	-0.000985	-0.010784	0.009886	-0.006092	0.016807
99	C	10	S	0.013268	-0.029550	0.034883	-0.026197	0.041846
100	C	10	X	0.028797	0.081021	0.028300	-0.053087	0.143183
101	C	10	Y	-0.041528	-0.138555	0.028984	-0.075301	0.100735
102	C	10	Z	0.006881	-0.061297	0.005418	-0.010199	-0.015703
103	C	10	S	0.048416	0.115218	0.086046	0.028832	0.089867
104	C	10	X	-0.035911	-0.009973	0.066694	0.035694	0.026590
105	C	10	Y	-0.032754	-0.004357	-0.015162	0.016820	-0.030585
106	C	10	Z	-0.003848	-0.005125	-0.007963	0.005168	-0.020543
107	C	11	S	0.011854	0.100283	-0.048733	0.005856	-0.047464
108	C	11	X	0.034763	0.071640	0.044516	-0.018062	0.025884
109	C	11	Y	0.017347	0.112012	0.001603	0.078239	-0.054919
110	C	11	Z	0.061120	-0.009482	-0.005401	0.038658	-0.101553
111	C	11	S	0.075568	0.203660	-0.249633	-0.140055	-0.213820
112	C	11	X	0.061042	0.009867	-0.189591	-0.139330	-0.043702
113	C	11	Y	-0.072795	-0.153231	-0.018927	0.001768	-0.009273
114	C	11	Z	-0.020778	-0.049941	-0.002781	0.009523	-0.024068
115	N	12	S	0.012363	-0.051248	0.034128	0.006196	0.012922
116	N	12	X	-0.002430	-0.114013	-0.044055	-0.105361	0.042890
117	N	12	Y	-0.101160	0.029127	-0.053477	0.089462	-0.022011
118	N	12	Z	0.110773	-0.090300	-0.012520	0.063881	-0.183022
119	N	12	S	0.014216	-0.078791	0.061210	0.054461	0.023402
120	N	12	X	-0.012731	-0.058872	-0.046137	-0.039904	0.038416
121	N	12	Y	-0.023087	0.015767	-0.021781	0.029815	-0.006603
122	N	12	Z	0.047715	-0.026359	-0.007849	0.029084	-0.078162
123	C	13	S	0.033568	0.008420	-0.045804	-0.049961	0.000044
124	C	13	X	-0.102666	0.094773	0.071238	0.079156	0.067523
125	C	13	Y	-0.010610	-0.044842	0.041514	-0.033307	0.087452
126	C	13	Z	0.075923	-0.031673	-0.010443	0.087543	-0.141913
127	C	13	S	0.254196	-0.053999	-0.177197	-0.067961	-0.045022
128	C	13	X	-0.104295	-0.033859	-0.075181	-0.095431	0.007707
129	C	13	Y	-0.029475	0.014448	0.054370	0.123645	0.013525
130	C	13	Z	0.009535	-0.022653	-0.027990	-0.033504	-0.037147
131	C	14	S	-0.067137	-0.013545	-0.048076	0.089666	0.048558
132	C	14	X	0.046394	-0.034940	-0.082961	-0.192069	-0.128826
133	C	14	Y	0.169630	-0.032137	0.008224	0.168463	-0.029968
134	C	14	Z	0.060246	-0.026729	0.014974	-0.033740	-0.037356
135	C	14	S	-0.197803	-0.042016	-0.173859	0.155064	0.136309

136	C	14	X	-0.168457	0.043470	0.099435	0.119569	0.095185
137	C	14	Y	-0.146255	0.015853	0.152378	-0.244675	-0.103693
138	C	14	Z	0.068935	-0.009011	-0.040735	0.111028	0.050937
139	C	15	S	-0.043840	0.037739	0.145480	-0.073752	-0.043499
140	C	15	X	-0.063030	-0.004108	-0.190502	-0.051104	0.090152
141	C	15	Y	-0.050796	-0.014036	0.010451	-0.082358	0.048874
142	C	15	Z	0.242132	-0.027126	0.046549	0.076489	0.016412
143	C	15	S	-0.244669	0.052693	0.318198	-0.311955	-0.071855
144	C	15	X	0.057049	-0.010510	0.048774	-0.091874	-0.144558
145	C	15	Y	0.035060	0.016648	0.078475	-0.163224	-0.116528
146	C	15	Z	0.032720	-0.016226	-0.014889	0.071424	0.030975
147	C	16	S	0.011856	-0.039904	-0.045720	0.015676	0.007066
148	C	16	X	0.028498	0.023664	0.212946	0.129698	-0.054674
149	C	16	Y	0.170489	0.007460	0.094965	-0.234009	-0.192261
150	C	16	Z	0.022299	-0.014114	0.006943	0.122416	0.081028
151	C	16	S	0.123610	-0.032173	0.063846	-0.090011	-0.184718
152	C	16	X	0.062469	-0.006320	-0.062323	0.021172	-0.037884
153	C	16	Y	0.025889	-0.016854	-0.032285	0.045175	0.010861
154	C	16	Z	0.016272	0.004547	0.014712	-0.013496	0.000816
155	C	17	S	0.004148	0.039645	0.062969	-0.048954	-0.048535
156	C	17	X	0.178042	-0.074649	-0.232423	-0.154115	-0.056348
157	C	17	Y	0.095268	-0.020206	0.027584	0.160559	0.012471
158	C	17	Z	0.013470	-0.004784	-0.017570	-0.063859	-0.007076
159	C	17	S	0.031365	0.029981	0.048622	-0.074019	-0.065870
160	C	17	X	-0.014903	0.012105	-0.013477	0.012391	0.020859
161	C	17	Y	0.002485	0.005983	0.100896	-0.051711	-0.047059
162	C	17	Z	-0.000553	-0.002821	-0.040207	0.023442	0.016790
163	C	18	S	-0.007904	-0.041042	-0.066807	0.047165	0.046053
164	C	18	X	0.107663	-0.024282	-0.260580	-0.101823	0.029614
165	C	18	Y	-0.099723	-0.003399	0.014025	-0.122963	-0.009477
166	C	18	Z	0.074129	-0.007389	-0.018538	0.050020	0.001924
167	C	18	S	0.119954	-0.088276	-0.266546	-0.007871	0.048693
168	C	18	X	0.064929	-0.036693	-0.060976	-0.104406	-0.040497
169	C	18	Y	0.042777	-0.002919	0.031281	-0.056221	-0.041525
170	C	18	Z	-0.004072	-0.002804	-0.014190	0.015852	0.014812
171	C	19	S	0.000055	0.036862	0.029774	-0.009535	-0.020198
172	C	19	X	-0.009312	0.034369	0.184331	0.198072	0.003341
173	C	19	Y	-0.029788	0.040741	0.238712	-0.202432	-0.192346
174	C	19	Z	0.057944	-0.027173	-0.064232	0.114453	0.059422
175	C	19	S	-0.077252	0.081661	0.110389	0.316032	0.135505
176	C	19	X	0.128038	-0.042021	-0.105479	0.017088	0.016200
177	C	19	Y	0.047516	-0.036259	-0.100643	-0.063840	-0.017379
178	C	19	Z	-0.002262	0.007656	0.029497	0.028871	0.001052
179	O	20	S	0.018327	-0.028667	-0.000601	0.026371	-0.003364
180	O	20	X	-0.021957	-0.057086	0.179673	0.093871	-0.026864
181	O	20	Y	0.275440	-0.046859	0.041606	0.103189	0.076990

182 O 20 Z 0.349842 -0.018256 0.125098 0.012655 0.087814
 183 O 20 S 0.030688 -0.043651 -0.021858 0.033114 0.007139
 184 O 20 X -0.026477 -0.046863 0.078668 0.028545 -0.019376
 185 O 20 Y 0.116822 -0.025306 0.007116 0.039025 0.042733
 186 O 20 Z 0.162506 -0.003994 0.056518 0.008130 0.041681
 187 N 21 S 0.012239 0.085009 -0.023233 0.001631 -0.004613
 188 N 21 X -0.079149 -0.229574 -0.064942 0.001854 -0.140913
 189 N 21 Y -0.006900 0.032724 -0.061408 0.032942 -0.102895
 190 N 21 Z 0.036478 0.266689 -0.032858 -0.005710 0.045190
 191 N 21 S 0.003373 0.119263 -0.060048 0.010444 -0.049753
 192 N 21 X -0.030447 -0.106891 -0.003865 0.017870 -0.075030
 193 N 21 Y -0.010418 0.028174 -0.047308 0.022281 -0.059228
 194 N 21 Z 0.015387 0.126787 -0.024854 -0.003093 0.015378
 195 H 22 S -0.000554 -0.025850 0.067655 0.041676 0.050690
 196 H 22 S 0.002932 0.028212 0.005952 0.040345 -0.019936
 197 H 23 S -0.040680 -0.148932 0.018848 0.035120 -0.024007
 198 H 23 S -0.013215 -0.057418 0.018738 0.022969 -0.011043
 199 H 24 S -0.025766 0.024180 0.000199 0.096709 -0.071095
 200 H 24 S -0.022208 -0.016881 -0.017973 0.044707 -0.053800
 201 H 25 S 0.009345 0.032268 -0.000288 0.025698 -0.061426
 202 H 25 S -0.001724 -0.034366 0.035655 0.011264 0.008627
 203 H 26 S -0.028045 0.031720 -0.059773 0.062261 -0.128459
 204 H 26 S -0.007474 0.016281 -0.025459 0.035753 -0.072191
 205 H 27 S -0.019569 -0.105501 0.012080 -0.005687 -0.034561
 206 H 27 S -0.018830 -0.057323 0.030718 0.003193 -0.000910
 207 H 28 S -0.003030 -0.024389 0.016574 -0.080480 0.071822
 208 H 28 S -0.025602 -0.015066 0.003597 -0.092769 0.012982
 209 H 29 S -0.093093 -0.028801 -0.105942 0.168032 0.151158
 210 H 29 S -0.040076 -0.014430 -0.077493 0.105068 0.087938
 211 H 30 S -0.110032 0.061599 0.146459 0.025184 0.007019
 212 H 30 S -0.048405 0.023682 0.058062 0.014171 0.012184
 213 H 31 S -0.092073 -0.007124 0.095432 0.017722 0.002971
 214 H 31 S -0.033237 -0.006412 0.030491 -0.018293 -0.007014
 215 H 32 S -0.028916 0.048163 0.186121 -0.138676 -0.135943
 216 H 32 S -0.036287 0.028200 0.118425 -0.056456 -0.057411
 217 H 33 S -0.036720 0.021972 -0.023469 -0.062447 -0.002210
 218 H 33 S -0.016704 -0.002500 0.005400 -0.005777 0.003526
 219 H 34 S 0.001804 -0.063951 0.019556 0.009694 -0.010091
 220 H 34 S 0.005608 -0.000187 0.001920 0.002388 -0.007003
 221 H 35 S -0.015661 -0.062017 0.019051 -0.016781 0.029234
 222 H 35 S 0.000196 -0.002932 0.001302 0.005103 0.009178

36 37 38 39 40
 -0.6773 -0.6663 -0.6614 -0.6422 -0.6288
 A A A A A

1 CO 1 S 0.023580 0.042057 0.000707 -0.014635 0.015436

2	CO	1	X	0.032092	0.031665	0.006608	0.018915	-0.013013
3	CO	1	Y	-0.009115	0.013677	0.001108	-0.042465	0.036500
4	CO	1	Z	-0.019533	-0.031984	-0.014021	-0.013988	0.011531
5	CO	1	XX	0.017853	0.020317	-0.004695	-0.045631	0.041964
6	CO	1	YY	0.023687	-0.013880	-0.003686	0.114075	-0.093784
7	CO	1	ZZ	-0.041541	-0.006437	0.008381	-0.068444	0.051821
8	CO	1	XY	-0.015434	0.013057	0.019313	-0.002987	0.015340
9	CO	1	XZ	0.010257	0.075224	0.057240	0.027208	0.003677
10	CO	1	YZ	-0.093176	0.050190	0.109934	-0.068370	0.086421
11	CO	1	XX	0.008170	0.012335	-0.000653	-0.029162	0.027161
12	CO	1	YY	0.012093	-0.007855	-0.000552	0.066855	-0.053927
13	CO	1	ZZ	-0.020263	-0.004481	0.001205	-0.037693	0.026766
14	CO	1	XY	-0.005158	0.010395	0.009953	-0.001110	0.009029
15	CO	1	XZ	0.007903	0.039908	0.029003	0.018750	-0.001125
16	CO	1	YZ	-0.050154	0.022431	0.055878	-0.035078	0.042851
17	CO	1	S	-0.066644	-0.112166	-0.000096	0.043702	-0.042448
18	CO	1	X	-0.029763	-0.008829	0.009276	0.001216	0.007285
19	CO	1	Y	-0.010870	-0.032842	0.004173	0.020882	-0.024643
20	CO	1	Z	0.018283	0.031832	0.012878	0.005797	-0.008482
21	CO	1	S	-0.008223	-0.016247	0.000937	0.006952	0.000995
22	CO	1	X	0.000673	-0.003258	0.005611	-0.000330	0.004601
23	CO	1	Y	0.003181	-0.004941	-0.005066	-0.001373	0.000768
24	CO	1	Z	-0.000385	0.002188	-0.002793	0.001955	-0.005959
25	CO	1	S	0.019811	0.036198	0.000567	-0.011970	0.012980
26	CO	1	X	-0.001898	-0.003863	-0.003145	-0.002838	0.001009
27	CO	1	Y	0.002417	0.001087	-0.000957	0.005846	-0.004345
28	CO	1	Z	0.000895	0.000856	0.000386	0.001677	-0.001603
29	CO	1	XX	0.004662	0.010352	-0.003970	0.005205	0.001640
30	CO	1	YY	0.000825	-0.006564	0.003139	0.013309	-0.012003
31	CO	1	ZZ	-0.005487	-0.003788	0.000831	-0.018514	0.010363
32	CO	1	XY	-0.013093	0.000386	0.014682	0.004258	-0.002666
33	CO	1	XZ	0.007842	0.016334	0.004489	-0.000909	-0.000826
34	CO	1	YZ	-0.012334	0.017105	0.022867	-0.011358	0.018372
35	C	2	S	-0.059897	-0.020199	-0.009138	0.081510	0.057591
36	C	2	X	-0.164656	-0.148555	-0.039460	-0.094255	0.070263
37	C	2	Y	-0.108873	0.157198	-0.047216	-0.097005	-0.109161
38	C	2	Z	-0.056969	0.020663	0.014311	-0.032391	-0.099775
39	C	2	S	0.093953	0.156123	0.008813	0.387353	-0.014527
40	C	2	X	-0.090006	-0.060594	-0.063477	-0.103030	0.039933
41	C	2	Y	0.102123	0.004281	0.105082	-0.045506	0.034288
42	C	2	Z	0.019139	-0.003566	0.030958	-0.016228	-0.002351
43	C	3	S	0.070146	0.024849	0.027157	-0.044616	-0.032188
44	C	3	X	-0.143149	-0.044439	-0.159562	-0.134001	-0.150486
45	C	3	Y	0.038501	-0.186917	0.025061	0.096895	0.170468
46	C	3	Z	-0.016782	-0.073686	0.020403	0.009674	-0.015449
47	C	3	S	0.113516	-0.003415	0.121581	-0.110454	0.034999

48	C	3	X	0.016619	0.002854	0.025646	0.050030	0.033934
49	C	3	Y	0.025917	-0.040101	0.042403	-0.102292	-0.037898
50	C	3	Z	0.005169	-0.013369	0.017324	-0.030641	-0.023970
51	C	4	S	-0.043642	-0.044381	0.022894	0.002675	0.050962
52	C	4	X	0.026132	0.205230	-0.001476	0.140314	0.040637
53	C	4	Y	0.161222	0.050228	0.156306	-0.158725	-0.045996
54	C	4	Z	0.004616	-0.015159	0.072253	-0.070519	-0.074238
55	C	4	S	0.092382	-0.089166	0.216398	-0.048690	0.125572
56	C	4	X	-0.045906	0.024216	-0.069327	-0.051480	-0.108421
57	C	4	Y	0.035760	-0.046727	0.012265	0.057342	0.060010
58	C	4	Z	-0.003790	-0.023696	0.003210	0.012232	0.000272
59	C	5	S	-0.027944	0.051969	-0.008411	-0.068288	-0.053627
60	C	5	X	-0.022880	-0.157093	0.020947	-0.171036	-0.045157
61	C	5	Y	-0.102374	0.180579	-0.096968	0.079972	0.049419
62	C	5	Z	-0.139022	-0.036885	0.013675	-0.028566	-0.066157
63	C	5	S	-0.372293	0.355394	-0.064915	-0.281819	-0.124145
64	C	5	X	-0.050762	0.023811	-0.173713	0.088226	-0.064189
65	C	5	Y	-0.051474	0.152193	0.083211	-0.052559	0.059371
66	C	5	Z	-0.035550	0.035113	0.026538	-0.027430	-0.009372
67	C	6	S	-0.018218	-0.049878	-0.000718	0.039692	0.035602
68	C	6	X	-0.125513	-0.046194	-0.213591	-0.001706	-0.071330
69	C	6	Y	0.133681	-0.217301	0.050803	-0.077480	0.035833
70	C	6	Z	-0.055927	-0.122015	0.124479	-0.018372	-0.140615
71	C	6	S	-0.035884	-0.267633	-0.132095	-0.085492	-0.015673
72	C	6	X	0.187785	-0.094548	0.172186	-0.029779	-0.189811
73	C	6	Y	-0.252789	0.224830	0.034194	-0.226886	0.049343
74	C	6	Z	-0.107386	0.060708	0.049121	-0.071931	-0.023996
75	C	7	S	0.021716	0.026363	-0.023544	-0.076932	-0.036740
76	C	7	X	0.062192	0.223378	0.050521	0.046738	-0.079597
77	C	7	Y	0.006369	0.047844	0.102713	-0.133357	0.112418
78	C	7	Z	-0.045791	-0.015186	0.092311	-0.032474	-0.094168
79	C	7	S	-0.050273	-0.206813	-0.240375	0.030622	0.019231
80	C	7	X	-0.147552	-0.110689	-0.019627	-0.274357	0.006772
81	C	7	Y	0.108786	-0.100845	0.010293	0.088165	-0.199972
82	C	7	Z	0.022185	-0.039468	0.012906	0.025456	-0.088852
83	C	8	S	0.029398	-0.052238	0.002481	0.074754	0.057633
84	C	8	X	0.173274	-0.042202	0.097062	-0.116739	-0.119503
85	C	8	Y	0.044378	-0.076269	-0.093099	0.148181	-0.049754
86	C	8	Z	-0.012615	-0.034427	0.012810	0.047203	-0.088466
87	C	8	S	-0.034828	0.016623	0.108273	-0.061486	0.317871
88	C	8	X	-0.037217	0.151460	-0.054961	0.077832	-0.067675
89	C	8	Y	0.057866	-0.117207	-0.004574	0.035674	-0.050988
90	C	8	Z	0.009692	-0.030968	0.007380	0.008458	-0.028876
91	C	9	S	-0.037719	0.072106	-0.005921	-0.054233	-0.019587
92	C	9	X	-0.060846	-0.074052	-0.120903	0.146899	0.048846
93	C	9	Y	0.137624	-0.121828	0.014858	-0.233439	-0.066507

94 C 9 Z 0.013065 -0.043950 0.049011 -0.054254 -0.079255
95 C 9 S -0.114383 0.192455 -0.020004 0.094550 -0.119217
96 C 9 X -0.001695 0.072777 -0.068786 -0.024457 -0.072600
97 C 9 Y 0.010252 -0.004484 0.005856 0.027058 0.074341
98 C 9 Z -0.000980 -0.006519 0.011161 0.015329 0.007293
99 C 10 S 0.024792 -0.010361 -0.032309 0.075273 -0.011802
100 C 10 X -0.078494 0.236087 0.049334 -0.035866 -0.132627
101 C 10 Y 0.070386 -0.052353 0.104052 -0.007914 0.160846
102 C 10 Z -0.030733 -0.045754 0.108107 0.026310 -0.018741
103 C 10 S -0.061766 0.170090 -0.063503 0.144495 -0.008100
104 C 10 X 0.005325 -0.013993 -0.036558 -0.000113 0.050330
105 C 10 Y 0.090331 -0.038040 -0.030366 -0.155703 -0.042957
106 C 10 Z 0.011674 -0.010503 0.012028 -0.045516 -0.028738
107 C 11 S 0.058320 0.037626 0.004995 -0.095701 -0.022934
108 C 11 X 0.113588 -0.081223 0.186822 0.057882 -0.044606
109 C 11 Y -0.028698 0.042220 -0.159434 0.008188 -0.121790
110 C 11 Z -0.148807 -0.007471 0.118885 0.049821 -0.167561
111 C 11 S 0.394781 -0.152095 0.157233 -0.133344 -0.251284
112 C 11 X 0.061295 -0.085948 0.044082 0.065109 -0.044815
113 C 11 Y 0.032030 -0.133208 -0.057026 -0.106367 0.063040
114 C 11 Z -0.011785 -0.049863 0.004933 -0.016030 -0.017143
115 N 12 S -0.005494 -0.010022 -0.013270 0.042424 -0.027195
116 N 12 X -0.037772 -0.005339 -0.109588 0.008467 -0.012909
117 N 12 Y -0.072689 0.137068 0.043585 -0.232941 0.202854
118 N 12 Z -0.209618 0.043417 0.263473 0.057777 -0.023276
119 N 12 S -0.008487 -0.005058 -0.022204 0.037965 -0.009762
120 N 12 X -0.001556 -0.014612 -0.030455 -0.013086 0.024673
121 N 12 Y -0.055301 0.033729 0.018575 -0.103952 0.098476
122 N 12 Z -0.092126 0.020256 0.115543 0.028705 -0.011796
123 C 13 S -0.016599 0.011504 0.039750 -0.003361 -0.018092
124 C 13 X 0.040318 -0.006075 0.089022 -0.005501 0.007604
125 C 13 Y -0.075662 -0.045137 0.135345 0.147566 -0.117724
126 C 13 Z -0.115190 0.069167 0.190900 -0.044337 0.147731
127 C 13 S -0.015601 0.089090 0.098379 -0.030415 -0.028675
128 C 13 X 0.000906 -0.108840 -0.082296 0.047169 0.009786
129 C 13 Y 0.024755 -0.019683 -0.012069 0.035045 -0.029288
130 C 13 Z -0.023954 -0.004318 0.038974 -0.003988 0.040611
131 C 14 S 0.004668 0.012425 -0.022131 -0.036786 0.042105
132 C 14 X -0.037220 0.033910 -0.116733 -0.082385 0.055677
133 C 14 Y 0.029163 0.052275 -0.004904 -0.050642 0.080750
134 C 14 Z -0.058315 0.022595 0.111917 0.016508 0.108878
135 C 14 S 0.007656 -0.087578 -0.062568 0.003108 0.040547
136 C 14 X 0.046701 -0.077209 -0.053275 0.043755 -0.022542
137 C 14 Y -0.037680 -0.038891 -0.042973 0.018431 0.046162
138 C 14 Z -0.000674 0.025175 0.048723 -0.001561 0.018555
139 C 15 S -0.005704 -0.011021 0.018047 0.026597 -0.031436

140	C	15	X	-0.044709	-0.041411	-0.006583	0.008715	0.001529
141	C	15	Y	-0.017273	-0.013197	0.034455	0.037066	0.003314
142	C	15	Z	0.042399	0.027083	-0.000444	-0.014071	0.067873
143	C	15	S	-0.012676	-0.077426	-0.002580	0.108265	-0.096814
144	C	15	X	-0.030320	0.056279	-0.012891	-0.055856	0.070197
145	C	15	Y	-0.020388	0.004002	-0.047776	-0.009571	0.036813
146	C	15	Z	0.017204	0.006259	0.020048	-0.001718	0.011841
147	C	16	S	0.008325	0.020601	-0.025907	-0.022003	0.021797
148	C	16	X	0.057865	0.025903	0.018116	-0.001105	-0.019199
149	C	16	Y	-0.021404	0.037861	-0.056383	-0.034214	0.037648
150	C	16	Z	0.029171	0.001255	0.035831	0.013618	0.044869
151	C	16	S	-0.020884	0.090364	-0.065660	-0.099853	0.118505
152	C	16	X	-0.008953	0.022407	-0.019171	-0.040634	0.057825
153	C	16	Y	-0.001918	0.015298	0.000500	-0.021412	0.037913
154	C	16	Z	0.005356	-0.000603	-0.002400	0.005287	0.002300
155	C	17	S	-0.006187	-0.003701	0.000214	-0.004298	0.003951
156	C	17	X	-0.039223	0.026348	-0.102194	-0.069182	0.076536
157	C	17	Y	0.046542	0.026565	-0.014062	-0.037904	0.071380
158	C	17	Z	-0.017368	0.001342	0.013926	0.010265	0.035926
159	C	17	S	0.001504	-0.001460	-0.022931	-0.004932	-0.005116
160	C	17	X	0.003876	-0.017787	0.019985	0.021802	-0.030287
161	C	17	Y	0.008917	0.005698	-0.010286	0.005602	-0.012367
162	C	17	Z	-0.004336	-0.002198	0.011532	0.000005	0.018128
163	C	18	S	0.001094	0.003988	-0.014904	-0.004754	0.005034
164	C	18	X	-0.047476	-0.043173	0.012771	0.037985	-0.059906
165	C	18	Y	-0.035767	-0.005555	0.019735	0.031097	-0.022314
166	C	18	Z	0.005169	0.009405	0.021974	-0.007304	0.069592
167	C	18	S	-0.039731	-0.007888	-0.040547	-0.006909	0.018993
168	C	18	X	-0.026677	0.000277	-0.046995	-0.008745	0.010591
169	C	18	Y	0.000076	0.007475	-0.020735	-0.001113	-0.005979
170	C	18	Z	-0.001406	0.000067	0.008644	-0.000478	0.017004
171	C	19	S	0.004643	-0.007032	0.021799	0.003619	-0.004244
172	C	19	X	0.068038	0.032919	-0.004938	-0.040741	0.051780
173	C	19	Y	-0.016920	0.044606	-0.035547	-0.054997	0.095635
174	C	19	Z	-0.005718	0.004807	0.072409	0.020907	0.060098
175	C	19	S	0.084480	-0.014938	0.075522	0.028133	-0.047389
176	C	19	X	-0.000270	-0.004609	-0.031448	0.006407	-0.017872
177	C	19	Y	-0.029872	0.003692	-0.005854	-0.008956	0.015967
178	C	19	Z	0.008324	-0.000773	0.010663	0.005532	0.015648
179	O	20	S	0.017979	0.026400	0.001279	-0.006902	0.007363
180	O	20	X	0.068909	0.062187	0.018055	0.001430	-0.007116
181	O	20	Y	0.094602	0.015273	-0.071720	-0.011108	-0.051690
182	O	20	Z	0.115144	-0.013647	-0.122334	-0.001670	-0.109458
183	O	20	S	0.020759	0.022636	-0.002799	-0.010660	0.009445
184	O	20	X	0.031447	0.034912	0.012698	-0.002312	-0.001384
185	O	20	Y	0.039492	0.005513	-0.028595	-0.004453	-0.029390

186	O	20	Z	0.057148	-0.003748	-0.061956	0.000154	-0.058843
187	N	21	S	-0.017546	-0.035215	0.009632	-0.030330	0.020653
188	N	21	X	0.232046	0.197037	0.033071	0.143309	-0.066088
189	N	21	Y	0.022183	-0.066314	0.038316	-0.001358	-0.002946
190	N	21	Z	-0.078216	-0.128588	-0.039736	-0.076052	0.084757
191	N	21	S	0.008184	-0.020719	-0.010702	-0.003834	0.027390
192	N	21	X	0.101948	0.077654	0.020823	0.080557	-0.031354
193	N	21	Y	0.027688	-0.007620	-0.016764	0.021562	0.001424
194	N	21	Z	-0.038122	-0.067211	-0.026976	-0.040308	0.041190
195	H	22	S	-0.147477	-0.024434	-0.039368	-0.050613	0.006350
196	H	22	S	-0.056060	-0.007238	-0.026368	-0.004496	-0.026728
197	H	23	S	-0.054565	0.034238	-0.086429	-0.128371	-0.156943
198	H	23	S	-0.036659	0.001885	-0.051850	-0.084490	-0.098842
199	H	24	S	-0.118265	-0.025892	-0.110025	0.151388	0.084252
200	H	24	S	-0.037071	-0.022536	-0.060620	0.115595	0.066617
201	H	25	S	0.108623	-0.077486	0.021167	0.026986	-0.067890
202	H	25	S	0.036171	-0.063509	0.017885	-0.030192	-0.019099
203	H	26	S	0.066821	-0.042842	0.021163	-0.194379	-0.071665
204	H	26	S	0.031983	-0.034767	0.004911	-0.109018	-0.058763
205	H	27	S	0.068149	-0.176819	0.012802	0.077269	0.127925
206	H	27	S	0.007378	-0.094232	0.018843	0.067101	0.097261
207	H	28	S	-0.029578	-0.059027	0.064243	0.131698	-0.129353
208	H	28	S	-0.016448	-0.042559	0.017656	0.042525	-0.021172
209	H	29	S	0.017239	-0.018664	0.032043	0.016428	-0.000181
210	H	29	S	0.003935	-0.012702	0.022943	0.006733	0.010259
211	H	30	S	0.008219	-0.024135	0.066512	0.052804	-0.066914
212	H	30	S	0.006123	-0.018241	0.036839	0.036533	-0.047746
213	H	31	S	0.009823	0.019610	-0.010670	-0.009365	0.013074
214	H	31	S	-0.003251	0.004490	-0.011886	-0.004484	0.011103
215	H	32	S	-0.001794	0.023460	-0.026641	-0.036737	0.047023
216	H	32	S	0.004359	0.007669	-0.013582	-0.008710	0.017862
217	H	33	S	-0.024544	-0.020626	-0.001025	0.006124	-0.005932
218	H	33	S	-0.002511	-0.008909	0.001362	0.003152	-0.001137
219	H	34	S	-0.019682	-0.009412	0.027510	-0.005687	-0.034893
220	H	34	S	-0.001442	-0.004733	-0.003844	0.003015	-0.015567
221	H	35	S	0.037384	0.096138	-0.026086	0.051137	-0.006082
222	H	35	S	-0.002229	0.031169	-0.033388	0.025231	0.001467

41	42	43	44	45
-0.6218	-0.6156	-0.6116	-0.6103	-0.6059

A	A	A	A	A
---	---	---	---	---

1	CO	1	S	-0.036422	-0.009902	-0.015063	-0.012671	-0.023085
2	CO	1	X	-0.001067	-0.012329	-0.004412	-0.003417	-0.011702
3	CO	1	Y	-0.014485	-0.016097	-0.015300	-0.022511	-0.001653
4	CO	1	Z	0.015339	0.013567	0.008608	-0.007539	-0.001156
5	CO	1	XX	-0.017190	0.001469	-0.021012	0.038490	-0.089741

6 CO 1 YY 0.069127 0.028582 0.053783 0.034614 -0.024750
7 CO 1 ZZ -0.051938 -0.030051 -0.032771 -0.073104 0.114491
8 CO 1 XY -0.008144 -0.061916 -0.020599 -0.122056 0.058933
9 CO 1 XZ -0.047623 0.043341 0.010045 0.025730 0.001208
10 CO 1 YZ -0.077690 0.020711 -0.029524 0.003012 0.206810
11 CO 1 XX -0.012203 -0.003640 -0.014859 0.012586 -0.042068
12 CO 1 YY 0.040475 0.018764 0.031777 0.022766 -0.013299
13 CO 1 ZZ -0.028272 -0.015124 -0.016918 -0.035352 0.055367
14 CO 1 XY -0.004396 -0.031726 -0.010342 -0.061063 0.023331
15 CO 1 XZ -0.021109 0.022435 0.007522 0.010449 -0.006117
16 CO 1 YZ -0.036494 0.009579 -0.014345 0.003510 0.102753
17 CO 1 S 0.099688 0.025387 0.038587 0.037117 0.066972
18 CO 1 X -0.003964 0.005030 -0.002199 -0.003528 0.013835
19 CO 1 Y 0.005783 0.010759 0.008016 0.013028 0.005706
20 CO 1 Z -0.015996 -0.014588 -0.007608 0.013015 0.002813
21 CO 1 S 0.001117 0.018295 0.016615 -0.000273 -0.003948
22 CO 1 X 0.003902 -0.010700 -0.001396 -0.007564 -0.000777
23 CO 1 Y -0.008108 0.004705 0.002219 0.000030 0.001104
24 CO 1 Z -0.003757 -0.002280 -0.005828 0.010056 0.010769
25 CO 1 S -0.030572 -0.008712 -0.014576 -0.010449 -0.018564
26 CO 1 X 0.000295 0.000670 0.001268 0.001230 0.000496
27 CO 1 Y 0.002826 0.002260 0.001676 0.003448 -0.000315
28 CO 1 Z -0.000598 -0.000678 -0.000425 0.000408 0.000787
29 CO 1 XX 0.000337 0.005043 0.004187 0.018595 -0.023255
30 CO 1 YY 0.012067 0.002204 0.007171 0.002302 -0.001338
31 CO 1 ZZ -0.012404 -0.007247 -0.011359 -0.020897 0.024592
32 CO 1 XY -0.003305 -0.014526 -0.004241 -0.029603 0.013836
33 CO 1 XZ -0.017940 0.006885 -0.001703 0.002605 -0.007742
34 CO 1 YZ -0.013438 0.007085 -0.006427 0.002141 0.040035
35 C 2 S -0.025503 -0.010282 -0.012385 0.024101 -0.018443
36 C 2 X 0.018770 0.002790 -0.014209 0.145348 -0.053191
37 C 2 Y 0.105383 0.010336 0.030655 0.204144 -0.118690
38 C 2 Z -0.070490 -0.015407 -0.002477 -0.028097 -0.140566
39 C 2 S -0.023912 -0.026617 -0.010557 0.057276 -0.146583
40 C 2 X -0.018476 -0.006052 -0.012262 -0.085346 0.078507
41 C 2 Y -0.004643 -0.005824 -0.012130 -0.045653 0.065141
42 C 2 Z -0.022080 -0.004804 -0.005321 -0.033327 -0.002897
43 C 3 S 0.002963 -0.000249 0.002060 -0.024680 0.012290
44 C 3 X 0.070036 0.022045 0.037146 -0.149118 0.077322
45 C 3 Y -0.058133 -0.006544 -0.032037 -0.122723 0.148195
46 C 3 Z -0.093197 -0.013855 -0.014569 -0.120708 -0.048944
47 C 3 S -0.020746 0.002541 0.001896 -0.064639 0.109392
48 C 3 X -0.007486 -0.006236 -0.014485 0.047491 -0.041136
49 C 3 Y 0.043117 0.013151 0.011536 0.009438 0.028699
50 C 3 Z -0.006664 -0.000751 0.000456 -0.014263 -0.017878
51 C 4 S -0.003759 -0.001158 -0.007018 0.051598 -0.019942

52	C	4	X	-0.031872	-0.013991	-0.016731	0.127982	-0.077781
53	C	4	Y	0.080902	0.004579	0.014624	0.198666	-0.087484
54	C	4	Z	-0.063374	-0.010243	-0.002115	-0.024072	-0.127050
55	C	4	S	-0.062197	-0.005661	-0.038813	0.058547	-0.053717
56	C	4	X	0.074046	0.009850	0.019444	0.034856	-0.023142
57	C	4	Y	-0.031293	-0.011000	-0.026460	-0.046983	0.009312
58	C	4	Z	-0.026247	-0.003198	-0.007479	-0.034666	-0.020355
59	C	5	S	0.018902	-0.003144	0.003124	-0.008624	0.001228
60	C	5	X	0.068095	0.016088	0.021749	-0.012664	0.015413
61	C	5	Y	0.019947	-0.012522	-0.015955	0.027418	0.029984
62	C	5	Z	-0.103133	-0.014421	-0.010091	-0.103896	-0.086461
63	C	5	S	0.057976	0.013363	0.064528	0.244667	-0.039728
64	C	5	X	0.070644	0.004217	0.024023	0.064224	-0.027329
65	C	5	Y	-0.025731	0.003736	0.013225	0.183520	-0.046443
66	C	5	Z	-0.038362	-0.004948	0.001681	0.024708	-0.054148
67	C	6	S	-0.022446	0.008535	-0.000091	0.010846	0.005927
68	C	6	X	0.059737	0.034068	0.030733	-0.017009	0.023679
69	C	6	Y	0.073704	0.040665	0.029448	0.075637	0.027351
70	C	6	Z	-0.151131	-0.017208	-0.005039	-0.077716	-0.114519
71	C	6	S	-0.038566	0.073758	0.074589	-0.009008	0.015466
72	C	6	X	0.080874	0.076478	0.059473	-0.139300	0.100813
73	C	6	Y	-0.033431	0.034128	0.060711	0.232315	-0.016006
74	C	6	Z	-0.060511	0.006140	0.016984	0.046098	-0.030775
75	C	7	S	0.017797	-0.012680	-0.005796	-0.013012	-0.007855
76	C	7	X	0.000775	-0.008797	0.011512	-0.062410	0.007535
77	C	7	Y	0.010923	-0.040265	-0.049838	0.091258	0.006982
78	C	7	Z	-0.158714	-0.041842	-0.030642	-0.089011	-0.149587
79	C	7	S	0.036986	-0.079826	-0.075072	-0.031736	-0.059941
80	C	7	X	-0.004941	0.055898	0.040338	-0.015237	0.111711
81	C	7	Y	0.105483	0.060401	0.068981	0.066943	-0.055141
82	C	7	Z	-0.014415	0.007148	0.013358	-0.015968	-0.062816
83	C	8	S	-0.031858	-0.005812	-0.012176	-0.030546	0.015006
84	C	8	X	0.044775	0.093185	0.070777	-0.163637	0.199469
85	C	8	Y	0.050194	0.060881	0.060002	-0.030987	0.052074
86	C	8	Z	-0.087633	-0.004131	0.003297	-0.071660	-0.077271
87	C	8	S	-0.156753	-0.049245	-0.070841	-0.095986	0.124756
88	C	8	X	0.032546	-0.025674	-0.007240	0.076910	-0.108213
89	C	8	Y	0.043116	0.001632	0.007202	0.057005	-0.048577
90	C	8	Z	-0.009141	-0.003286	-0.000644	0.003560	-0.030210
91	C	9	S	0.010363	-0.013044	-0.005023	0.019271	-0.014464
92	C	9	X	-0.013986	-0.054068	-0.037704	0.142447	-0.179164
93	C	9	Y	0.081271	0.002664	-0.004119	0.093254	-0.028275
94	C	9	Z	-0.061670	-0.017511	-0.014488	-0.010065	-0.064430
95	C	9	S	0.073619	-0.024403	-0.002194	0.099118	-0.098665
96	C	9	X	0.021253	0.015813	0.016856	-0.009117	-0.017320
97	C	9	Y	-0.037415	0.004736	-0.001771	-0.052315	0.047022

98	C	9	Z	-0.029609	-0.004175	-0.003558	-0.022292	-0.004270
99	C	10	S	0.001360	0.022604	0.015209	-0.046369	0.024448
100	C	10	X	0.036707	0.071070	0.073330	-0.151420	0.178935
101	C	10	Y	-0.054893	-0.010784	-0.022993	-0.055689	0.057136
102	C	10	Z	-0.111476	-0.030556	-0.029223	-0.011039	-0.031054
103	C	10	S	-0.001898	0.045136	0.047401	-0.060613	0.079966
104	C	10	X	-0.043072	-0.002757	0.012466	0.005710	-0.021636
105	C	10	Y	0.009367	0.009146	-0.006435	-0.039305	0.005643
106	C	10	Z	-0.020148	-0.001650	-0.009007	-0.014558	-0.002526
107	C	11	S	0.012723	-0.021334	-0.016954	-0.008794	-0.013629
108	C	11	X	0.005221	0.043245	0.043623	0.038737	0.003826
109	C	11	Y	0.108943	0.055793	0.052608	0.030230	-0.001573
110	C	11	Z	-0.076705	-0.007224	0.004640	0.028371	0.001308
111	C	11	S	0.111563	0.019548	0.001438	-0.205401	0.063222
112	C	11	X	0.073533	0.004490	-0.046470	-0.151928	0.092490
113	C	11	Y	-0.025102	-0.013825	-0.038640	-0.012115	-0.029933
114	C	11	Z	-0.034873	-0.016188	-0.014316	0.006940	-0.026921
115	N	12	S	0.022068	0.050038	0.030241	0.014765	0.017874
116	N	12	X	0.042900	-0.032348	-0.003681	-0.034657	0.005472
117	N	12	Y	-0.163323	-0.079389	-0.101259	-0.100260	0.036626
118	N	12	Z	0.048279	0.008901	0.015366	0.152701	0.174842
119	N	12	S	0.024716	0.079975	0.047863	0.000478	0.043331
120	N	12	X	-0.000244	-0.016464	-0.025320	-0.025731	0.002585
121	N	12	Y	-0.058513	-0.034079	-0.052628	-0.051797	0.032010
122	N	12	Z	0.021640	0.002982	0.004427	0.070572	0.091058
123	C	13	S	0.021379	-0.043599	-0.056292	-0.028276	0.013583
124	C	13	X	-0.091844	0.047168	0.071173	0.007957	-0.005760
125	C	13	Y	0.092018	0.087298	0.132118	0.075189	0.055647
126	C	13	Z	0.063142	0.002965	-0.005348	0.016508	0.049355
127	C	13	S	0.059601	-0.108113	-0.180476	-0.054151	0.085172
128	C	13	X	0.009594	-0.007443	-0.010338	-0.015601	-0.041940
129	C	13	Y	0.016853	0.033030	0.067827	0.032307	-0.016091
130	C	13	Z	0.018147	-0.006479	-0.017546	0.006538	0.009130
131	C	14	S	-0.040940	0.057606	-0.023114	-0.010799	-0.012446
132	C	14	X	0.015684	-0.201845	-0.042234	-0.053564	0.004944
133	C	14	Y	0.034637	0.126871	-0.147710	-0.058325	-0.051469
134	C	14	Z	0.174532	0.011036	0.126808	-0.104957	-0.101394
135	C	14	S	0.004647	0.123364	-0.204081	-0.030162	-0.066635
136	C	14	X	-0.026837	-0.009341	0.176955	0.039621	-0.051568
137	C	14	Y	-0.032553	0.104583	0.053530	-0.015999	-0.034838
138	C	14	Z	0.068874	-0.012620	0.023183	-0.034500	-0.022509
139	C	15	S	0.046850	-0.066313	0.002151	-0.007685	0.007913
140	C	15	X	-0.054313	0.029470	0.163395	0.029899	0.009689
141	C	15	Y	0.007085	0.018223	0.187707	-0.008684	-0.035193
142	C	15	Z	0.096210	0.046574	-0.021487	-0.116488	-0.114001
143	C	15	S	0.069452	0.044917	-0.028754	0.005171	-0.017330

144	C	15	X	-0.042897	-0.071900	0.054372	-0.018930	0.037215
145	C	15	Y	-0.041611	0.068434	0.091927	0.000746	-0.018888
146	C	15	Z	0.039894	-0.017782	-0.022212	-0.034134	-0.032041
147	C	16	S	-0.049348	0.061022	0.006092	0.007920	-0.002442
148	C	16	X	0.077890	-0.200072	-0.110423	-0.028619	0.019747
149	C	16	Y	0.018813	0.176835	-0.144881	-0.048138	-0.062384
150	C	16	Z	0.100703	-0.030373	0.094774	-0.113376	-0.123604
151	C	16	S	-0.160816	0.119346	0.079481	0.011354	0.031693
152	C	16	X	-0.038037	-0.081882	0.112168	-0.007373	0.005591
153	C	16	Y	-0.046811	0.015018	0.077638	-0.001036	-0.000150
154	C	16	Z	0.038763	0.000427	-0.008457	-0.035620	-0.038530
155	C	17	S	0.018123	-0.057725	0.013165	-0.008980	0.000111
156	C	17	X	-0.173860	0.187955	0.181229	0.049186	-0.002601
157	C	17	Y	-0.034722	-0.157920	0.284339	-0.030686	-0.039777
158	C	17	Z	0.099288	0.128954	-0.045671	-0.105981	-0.128943
159	C	17	S	0.057429	-0.180296	0.071724	-0.020350	-0.012921
160	C	17	X	0.077276	-0.104346	-0.054677	-0.019225	-0.004767
161	C	17	Y	0.019516	0.015017	-0.028047	-0.007051	-0.012797
162	C	17	Z	0.025288	0.000107	0.019679	-0.029795	-0.034074
163	C	18	S	-0.020502	0.034881	0.013657	0.005090	-0.000270
164	C	18	X	0.166812	-0.279895	-0.116231	-0.047679	0.022790
165	C	18	Y	0.080140	0.234490	-0.247108	-0.044023	-0.055719
166	C	18	Z	0.091866	-0.060198	0.143382	-0.103846	-0.113495
167	C	18	S	-0.036423	0.057578	0.030791	0.005684	0.020430
168	C	18	X	-0.044316	0.102691	-0.000953	0.014669	0.007961
169	C	18	Y	0.025870	-0.064606	0.043289	-0.010626	-0.008218
170	C	18	Z	0.010095	0.045975	-0.003009	-0.023335	-0.029045
171	C	19	S	0.030262	-0.066567	-0.025537	-0.011372	0.000696
172	C	19	X	-0.169440	0.193345	0.123660	0.058404	-0.001232
173	C	19	Y	-0.031897	-0.077785	0.247907	-0.034051	-0.043517
174	C	19	Z	0.139765	0.111188	-0.016776	-0.104209	-0.119520
175	C	19	S	0.067500	-0.190214	0.075896	0.010792	-0.018922
176	C	19	X	0.005771	-0.055041	0.064665	0.014193	0.016129
177	C	19	Y	0.019576	0.087588	-0.128409	-0.025388	-0.004367
178	C	19	Z	0.029506	-0.022634	0.071574	-0.021098	-0.037582
179	O	20	S	-0.022505	0.034579	-0.030788	-0.006349	-0.003112
180	O	20	X	0.012055	-0.127295	-0.029857	-0.025053	0.010703
181	O	20	Y	-0.104963	0.000931	-0.080379	0.046422	0.064523
182	O	20	Z	-0.151935	-0.090745	-0.065884	0.111574	0.125107
183	O	20	S	-0.037080	0.079792	-0.046142	-0.009784	-0.011004
184	O	20	X	0.001439	-0.071060	-0.024387	-0.019778	0.006480
185	O	20	Y	-0.058088	0.001604	-0.042610	0.025699	0.034070
186	O	20	Z	-0.079608	-0.047482	-0.036956	0.060089	0.067584
187	N	21	S	0.009600	0.010695	0.003108	0.025431	0.008554
188	N	21	X	-0.043829	-0.024539	-0.005553	0.045345	-0.093244
189	N	21	Y	-0.021809	0.012455	0.004657	0.010256	-0.001441

190	N	21	Z	0.068606	0.030507	0.012380	0.031666	0.079470
191	N	21	S	0.013236	0.012730	0.008739	0.078809	-0.016112
192	N	21	X	-0.023589	-0.008857	-0.001783	0.027997	-0.051938
193	N	21	Y	0.001078	0.008140	0.003923	0.010131	-0.008297
194	N	21	Z	0.029405	0.016045	0.004148	0.017368	0.038064
195	H	22	S	0.034510	0.003056	0.001918	0.177961	-0.105915
196	H	22	S	0.031736	0.011316	0.013759	0.127861	-0.084773
197	H	23	S	0.067758	0.017076	0.035817	-0.072607	0.020099
198	H	23	S	0.044478	0.014509	0.027195	-0.050175	0.022844
199	H	24	S	-0.052702	-0.005109	-0.017998	-0.105730	0.078345
200	H	24	S	-0.050799	-0.008862	-0.021022	-0.097342	0.051538
201	H	25	S	0.021580	0.077561	0.061499	-0.128909	0.140477
202	H	25	S	0.003026	0.052707	0.038419	-0.096340	0.115608
203	H	26	S	0.049134	-0.005234	-0.006205	0.065166	-0.029738
204	H	26	S	0.038735	0.000555	0.001136	0.051959	-0.026147
205	H	27	S	-0.055129	-0.042854	-0.046486	0.072112	-0.099127
206	H	27	S	-0.040241	-0.028937	-0.014368	0.064572	-0.068344
207	H	28	S	0.074089	0.031239	0.093436	0.058275	0.029472
208	H	28	S	0.016270	0.008211	0.034469	0.023996	0.003259
209	H	29	S	-0.025436	-0.084656	0.168751	0.015040	0.008813
210	H	29	S	-0.026747	-0.060549	0.141606	0.012860	0.008038
211	H	30	S	0.144171	-0.112448	-0.204254	-0.036974	0.006358
212	H	30	S	0.100984	-0.080273	-0.136488	-0.024651	0.001139
213	H	31	S	-0.091590	0.290652	-0.058924	0.034173	-0.013168
214	H	31	S	-0.061383	0.196133	-0.041454	0.022242	-0.007484
215	H	32	S	-0.058230	-0.103826	0.202056	0.008438	0.002646
216	H	32	S	-0.038668	-0.074637	0.176336	0.013378	-0.001079
217	H	33	S	-0.001494	-0.008127	0.043237	0.022009	0.003111
218	H	33	S	-0.003264	-0.010441	0.028273	0.007347	0.001039
219	H	34	S	-0.037414	-0.003925	-0.002923	-0.028662	-0.030958
220	H	34	S	-0.014327	-0.002588	-0.004017	-0.000604	-0.012893
221	H	35	S	0.003098	-0.015856	-0.005518	0.001095	-0.023119
222	H	35	S	0.002212	-0.002773	-0.002183	0.001122	0.000344

46	47	48	49	50
-0.5928	-0.5898	-0.5850	-0.5778	-0.5605
A	A	A	A	A

1	CO	1	S	0.009468	-0.049858	-0.001961	-0.018389	0.006567
2	CO	1	X	0.010688	0.008200	0.002017	0.010807	0.009934
3	CO	1	Y	0.002299	-0.019020	0.003169	-0.018884	-0.012113
4	CO	1	Z	-0.007223	0.007630	-0.002320	-0.003486	-0.014832
5	CO	1	XX	-0.382696	-0.171557	0.082228	-0.079670	-0.020681
6	CO	1	YY	0.104186	-0.016494	-0.089839	0.051935	0.051559
7	CO	1	ZZ	0.278510	0.188051	0.007611	0.027735	-0.030878
8	CO	1	XY	0.509443	0.101491	-0.090082	0.047598	0.014422
9	CO	1	XZ	-0.245239	0.244289	0.208522	0.090840	0.021912

10	CO	1	YZ	-0.042718	0.469785	0.250154	0.100957	-0.024241
11	CO	1	XX	-0.179283	-0.082607	0.042328	-0.040792	-0.011046
12	CO	1	YY	0.049157	-0.005030	-0.046142	0.030407	0.028312
13	CO	1	ZZ	0.130126	0.087637	0.003815	0.010385	-0.017266
14	CO	1	XY	0.240082	0.047136	-0.037819	0.023445	0.007662
15	CO	1	XZ	-0.114672	0.115836	0.097758	0.046100	0.013785
16	CO	1	YZ	-0.020969	0.220198	0.115863	0.045223	-0.012409
17	CO	1	S	-0.026064	0.141716	0.007741	0.055045	-0.019082
18	CO	1	X	0.003902	-0.024777	-0.005159	-0.007994	-0.011305
19	CO	1	Y	-0.000817	0.018633	-0.004671	0.006655	0.022575
20	CO	1	Z	0.004354	-0.001886	0.008717	0.002189	0.019852
21	CO	1	S	-0.005572	-0.002627	-0.003940	0.000634	0.002551
22	CO	1	X	0.013102	-0.007501	-0.000740	-0.001651	0.004398
23	CO	1	Y	0.000771	-0.008815	0.003031	-0.003717	0.003937
24	CO	1	Z	-0.003101	0.005218	0.003565	0.002938	0.001668
25	CO	1	S	0.008939	-0.041606	0.000130	-0.014900	0.005746
26	CO	1	X	-0.003129	0.000843	0.001363	-0.000441	-0.000754
27	CO	1	Y	-0.000322	0.000779	0.000178	0.002647	0.000885
28	CO	1	Z	0.001324	0.000634	-0.000744	0.000696	0.000707
29	CO	1	XX	-0.078848	-0.034290	0.017459	-0.007040	-0.009121
30	CO	1	YY	0.023867	0.002784	-0.015524	0.006005	0.017587
31	CO	1	ZZ	0.054981	0.031507	-0.001935	0.001035	-0.008466
32	CO	1	XY	0.105029	0.014739	-0.023157	0.007924	0.003999
33	CO	1	XZ	-0.047702	0.053101	0.048654	0.019667	0.005268
34	CO	1	YZ	-0.010307	0.088148	0.052162	0.019651	-0.006179
35	C	2	S	0.002544	0.007815	-0.005802	-0.006883	0.001816
36	C	2	X	0.073456	-0.131403	0.168968	0.196095	0.016074
37	C	2	Y	0.091933	0.043733	0.113302	-0.173504	-0.029241
38	C	2	Z	0.024765	0.014761	0.055767	-0.017766	0.131754
39	C	2	S	0.050491	0.171010	0.032643	-0.424072	0.050147
40	C	2	X	-0.063900	-0.046765	-0.081198	0.164036	-0.028188
41	C	2	Y	-0.019425	-0.022900	-0.061835	0.097621	-0.023288
42	C	2	Z	-0.009915	-0.005910	-0.013973	0.038341	0.038742
43	C	3	S	-0.008946	0.010594	-0.026679	0.008741	0.001480
44	C	3	X	-0.076229	0.091152	-0.122155	-0.181107	-0.035799
45	C	3	Y	-0.084127	-0.054917	-0.118197	0.163709	-0.071121
46	C	3	Z	-0.032161	0.006974	-0.022478	0.057972	0.222267
47	C	3	S	-0.049089	-0.061234	-0.103494	0.260996	-0.046835
48	C	3	X	0.026319	-0.016327	0.055275	-0.038096	0.021702
49	C	3	Y	0.013733	-0.006796	0.002803	0.029502	-0.021654
50	C	3	Z	0.005665	0.002132	0.006700	0.010466	0.059792
51	C	4	S	0.013761	-0.020580	0.032601	0.009612	0.000577
52	C	4	X	0.077199	-0.064173	0.124443	0.139966	0.015887
53	C	4	Y	0.087506	-0.002225	0.098467	-0.080811	-0.075989
54	C	4	Z	0.020811	0.027125	0.046343	-0.001778	0.270348
55	C	4	S	-0.023978	-0.097521	0.102351	-0.075665	0.055861

56	C	4	X	0.058914	0.055605	0.035225	-0.063695	0.002079
57	C	4	Y	-0.009927	-0.013165	0.000241	-0.051474	0.014316
58	C	4	Z	-0.006949	0.006882	0.006243	-0.013243	0.093063
59	C	5	S	-0.018423	0.042761	-0.059100	0.005721	-0.009194
60	C	5	X	-0.023046	0.017911	-0.036504	-0.148380	-0.033380
61	C	5	Y	-0.028614	-0.051400	-0.080139	0.132915	-0.075702
62	C	5	Z	-0.023659	0.021669	-0.029676	0.048795	0.192413
63	C	5	S	-0.030545	0.008657	-0.099224	0.414177	-0.107407
64	C	5	X	0.083184	0.038421	0.019922	0.027453	-0.041548
65	C	5	Y	-0.031339	-0.124567	0.028518	0.243597	-0.076876
66	C	5	Z	-0.004970	-0.021623	0.009155	0.089215	0.066869
67	C	6	S	0.025082	-0.043185	0.046821	-0.009332	0.006782
68	C	6	X	0.047820	-0.098548	0.189577	0.112720	0.016226
69	C	6	Y	0.058766	-0.013252	0.143287	-0.115140	0.014012
70	C	6	Z	0.021398	-0.008075	0.059460	-0.015645	0.003404
71	C	6	S	0.102626	-0.065876	0.097595	0.000243	0.026339
72	C	6	X	0.006213	0.028619	0.185944	-0.379827	0.066885
73	C	6	Y	-0.041616	-0.169606	0.007717	0.449549	-0.074497
74	C	6	Z	-0.016820	-0.056074	0.005702	0.143608	-0.026066
75	C	7	S	-0.025031	0.039538	-0.053414	0.001762	-0.003071
76	C	7	X	-0.059165	0.130617	-0.184286	-0.180767	-0.024830
77	C	7	Y	-0.054835	0.000487	-0.183862	0.210307	-0.008668
78	C	7	Z	-0.010904	-0.007753	-0.020392	0.083089	-0.020004
79	C	7	S	-0.058866	0.160725	-0.242855	0.031736	-0.022384
80	C	7	X	-0.029667	-0.177761	0.071975	0.275436	-0.022197
81	C	7	Y	0.077932	0.120807	0.142887	-0.388113	0.051007
82	C	7	Z	0.025966	0.030388	0.052147	-0.096032	0.008688
83	C	8	S	-0.009295	-0.005415	-0.007075	-0.000960	0.000877
84	C	8	X	0.004673	-0.154304	0.113382	0.123845	0.007216
85	C	8	Y	0.063010	0.002344	0.175269	-0.222680	0.055846
86	C	8	Z	0.024879	-0.022490	0.072632	-0.047611	-0.153056
87	C	8	S	-0.086367	-0.169587	-0.096909	0.393145	-0.043631
88	C	8	X	0.019375	0.094634	-0.038292	-0.136060	0.004397
89	C	8	Y	0.009424	0.092084	-0.020651	-0.119860	0.029115
90	C	8	Z	0.004503	0.017458	-0.000462	-0.029018	-0.045847
91	C	9	S	-0.010358	0.008917	-0.023916	-0.010439	0.000920
92	C	9	X	0.013241	0.162911	-0.094210	-0.120596	-0.012875
93	C	9	Y	-0.025506	0.037344	-0.139940	0.224594	0.056276
94	C	9	Z	0.003283	-0.026283	-0.019759	0.063109	-0.243934
95	C	9	S	0.011181	0.105297	-0.044593	-0.244711	0.036055
96	C	9	X	0.022758	-0.002480	0.032534	-0.005125	-0.008580
97	C	9	Y	0.006417	-0.039419	0.046619	0.029925	0.003720
98	C	9	Z	0.002959	-0.017403	0.016112	0.007085	-0.069522
99	C	10	S	0.014733	-0.004837	0.040347	-0.004073	0.002289
100	C	10	X	-0.002732	-0.142736	0.107486	0.047291	-0.009227
101	C	10	Y	0.003586	-0.047898	0.111504	-0.165498	0.085395

102	C	10	Z	0.014854	-0.050236	0.029005	-0.062580	-0.264715
103	C	10	S	0.027138	-0.027093	0.123988	0.040413	-0.025602
104	C	10	X	0.004634	-0.010522	0.014679	0.064676	-0.042223
105	C	10	Y	0.000836	-0.040012	0.009033	0.064229	0.020767
106	C	10	Z	0.007174	-0.025602	0.004070	0.011085	-0.078756
107	C	11	S	-0.038180	0.016920	-0.049727	-0.011023	-0.012216
108	C	11	X	0.023551	0.078132	-0.083587	-0.095520	-0.014495
109	C	11	Y	0.019296	0.032208	-0.056795	0.197574	0.051307
110	C	11	Z	0.015013	-0.051329	-0.020861	0.062525	-0.186286
111	C	11	S	-0.079674	0.087873	0.041122	-0.395998	0.043042
112	C	11	X	0.040854	0.025734	0.107448	-0.270880	0.073543
113	C	11	Y	0.034744	-0.035512	-0.042942	0.089354	0.038241
114	C	11	Z	0.007814	-0.022558	-0.018399	0.038632	-0.076375
115	N	12	S	0.012015	-0.003835	0.034009	0.020729	0.016810
116	N	12	X	-0.027010	-0.041683	0.111122	0.021445	0.004449
117	N	12	Y	0.013168	-0.148654	0.070891	-0.107497	-0.026777
118	N	12	Z	-0.019025	-0.070077	-0.070428	-0.027881	0.073878
119	N	12	S	0.011834	-0.052659	0.065312	0.009570	0.043775
120	N	12	X	0.035969	-0.003538	0.043395	0.003899	0.012540
121	N	12	Y	0.013105	-0.067264	0.036904	-0.069142	-0.002085
122	N	12	Z	-0.001066	-0.031986	-0.038000	-0.018174	0.042526
123	C	13	S	0.014515	-0.010429	-0.003192	-0.012657	-0.016586
124	C	13	X	0.030536	0.021417	-0.051707	-0.024246	-0.035013
125	C	13	Y	-0.035769	-0.017470	-0.034254	0.024380	0.042198
126	C	13	Z	0.018376	-0.104483	-0.081758	-0.105650	0.134172
127	C	13	S	0.049219	0.009153	-0.010055	-0.024455	-0.011841
128	C	13	X	0.035568	0.041307	0.036250	-0.006687	0.013350
129	C	13	Y	-0.033366	-0.017547	-0.013073	0.007542	0.020763
130	C	13	Z	0.016555	-0.022651	-0.024513	-0.038696	0.047550
131	C	14	S	0.010946	-0.017651	0.006930	-0.011669	0.000422
132	C	14	X	-0.004060	-0.035706	0.067110	-0.005713	-0.001711
133	C	14	Y	0.022957	-0.015579	-0.003325	-0.022471	0.031308
134	C	14	Z	-0.002592	-0.017300	-0.014780	-0.017241	0.067210
135	C	14	S	-0.023694	-0.023842	0.052672	-0.039147	0.025503
136	C	14	X	-0.015775	0.010833	-0.009386	0.024292	-0.002953
137	C	14	Y	0.053793	0.018845	0.028081	0.002838	0.004411
138	C	14	Z	-0.018478	-0.016216	-0.015708	-0.006222	0.029005
139	C	15	S	0.008333	-0.004944	0.000292	0.006932	-0.001136
140	C	15	X	0.043951	-0.023396	-0.045620	-0.002533	-0.002334
141	C	15	Y	-0.027208	0.036004	0.011726	0.028300	-0.015769
142	C	15	Z	0.008733	0.045577	0.035997	0.028775	-0.028252
143	C	15	S	0.070935	0.041817	0.013532	0.044356	-0.019970
144	C	15	X	0.033772	-0.004885	0.010722	-0.010526	0.013343
145	C	15	Y	0.022907	0.018195	0.007698	0.013879	-0.012608
146	C	15	Z	-0.010433	0.013615	0.010954	0.006545	-0.007967
147	C	16	S	0.003638	0.004270	-0.000305	-0.002020	0.001497

148	C	16	X	-0.030744	0.006967	0.046676	-0.001078	0.013239
149	C	16	Y	0.003576	0.016303	0.015331	0.013116	-0.036835
150	C	16	Z	-0.009638	0.066017	0.053541	0.060938	-0.099202
151	C	16	S	0.019684	0.007370	0.003783	-0.017739	0.019303
152	C	16	X	0.003959	-0.017380	0.003711	-0.010707	0.003932
153	C	16	Y	0.000932	0.009407	-0.001133	0.000517	-0.002528
154	C	16	Z	-0.001564	0.016468	0.018773	0.020557	-0.038986
155	C	17	S	0.000272	-0.005805	0.002675	-0.001497	-0.000812
156	C	17	X	0.032691	-0.017440	-0.047178	-0.012901	0.004946
157	C	17	Y	-0.007557	0.025751	0.020825	0.024676	-0.043051
158	C	17	Z	0.002344	0.047666	0.034525	0.051789	-0.106875
159	C	17	S	-0.007225	-0.018082	0.007387	0.007470	-0.011549
160	C	17	X	-0.005460	-0.005587	0.009175	0.003403	-0.003054
161	C	17	Y	-0.006499	0.017026	0.008346	0.013000	-0.011924
162	C	17	Z	0.001634	0.008186	0.008827	0.011787	-0.031060
163	C	18	S	0.003737	-0.002505	-0.000243	0.001783	0.000249
164	C	18	X	-0.022468	-0.013728	0.051285	0.007143	0.008687
165	C	18	Y	0.004821	0.009911	0.006084	0.011239	-0.025793
166	C	18	Z	-0.004165	0.033297	0.030309	0.038680	-0.071229
167	C	18	S	0.008154	-0.008269	0.009407	-0.004890	0.013559
168	C	18	X	0.005690	0.000953	0.002193	-0.001117	0.008069
169	C	18	Y	-0.008635	0.004014	0.006655	0.013263	-0.008402
170	C	18	Z	0.003554	0.008734	0.006241	0.007209	-0.021062
171	C	19	S	-0.000428	0.002692	0.000524	-0.004570	0.000416
172	C	19	X	0.025185	0.011811	-0.056306	-0.014000	-0.001611
173	C	19	Y	-0.003294	-0.001998	0.007111	0.003558	-0.005165
174	C	19	Z	0.005929	0.013847	-0.002417	0.009750	-0.005595
175	C	19	S	-0.031992	0.005550	-0.040764	0.012337	-0.006298
176	C	19	X	-0.012346	0.003672	-0.005395	0.008801	0.009300
177	C	19	Y	0.006083	-0.003958	0.015486	-0.012220	0.003549
178	C	19	Z	-0.002772	0.007904	-0.005174	0.009826	-0.006829
179	O	20	S	0.011963	0.012650	0.008541	0.002096	0.002714
180	O	20	X	-0.015869	0.041294	0.057355	0.017159	0.006847
181	O	20	Y	0.035690	0.018938	-0.000778	-0.000156	0.011111
182	O	20	Z	-0.037941	0.022749	0.024604	-0.001816	0.018207
183	O	20	S	0.019233	0.016351	0.006267	-0.000075	0.001227
184	O	20	X	0.003213	0.018164	0.030933	0.007147	0.006189
185	O	20	Y	0.000560	0.005056	0.002743	-0.004283	0.006096
186	O	20	Z	-0.009776	0.014344	0.011398	0.001360	0.011879
187	N	21	S	0.017108	-0.018347	0.043792	-0.014345	-0.010481
188	N	21	X	0.088921	-0.020937	0.093227	0.061591	0.058665
189	N	21	Y	-0.010387	-0.005366	0.085846	-0.005394	0.025492
190	N	21	Z	0.031488	0.010652	0.024290	-0.026182	-0.081396
191	N	21	S	0.048394	-0.037543	0.103861	0.010704	-0.027780
192	N	21	X	0.036618	-0.040508	0.052499	0.039544	0.028982
193	N	21	Y	0.017991	-0.008959	0.050602	0.002516	0.008931

194	N	21	Z	0.007755	0.007370	0.023959	-0.016570	-0.038858
195	H	22	S	0.095334	-0.061499	0.176625	0.033577	0.018220
196	H	22	S	0.077080	-0.023448	0.144897	-0.040320	0.020357
197	H	23	S	-0.032007	0.087600	-0.066651	-0.184217	-0.018141
198	H	23	S	-0.020056	0.056390	-0.045486	-0.103720	-0.016315
199	H	24	S	-0.056201	-0.028152	-0.063697	0.099512	-0.005305
200	H	24	S	-0.043214	-0.020739	-0.050830	0.054006	0.013892
201	H	25	S	0.033126	-0.111035	0.168028	-0.017430	0.013014
202	H	25	S	0.016290	-0.109119	0.122416	0.047445	0.005888
203	H	26	S	-0.024965	0.016146	-0.117718	0.190946	-0.009253
204	H	26	S	-0.015914	0.016910	-0.078443	0.115017	-0.000807
205	H	27	S	0.013347	0.081304	-0.022078	-0.116947	-0.003589
206	H	27	S	0.002748	0.056613	-0.022664	-0.066879	-0.014716
207	H	28	S	-0.031164	0.029255	-0.018971	0.041627	0.004163
208	H	28	S	-0.001994	0.029309	-0.008801	0.009919	0.009119
209	H	29	S	-0.003174	0.008518	-0.003247	0.007179	-0.001477
210	H	29	S	-0.001721	0.003017	-0.008170	0.002063	0.003335
211	H	30	S	-0.022005	0.004814	0.033525	0.004636	0.002887
212	H	30	S	-0.014511	0.005512	0.022532	0.005783	0.000720
213	H	31	S	0.019069	0.004155	-0.036676	-0.007376	-0.000938
214	H	31	S	0.013293	0.004233	-0.020252	-0.006049	0.000959
215	H	32	S	-0.004461	0.000506	-0.001621	-0.000404	-0.002706
216	H	32	S	-0.002584	0.004099	-0.004319	0.008543	-0.004206
217	H	33	S	-0.053353	-0.008160	0.005681	-0.003188	-0.002336
218	H	33	S	-0.028125	-0.000027	0.009815	0.000174	-0.001112
219	H	34	S	-0.065227	-0.003952	-0.004357	-0.008729	0.054327
220	H	34	S	-0.036239	0.006006	0.012393	0.006600	0.027709
221	H	35	S	0.046329	-0.016076	-0.042357	0.033419	-0.003002
222	H	35	S	0.018069	-0.008353	-0.025634	0.029418	-0.007202

51	52	53	54	55
-0.5306	-0.5088	-0.5076	-0.4861	-0.4529
A	A	A	A	A

1	CO	1	S	-0.021312	-0.004467	0.004175	-0.003746	0.000629
2	CO	1	X	-0.000790	-0.000575	-0.000903	-0.004869	-0.001990
3	CO	1	Y	-0.004008	0.004418	-0.006934	-0.001357	0.004875
4	CO	1	Z	0.013988	0.001607	-0.011579	-0.001823	0.014497
5	CO	1	XX	-0.040943	-0.006392	-0.028271	0.017655	0.035575
6	CO	1	YY	0.010945	0.033965	-0.007208	-0.007059	-0.095471
7	CO	1	ZZ	0.029999	-0.027573	0.035480	-0.010596	0.059896
8	CO	1	XY	-0.034896	-0.024149	-0.051239	0.004898	-0.030209
9	CO	1	XZ	0.022366	-0.100916	-0.077801	-0.013635	-0.042980
10	CO	1	YZ	0.082221	-0.004468	0.025815	-0.004365	0.016603
11	CO	1	XX	-0.022003	-0.003693	-0.015868	0.009050	0.019385
12	CO	1	YY	0.007832	0.018862	-0.003592	-0.004355	-0.052160
13	CO	1	ZZ	0.014171	-0.015169	0.019460	-0.004694	0.032774

14 CO 1 XY -0.017748 -0.013487 -0.028902 0.001630 -0.014942
15 CO 1 XZ 0.008907 -0.053017 -0.043340 -0.007102 -0.024577
16 CO 1 YZ 0.037134 0.003670 0.015966 -0.001263 0.007934
17 CO 1 S 0.061555 0.016654 -0.010548 0.019502 -0.003578
18 CO 1 X -0.005632 -0.014935 0.001120 0.031713 0.026655
19 CO 1 Y -0.012373 -0.006190 0.013848 -0.001463 -0.034358
20 CO 1 Z -0.017580 -0.003000 0.015010 0.000632 -0.036422
21 CO 1 S 0.001253 -0.003220 -0.009397 0.003975 -0.015183
22 CO 1 X -0.004300 -0.000258 -0.007868 -0.003556 -0.002355
23 CO 1 Y -0.002639 0.000250 0.005945 -0.001731 -0.001813
24 CO 1 Z -0.001910 0.000965 0.016157 0.001339 -0.007426
25 CO 1 S -0.017366 -0.002331 0.004382 -0.002191 0.000800
26 CO 1 X 0.001418 0.002345 0.002008 -0.001959 -0.000618
27 CO 1 Y 0.002714 0.001198 0.000517 -0.000809 -0.000269
28 CO 1 Z -0.001037 -0.000369 0.000520 -0.000383 -0.000693
29 CO 1 XX -0.013873 -0.007282 -0.012503 0.015001 0.007915
30 CO 1 YY 0.002750 0.016175 -0.002843 -0.008831 -0.032636
31 CO 1 ZZ 0.011122 -0.008893 0.015346 -0.006170 0.024720
32 CO 1 XY -0.027912 -0.017312 -0.026588 0.012496 -0.010203
33 CO 1 XZ -0.007770 -0.023429 -0.021749 -0.009460 -0.014945
34 CO 1 YZ 0.025134 0.005996 0.006819 0.003593 0.012720
35 C 2 S -0.003996 0.001915 0.001343 -0.002858 -0.000323
36 C 2 X 0.005167 -0.015641 -0.006746 0.001972 -0.007197
37 C 2 Y -0.050321 -0.055616 -0.026114 -0.002866 -0.068215
38 C 2 Z 0.175915 0.218192 0.102286 0.017194 0.260754
39 C 2 S -0.004063 0.039874 0.008906 -0.026263 -0.020369
40 C 2 X 0.002588 -0.019892 -0.005313 0.010542 0.003839
41 C 2 Y -0.009157 -0.024695 -0.007999 0.018597 -0.025348
42 C 2 Z 0.054018 0.074528 0.036619 0.013429 0.109876
43 C 3 S -0.001221 -0.001816 0.000302 -0.001711 -0.001321
44 C 3 X -0.000783 0.003032 -0.002685 0.011679 -0.005132
45 C 3 Y -0.013134 -0.043791 -0.024277 0.067689 -0.058363
46 C 3 Z 0.063950 0.162496 0.085663 -0.249194 0.217922
47 C 3 S 0.003387 -0.027199 0.001051 0.024191 0.028045
48 C 3 X 0.003641 0.014031 0.000553 -0.005652 -0.014324
49 C 3 Y -0.006390 -0.018053 -0.008546 0.037575 -0.024791
50 C 3 Z 0.018901 0.053432 0.028788 -0.083881 0.099284
51 C 4 S 0.003125 0.007028 0.001017 -0.001367 0.001918
52 C 4 X 0.000348 -0.016501 -0.002262 0.013738 0.000681
53 C 4 Y 0.027854 0.007415 -0.000643 0.094744 0.033843
54 C 4 Z -0.091481 -0.019840 0.002117 -0.299195 -0.112118
55 C 4 S 0.021210 0.047108 0.007345 -0.068424 -0.042608
56 C 4 X -0.008692 -0.006407 -0.003550 0.029805 0.000147
57 C 4 Y 0.009740 0.017848 -0.001918 0.021608 -0.018718
58 C 4 Z -0.023845 0.006388 0.003972 -0.134844 -0.057319
59 C 5 S 0.005202 -0.000071 0.002237 -0.001516 0.002988

60	C	5	X	0.014015	0.025807	0.004700	0.007557	0.023147
61	C	5	Y	0.070108	0.060979	0.026353	0.009851	0.104375
62	C	5	Z	-0.186547	-0.185579	-0.083958	-0.028324	-0.274204
63	C	5	S	-0.004322	-0.067086	-0.009802	0.006838	0.042710
64	C	5	X	-0.007233	-0.014309	0.003653	0.078521	0.074379
65	C	5	Y	0.037875	0.010688	0.017205	-0.001029	0.102751
66	C	5	Z	-0.071298	-0.087537	-0.033697	-0.014727	-0.120538
67	C	6	S	-0.010126	0.010253	0.007281	0.002794	-0.000393
68	C	6	X	0.018203	-0.025128	-0.012376	0.000910	-0.001990
69	C	6	Y	0.034009	0.054990	0.021598	-0.094742	-0.017191
70	C	6	Z	-0.135280	-0.161445	-0.069082	0.305183	0.019824
71	C	6	S	-0.050763	-0.019046	-0.005720	0.002356	0.040829
72	C	6	X	0.019169	0.052899	-0.005921	-0.120011	-0.084569
73	C	6	Y	0.022793	-0.019260	0.001537	-0.096049	0.047817
74	C	6	Z	-0.045674	-0.067889	-0.026463	0.128472	0.029580
75	C	7	S	0.002967	-0.005908	-0.003730	-0.000243	-0.006665
76	C	7	X	-0.012678	0.012168	0.005792	-0.005119	0.009772
77	C	7	Y	-0.053136	-0.033371	-0.011518	-0.080958	0.011232
78	C	7	Z	0.218338	0.123021	0.044901	0.301590	-0.006357
79	C	7	S	-0.013611	-0.019143	0.004261	0.102192	0.011007
80	C	7	X	-0.001570	-0.016264	-0.008186	-0.044763	0.011119
81	C	7	Y	-0.036444	0.024249	-0.001130	-0.079319	-0.017985
82	C	7	Z	0.081200	0.059079	0.018601	0.091621	-0.008757
83	C	8	S	-0.002599	0.001086	0.001162	0.004974	0.002560
84	C	8	X	0.003813	-0.003050	-0.001723	-0.005108	-0.000012
85	C	8	Y	-0.076524	-0.019466	-0.003085	-0.001993	0.074051
86	C	8	Z	0.250881	0.087696	0.017610	0.003809	-0.290258
87	C	8	S	0.020924	-0.018755	0.000875	0.002433	0.013114
88	C	8	X	-0.007062	0.002991	0.002863	0.021853	0.001548
89	C	8	Y	-0.034036	0.012712	0.005858	-0.010204	0.027810
90	C	8	Z	0.075148	0.034862	0.007397	0.001233	-0.123568
91	C	9	S	-0.004815	0.004704	0.002853	0.001831	-0.001317
92	C	9	X	0.004849	-0.004666	-0.003432	-0.003142	0.001669
93	C	9	Y	-0.029534	-0.013321	-0.003077	0.068784	0.065681
94	C	9	Z	0.169725	-0.003558	-0.019467	-0.263801	-0.219372
95	C	9	S	-0.040891	0.060051	0.027712	0.012629	-0.027577
96	C	9	X	0.011644	-0.031821	-0.016108	0.018279	0.009538
97	C	9	Y	0.005350	-0.016915	-0.005830	0.012335	0.029003
98	C	9	Z	0.056437	-0.007373	-0.008653	-0.099831	-0.098155
99	C	10	S	0.004258	-0.014196	-0.007494	0.002274	0.008943
100	C	10	X	0.001670	-0.000811	-0.000502	-0.028146	-0.000537
101	C	10	Y	-0.021440	0.051676	0.027043	0.093603	-0.046628
102	C	10	Z	-0.027638	-0.079337	-0.033194	-0.299466	0.136932
103	C	10	S	0.072874	-0.015394	-0.019992	-0.070583	-0.011242
104	C	10	X	0.025897	-0.053310	-0.017476	-0.013211	0.034454
105	C	10	Y	-0.009357	-0.030253	-0.012867	0.087805	0.003232

106	C	10	Z	-0.004602	-0.031889	-0.016311	-0.113004	0.060483
107	C	11	S	0.002697	0.001962	0.002502	-0.003218	0.000419
108	C	11	X	-0.012712	0.007304	0.000990	-0.007276	0.023476
109	C	11	Y	0.076146	0.007478	-0.006045	-0.000662	-0.082514
110	C	11	Z	-0.194401	-0.111784	-0.031914	-0.024480	0.313082
111	C	11	S	0.008961	0.016438	-0.010411	-0.008455	-0.049025
112	C	11	X	-0.001519	0.066871	0.009365	-0.019473	-0.083223
113	C	11	Y	-0.027591	-0.021788	-0.003119	0.095979	-0.009983
114	C	11	Z	-0.082189	-0.066078	-0.017637	0.015524	0.164597
115	N	12	S	0.016023	0.005591	0.003160	-0.003742	-0.001893
116	N	12	X	0.021862	-0.019525	-0.008694	-0.006739	0.007387
117	N	12	Y	-0.074564	0.019629	0.014702	0.008116	0.003843
118	N	12	Z	-0.085574	0.206985	0.108727	0.014505	-0.090985
119	N	12	S	0.025978	0.030531	0.016472	0.005074	-0.022954
120	N	12	X	-0.005754	-0.010971	-0.005873	0.002152	0.015138
121	N	12	Y	-0.039275	0.034168	0.014732	-0.014059	-0.028617
122	N	12	Z	-0.061135	0.129254	0.064685	0.008679	-0.056668
123	C	13	S	-0.020646	-0.006781	-0.004108	-0.004358	0.018864
124	C	13	X	-0.041444	-0.008824	-0.004220	0.003085	0.033977
125	C	13	Y	0.050725	0.019292	-0.000617	-0.014312	-0.045600
126	C	13	Z	0.120262	0.029669	-0.017286	0.015911	-0.157963
127	C	13	S	-0.089036	-0.015400	-0.000278	-0.052019	0.138909
128	C	13	X	0.025310	-0.009241	-0.016737	0.040826	-0.048833
129	C	13	Y	0.050065	0.012341	0.002599	0.009800	-0.068131
130	C	13	Z	0.050399	0.002484	-0.012289	0.003525	-0.073816
131	C	14	S	-0.001499	-0.000591	-0.003872	0.004517	-0.003757
132	C	14	X	-0.018992	0.016034	0.012153	0.005668	-0.016718
133	C	14	Y	0.084005	-0.085755	-0.054669	-0.000145	0.024740
134	C	14	Z	0.219269	-0.214254	-0.159796	-0.012287	0.087634
135	C	14	S	0.036585	-0.008570	-0.016908	0.045382	-0.065709
136	C	14	X	0.033331	0.027670	0.011831	0.043664	-0.087044
137	C	14	Y	0.063341	-0.052963	-0.040544	0.003715	-0.021556
138	C	14	Z	0.080815	-0.088401	-0.055391	-0.002388	0.052213
139	C	15	S	-0.001410	0.001605	-0.000464	-0.002015	0.001655
140	C	15	X	-0.004374	-0.000204	0.025770	0.000745	-0.006681
141	C	15	Y	0.001563	0.031563	-0.142259	-0.009052	0.042736
142	C	15	Z	-0.002793	0.086322	-0.358122	-0.006636	0.086271
143	C	15	S	0.023617	0.005055	0.006116	-0.012860	-0.019983
144	C	15	X	0.003874	-0.018360	0.007954	-0.006291	-0.001899
145	C	15	Y	0.011119	0.009353	-0.066852	-0.005471	-0.001328
146	C	15	Z	-0.010583	0.042209	-0.135725	-0.003658	0.044154
147	C	16	S	0.000467	-0.002871	0.002840	0.000294	-0.002856
148	C	16	X	0.018460	-0.028699	0.018139	-0.000279	-0.001249
149	C	16	Y	-0.074878	0.110896	-0.059776	0.003341	-0.016964
150	C	16	Z	-0.193545	0.284882	-0.158848	0.003695	-0.039352
151	C	16	S	0.007711	-0.025500	-0.000438	-0.002632	-0.011359

152	C	16	X	0.004806	-0.012625	-0.010166	0.003363	-0.002865
153	C	16	Y	-0.024984	0.034885	-0.017973	0.005324	-0.013631
154	C	16	Z	-0.077585	0.117843	-0.057361	0.001541	-0.018689
155	C	17	S	-0.001251	0.001911	-0.001183	0.000836	-0.000312
156	C	17	X	0.014164	-0.010666	-0.018662	0.000404	0.008983
157	C	17	Y	-0.083177	0.070053	0.076361	0.003777	-0.041151
158	C	17	Z	-0.212307	0.184616	0.198103	0.012164	-0.106280
159	C	17	S	-0.006678	0.017792	-0.007238	0.004102	0.001183
160	C	17	X	0.004185	0.002769	-0.006522	0.001597	0.004619
161	C	17	Y	-0.023528	0.026016	0.038710	0.000583	-0.019039
162	C	17	Z	-0.067509	0.059217	0.071887	0.004745	-0.045271
163	C	18	S	0.000211	0.000595	0.000145	-0.000456	-0.000620
164	C	18	X	0.009051	0.005399	-0.028809	-0.001563	0.001199
165	C	18	Y	-0.033528	-0.027215	0.146121	0.002809	-0.012994
166	C	18	Z	-0.088479	-0.070359	0.368536	0.006247	-0.031289
167	C	18	S	-0.005576	-0.006662	-0.008721	-0.007254	0.010243
168	C	18	X	0.004754	-0.001135	-0.011391	-0.003432	0.000658
169	C	18	Y	-0.014158	-0.000570	0.055807	0.002718	-0.006123
170	C	18	Z	-0.030961	-0.022798	0.125985	0.001778	-0.014237
171	C	19	S	-0.000808	-0.001127	-0.000009	0.001779	-0.000903
172	C	19	X	-0.010409	0.022911	-0.019786	0.002971	-0.006882
173	C	19	Y	0.035116	-0.103229	0.084847	-0.002626	0.032306
174	C	19	Z	0.094102	-0.265584	0.233107	-0.004913	0.079786
175	C	19	S	0.002747	0.022739	0.017266	0.024778	-0.023904
176	C	19	X	-0.007729	0.017754	-0.001715	0.002431	-0.000003
177	C	19	Y	0.003155	-0.049129	0.030423	-0.013254	0.035195
178	C	19	Z	0.031375	-0.096718	0.101089	0.002749	0.029186
179	O	20	S	-0.000426	-0.007826	-0.003356	-0.003681	0.000735
180	O	20	X	0.002900	-0.012514	-0.002103	-0.006278	-0.005184
181	O	20	Y	-0.001652	-0.041749	0.084978	-0.000182	-0.023952
182	O	20	Z	0.002723	-0.076829	0.172824	0.003104	-0.040523
183	O	20	S	0.001913	-0.009134	-0.007662	-0.006044	0.006633
184	O	20	X	0.001311	-0.007429	0.007420	-0.005373	0.001717
185	O	20	Y	-0.008706	-0.027209	0.050350	0.003206	-0.012098
186	O	20	Z	-0.000104	-0.045875	0.101017	0.001737	-0.030546
187	N	21	S	0.004251	0.013176	0.004145	0.004891	0.010756
188	N	21	X	-0.024418	-0.038280	-0.004098	-0.005716	-0.020339
189	N	21	Y	-0.018003	-0.009972	-0.002259	-0.000556	-0.015943
190	N	21	Z	0.068546	0.052805	0.015359	0.005404	0.056898
191	N	21	S	0.004076	0.025821	0.009620	0.024094	0.051842
192	N	21	X	-0.013364	-0.024102	0.002040	0.008519	0.008624
193	N	21	Y	0.011271	0.006932	0.002944	-0.000931	0.015134
194	N	21	Z	0.025711	0.021370	0.004831	-0.012508	0.010992
195	H	22	S	0.002291	-0.005388	-0.001835	0.000636	-0.000833
196	H	22	S	-0.001329	0.001412	-0.000603	-0.007454	-0.002267
197	H	23	S	-0.001359	0.006287	0.000712	0.002474	0.001073

198	H	23	S	-0.003287	-0.000808	-0.000340	0.004880	0.003550
199	H	24	S	0.003807	0.000765	0.000025	0.000917	0.005684
200	H	24	S	0.000739	0.003279	-0.000584	-0.005423	-0.009787
201	H	25	S	-0.001573	0.000399	0.000091	-0.001736	-0.003522
202	H	25	S	0.003656	-0.005328	-0.003429	-0.008301	-0.003450
203	H	26	S	0.013153	-0.010354	-0.006160	-0.004713	0.002850
204	H	26	S	0.002410	-0.003897	-0.003049	0.003502	0.005546
205	H	27	S	-0.008300	0.001206	0.001148	0.002868	0.008681
206	H	27	S	-0.001454	-0.006618	0.005272	-0.010091	0.017170
207	H	28	S	0.006644	0.015663	0.007858	-0.008000	-0.000361
208	H	28	S	0.006687	0.006719	-0.000008	0.009837	-0.008199
209	H	29	S	0.000389	-0.001590	-0.000365	-0.002005	0.002103
210	H	29	S	0.002596	-0.002937	-0.001346	0.002251	-0.001391
211	H	30	S	0.001880	-0.001953	0.002425	-0.000589	-0.000621
212	H	30	S	0.002583	0.000905	0.004040	0.000361	-0.001298
213	H	31	S	-0.000733	0.000670	0.000821	0.000630	0.000451
214	H	31	S	0.002543	-0.002070	-0.001158	0.000119	-0.002111
215	H	32	S	-0.000638	-0.000936	-0.003393	-0.000390	0.002296
216	H	32	S	0.004229	0.003792	-0.000029	0.004422	-0.008588
217	H	33	S	-0.000302	0.000460	0.015644	0.002747	0.000590
218	H	33	S	0.001278	0.002427	0.006874	0.000068	0.000469
219	H	34	S	-0.056506	-0.043376	-0.020157	-0.009063	-0.070236
220	H	34	S	-0.032383	-0.038573	-0.009551	-0.009743	-0.061515
221	H	35	S	0.010528	-0.000131	-0.000672	-0.004194	0.013610
222	H	35	S	0.014840	0.007099	0.006433	-0.007030	0.017419

56	57	58	59	60
-0.3926	-0.3794	-0.3630	-0.3423	-0.2993

A	A	A	A	A
---	---	---	---	---

1	CO	1	S	-0.075066	0.014535	-0.039260	0.032194	-0.098979
2	CO	1	X	-0.014081	0.043686	-0.003561	0.006215	-0.016689
3	CO	1	Y	0.015016	-0.024073	0.108182	-0.021543	0.022280
4	CO	1	Z	-0.014335	-0.021327	-0.010207	0.038703	-0.083579
5	CO	1	XX	-0.086467	-0.251370	-0.421210	0.004920	0.210163
6	CO	1	YY	-0.254119	-0.199602	0.529983	0.056526	-0.120372
7	CO	1	ZZ	0.340586	0.450972	-0.108773	-0.061446	-0.089791
8	CO	1	XY	0.026025	-0.407605	-0.215311	-0.003974	0.040480
9	CO	1	XZ	0.377821	-0.280413	0.080309	-0.008769	-0.258628
10	CO	1	YZ	-0.344270	0.046208	-0.030430	0.121912	0.112156
11	CO	1	XX	-0.047966	-0.133980	-0.221151	0.004227	0.101402
12	CO	1	YY	-0.135968	-0.103549	0.276947	0.031409	-0.060601
13	CO	1	ZZ	0.183934	0.237529	-0.055796	-0.035636	-0.040801
14	CO	1	XY	0.011574	-0.212683	-0.113361	0.000094	0.019771
15	CO	1	XZ	0.204763	-0.145346	0.042874	-0.009319	-0.123086
16	CO	1	YZ	-0.181382	0.022094	-0.017031	0.055007	0.060755
17	CO	1	S	0.225893	-0.043523	0.135943	-0.100018	0.324563

18	CO	1	X	0.016800	-0.031754	-0.020762	0.007649	0.106824
19	CO	1	Y	-0.030264	0.018716	-0.142895	0.044200	-0.129174
20	CO	1	Z	0.023369	0.010663	0.046217	-0.109782	0.198253
21	CO	1	S	0.172180	-0.018906	0.125634	-0.141693	0.633466
22	CO	1	X	0.011116	-0.029660	0.001155	-0.020199	0.054365
23	CO	1	Y	-0.001370	0.020872	-0.117651	0.019100	-0.091112
24	CO	1	Z	0.010447	0.005935	0.007160	-0.031086	0.116029
25	CO	1	S	-0.069130	0.014327	-0.032825	0.032306	-0.104885
26	CO	1	X	0.000170	0.001806	0.002590	-0.002020	-0.001094
27	CO	1	Y	-0.001760	0.001254	0.001716	0.001687	0.001514
28	CO	1	Z	0.005291	-0.000623	-0.000119	0.000383	-0.001528
29	CO	1	XX	-0.037874	-0.079908	-0.178780	-0.002972	0.102143
30	CO	1	YY	-0.076362	-0.075116	0.215952	0.009451	-0.073980
31	CO	1	ZZ	0.114236	0.155024	-0.037173	-0.006479	-0.028163
32	CO	1	XY	0.012373	-0.141733	-0.080328	-0.014359	0.024354
33	CO	1	XZ	0.118528	-0.098895	0.048849	-0.025620	-0.117446
34	CO	1	YZ	-0.123975	0.021700	-0.012230	0.028095	0.037739
35	C	2	S	-0.001646	0.000820	0.004117	-0.004422	-0.005257
36	C	2	X	-0.000741	0.004547	-0.003842	0.004454	0.001922
37	C	2	Y	-0.010492	0.019707	-0.004821	-0.018814	-0.009107
38	C	2	Z	0.047911	-0.081790	0.015872	0.063380	0.048031
39	C	2	S	0.005619	-0.027216	-0.008300	0.003983	-0.027079
40	C	2	X	-0.013188	0.015241	-0.008188	0.007294	0.008258
41	C	2	Y	0.002005	0.031615	-0.004662	0.000961	-0.023524
42	C	2	Z	0.025150	-0.040310	0.008333	0.034160	0.033046
43	C	3	S	0.001488	0.010984	0.003135	-0.001454	0.010230
44	C	3	X	-0.002777	-0.017569	-0.005093	0.001278	-0.014719
45	C	3	Y	-0.007341	0.000523	-0.001216	0.000719	-0.016293
46	C	3	Z	0.014658	-0.036474	-0.007147	0.001635	0.009252
47	C	3	S	-0.015097	0.109136	-0.066327	0.026764	0.024709
48	C	3	X	0.002581	-0.050893	0.018733	0.000918	-0.010813
49	C	3	Y	0.013216	0.006438	0.022410	-0.017708	-0.022593
50	C	3	Z	0.012786	-0.018028	0.002514	0.005617	0.011831
51	C	4	S	-0.002614	-0.022801	-0.001241	0.000824	-0.026668
52	C	4	X	0.002336	0.035039	0.009863	0.002904	0.021942
53	C	4	Y	0.019752	-0.029676	-0.001722	0.023734	0.032190
54	C	4	Z	-0.042086	0.072550	-0.023098	-0.074663	-0.059584
55	C	4	S	-0.036452	-0.215465	0.040401	0.069949	-0.001057
56	C	4	X	0.039404	0.024515	0.065344	-0.053760	-0.028470
57	C	4	Y	0.028677	-0.090734	0.048850	0.012371	0.044279
58	C	4	Z	-0.016746	0.017566	0.011313	-0.061188	-0.051949
59	C	5	S	-0.005352	0.031874	0.029479	0.001909	-0.010546
60	C	5	X	0.001170	-0.053120	-0.040967	0.003690	-0.018926
61	C	5	Y	0.004751	-0.027711	-0.032964	0.003308	-0.028716
62	C	5	Z	-0.039763	0.041925	-0.022407	0.020927	0.006428
63	C	5	S	-0.006901	0.067161	0.115278	0.003996	0.023572

64	C	5	X	0.005069	0.142041	-0.095106	-0.054940	-0.090401
65	C	5	Y	-0.094511	-0.018448	-0.098328	0.096143	0.025672
66	C	5	Z	-0.036689	0.029616	-0.054109	0.043869	0.014153
67	C	6	S	-0.006190	0.016586	0.014200	-0.017357	-0.024267
68	C	6	X	0.001427	0.005283	-0.022233	0.027664	0.013433
69	C	6	Y	0.018187	-0.044451	0.004715	-0.043884	-0.002106
70	C	6	Z	-0.028923	0.061625	0.049024	0.100412	0.039384
71	C	6	S	0.056822	0.086763	0.054419	-0.199878	-0.002434
72	C	6	X	0.021937	-0.101429	0.009437	0.039646	0.078323
73	C	6	Y	-0.041652	-0.033975	-0.022340	0.025467	0.091395
74	C	6	Z	-0.039814	0.021611	0.032855	0.086741	0.082407
75	C	7	S	0.001387	-0.003094	-0.000206	0.005168	0.006403
76	C	7	X	-0.003863	-0.000007	-0.002139	-0.007260	-0.012791
77	C	7	Y	-0.005375	0.002139	-0.008462	-0.002796	0.002249
78	C	7	Z	0.004890	0.007007	0.010386	0.002188	-0.036145
79	C	7	S	0.000788	0.074483	-0.014286	-0.021764	-0.077967
80	C	7	X	-0.020764	-0.023859	0.009884	-0.009877	0.061222
81	C	7	Y	0.012766	-0.009574	-0.017969	-0.032910	0.028415
82	C	7	Z	0.007830	0.008273	-0.000397	0.001299	-0.029482
83	C	8	S	-0.003709	0.003036	0.000022	-0.005691	-0.004884
84	C	8	X	0.004246	-0.000334	-0.001219	0.010217	0.000916
85	C	8	Y	0.005847	-0.007535	0.023097	0.040058	0.023061
86	C	8	Z	-0.013881	0.008884	-0.061014	-0.171683	-0.069906
87	C	8	S	-0.011282	-0.012257	0.001376	0.055079	-0.003045
88	C	8	X	0.002354	0.002617	0.010000	-0.010094	-0.024606
89	C	8	Y	0.012412	0.005020	0.005054	0.010529	0.004050
90	C	8	Z	-0.004059	0.002553	-0.035319	-0.114912	-0.053329
91	C	9	S	0.004317	0.001369	0.012737	-0.005194	-0.002474
92	C	9	X	-0.008160	-0.001534	-0.017964	0.003099	0.001328
93	C	9	Y	-0.000408	-0.000919	-0.009876	0.010433	-0.013178
94	C	9	Z	-0.013486	-0.000985	-0.026506	-0.001587	0.056240
95	C	9	S	0.030527	-0.015194	0.062724	-0.049345	-0.104350
96	C	9	X	-0.020173	0.004222	-0.006832	-0.010795	0.033018
97	C	9	Y	-0.005964	-0.007519	-0.020794	0.055468	0.020458
98	C	9	Z	-0.008018	0.001076	-0.022146	0.013676	0.048959
99	C	10	S	-0.008182	-0.001602	-0.022841	0.015291	0.003545
100	C	10	X	0.014088	-0.000005	0.002993	0.033625	0.005578
101	C	10	Y	-0.003033	0.005953	0.029029	-0.102786	-0.022539
102	C	10	Z	0.011127	-0.014761	0.072438	0.156810	0.045365
103	C	10	S	-0.026514	-0.037375	-0.116091	0.192835	0.095467
104	C	10	X	-0.001706	0.035448	-0.045003	0.067359	0.087439
105	C	10	Y	-0.031942	0.021203	0.036314	-0.153956	0.010298
106	C	10	Z	-0.004902	-0.007960	0.061282	0.088015	0.043670
107	C	11	S	-0.003806	0.017208	0.030879	-0.009273	-0.018350
108	C	11	X	-0.005085	-0.018493	-0.042705	0.017724	-0.015168
109	C	11	Y	-0.002817	-0.013731	-0.045040	0.033411	0.036271

110	C	11	Z	0.007926	-0.005913	0.006506	-0.030856	-0.084664
111	C	11	S	-0.009269	0.017777	0.071134	-0.129852	0.008233
112	C	11	X	0.006177	-0.109914	0.032334	0.039606	-0.076558
113	C	11	Y	-0.017932	0.014745	0.059327	-0.123256	-0.040414
114	C	11	Z	0.009062	0.010946	0.015144	-0.087055	-0.083629
115	N	12	S	-0.018095	0.026222	-0.097996	0.020685	-0.029736
116	N	12	X	0.002575	0.026737	-0.009340	0.049440	-0.002321
117	N	12	Y	0.022040	-0.052827	0.201447	-0.099013	0.006750
118	N	12	Z	0.004383	-0.025134	-0.061567	-0.327241	-0.088457
119	N	12	S	-0.036452	0.051559	-0.178209	0.049663	-0.081408
120	N	12	X	-0.003962	-0.030793	-0.005757	0.033601	-0.029046
121	N	12	Y	0.016095	-0.066881	0.193688	-0.060794	-0.058343
122	N	12	Z	-0.001669	-0.025960	-0.056363	-0.271003	-0.043228
123	C	13	S	-0.008044	-0.032388	0.027554	0.005845	-0.017989
124	C	13	X	-0.012983	-0.045247	0.036357	-0.052453	0.029140
125	C	13	Y	0.060987	0.022517	-0.014373	0.138029	0.019913
126	C	13	Z	0.161501	-0.008193	0.004523	0.402178	0.013127
127	C	13	S	0.012246	-0.060949	-0.122349	0.076167	-0.326881
128	C	13	X	-0.012490	-0.048531	0.081191	-0.055075	0.177610
129	C	13	Y	0.005395	0.008710	0.028425	0.121599	0.115161
130	C	13	Z	0.102085	-0.011564	-0.002246	0.292977	-0.012489
131	C	14	S	-0.010533	-0.005690	0.017167	0.003883	-0.015723
132	C	14	X	-0.003591	-0.009809	0.037352	-0.003487	-0.000874
133	C	14	Y	0.004244	0.012749	0.027928	0.032679	0.049514
134	C	14	Z	-0.021672	0.049770	-0.010029	0.094222	0.036353
135	C	14	S	-0.058813	-0.004299	0.010229	0.068640	-0.100010
136	C	14	X	-0.040068	-0.034233	0.082987	-0.063348	0.331051
137	C	14	Y	0.035797	-0.003670	0.206403	-0.033897	0.207715
138	C	14	Z	-0.042075	0.049238	-0.068585	0.082129	0.020320
139	C	15	S	0.003717	-0.016410	0.009492	-0.015816	0.064693
140	C	15	X	0.019142	-0.029234	0.014569	-0.008988	0.132012
141	C	15	Y	-0.043635	0.019162	-0.023296	-0.074244	-0.114943
142	C	15	Z	-0.054418	-0.014970	0.015772	-0.247643	-0.002303
143	C	15	S	0.038904	-0.079605	0.220010	-0.128108	0.402540
144	C	15	X	0.074412	0.043356	0.103351	0.026318	-0.027218
145	C	15	Y	0.006261	-0.006562	0.099985	-0.100353	0.068463
146	C	15	Z	-0.044491	-0.017830	-0.029107	-0.149542	-0.083900
147	C	16	S	-0.000872	0.006067	0.011276	0.008981	-0.041745
148	C	16	X	-0.003062	0.008238	0.012288	0.011054	-0.035991
149	C	16	Y	0.010313	0.020600	-0.003276	0.004903	0.013724
150	C	16	Z	0.019820	0.049630	-0.002517	0.013874	-0.010663
151	C	16	S	0.069790	0.076499	0.115168	0.070817	-0.285451
152	C	16	X	0.001866	0.010851	-0.000067	-0.004195	0.040288
153	C	16	Y	0.026049	0.046918	0.014989	0.042437	-0.104690
154	C	16	Z	0.010778	0.017848	-0.009588	-0.003560	0.045826
155	C	17	S	0.002150	-0.005742	0.000298	-0.004736	0.032426

156	C	17	X	-0.001582	-0.009248	-0.002171	-0.027541	0.034904
157	C	17	Y	0.022260	0.007097	0.003948	0.102418	-0.013565
158	C	17	Z	0.067093	0.005868	-0.001670	0.240125	0.061921
159	C	17	S	-0.026814	-0.046425	-0.043439	-0.061783	0.288756
160	C	17	X	-0.016957	-0.020188	-0.014514	-0.042418	0.105875
161	C	17	Y	0.013789	0.000888	0.008075	0.066751	0.000005
162	C	17	Z	0.032100	0.005166	-0.004169	0.160443	0.051504
163	C	18	S	-0.000541	0.000344	0.002361	-0.001247	-0.000300
164	C	18	X	-0.001571	0.006137	0.002028	0.003714	0.002036
165	C	18	Y	0.000108	-0.018521	0.000642	-0.022563	-0.003229
166	C	18	Z	-0.001941	-0.049878	0.004698	-0.053620	-0.028285
167	C	18	S	0.010467	0.028156	-0.067503	0.037608	-0.142513
168	C	18	X	0.010409	0.016024	-0.014901	0.023349	-0.061688
169	C	18	Y	-0.008326	-0.017358	-0.020498	-0.028427	0.048533
170	C	18	Z	-0.000631	-0.023326	0.010632	-0.041299	-0.047095
171	C	19	S	0.005393	-0.005077	0.006295	-0.002355	0.021741
172	C	19	X	0.013055	-0.004667	0.000779	0.012526	0.033467
173	C	19	Y	-0.028836	-0.007451	0.007363	-0.076292	-0.027105
174	C	19	Z	-0.058336	-0.017643	-0.002690	-0.220338	-0.022255
175	C	19	S	-0.035715	-0.032430	-0.011933	-0.043373	0.254676
176	C	19	X	-0.004399	0.007212	-0.091817	0.019063	0.013507
177	C	19	Y	-0.000706	0.005713	-0.035266	-0.015068	-0.154810
178	C	19	Z	-0.029389	-0.017288	0.002833	-0.148287	0.023857
179	O	20	S	-0.030628	0.032070	0.019186	0.039400	-0.211912
180	O	20	X	-0.010132	0.033506	0.055918	0.022097	-0.063163
181	O	20	Y	0.034036	-0.064968	0.043209	0.041942	0.020467
182	O	20	Z	0.050246	-0.123154	0.000086	0.091967	-0.045131
183	O	20	S	-0.069228	0.059566	0.040597	0.082960	-0.524569
184	O	20	X	0.004665	0.033592	0.076957	0.021936	-0.049280
185	O	20	Y	0.016962	-0.045189	-0.010971	0.039273	0.013900
186	O	20	Z	0.040010	-0.088143	0.013345	0.060508	-0.033066
187	N	21	S	-0.019792	-0.032313	0.001560	0.008745	-0.152880
188	N	21	X	-0.000675	0.113226	-0.024559	0.000978	0.111520
189	N	21	Y	-0.014188	0.010126	0.043219	-0.007497	0.024855
190	N	21	Z	0.033921	-0.061125	0.028825	0.012460	-0.106272
191	N	21	S	-0.067332	-0.024931	-0.023462	0.010883	-0.467595
192	N	21	X	-0.041368	0.112979	-0.087950	0.029247	0.149719
193	N	21	Y	-0.009388	0.041472	-0.021571	0.005556	-0.017752
194	N	21	Z	0.034213	-0.072088	0.052279	-0.006788	-0.121373
195	H	22	S	0.001542	0.002054	-0.000648	0.002451	0.006210
196	H	22	S	0.004665	-0.006305	0.002641	-0.002923	0.011011
197	H	23	S	0.000379	-0.010564	-0.003812	-0.000177	-0.004516
198	H	23	S	0.004029	0.001071	-0.002517	-0.004944	-0.009024
199	H	24	S	-0.004393	-0.004296	-0.001651	0.003419	-0.017402
200	H	24	S	0.006028	-0.017894	0.001436	0.002688	0.022923
201	H	25	S	0.003748	-0.001712	0.004223	0.002413	0.003144

202	H	25	S	0.001525	-0.002749	0.000397	0.009601	0.017522
203	H	26	S	-0.000665	-0.000293	-0.013291	0.014418	0.002621
204	H	26	S	0.000161	0.005119	-0.010104	-0.006684	-0.002979
205	H	27	S	-0.007226	-0.001401	-0.002301	-0.002749	-0.003790
206	H	27	S	0.014993	0.019087	-0.031925	0.051571	0.012573
207	H	28	S	0.001331	0.023937	-0.058817	-0.008473	-0.006450
208	H	28	S	0.007083	0.030784	-0.076410	-0.048191	-0.037532
209	H	29	S	-0.004979	0.004948	-0.001740	0.006987	-0.041422
210	H	29	S	-0.003246	0.018394	-0.016551	0.017136	-0.037202
211	H	30	S	-0.001469	0.004901	0.000068	0.003479	-0.015169
212	H	30	S	-0.005456	0.002657	-0.002173	-0.001821	-0.010562
213	H	31	S	0.002422	-0.001267	-0.003507	-0.002576	0.008762
214	H	31	S	0.007035	0.004881	0.003010	0.004884	-0.018244
215	H	32	S	-0.003876	0.000419	-0.001941	0.003425	-0.017272
216	H	32	S	-0.006915	0.000326	0.011798	-0.014029	0.024261
217	H	33	S	0.005581	-0.004146	-0.054025	0.000443	0.101636
218	H	33	S	0.020453	-0.004183	-0.030420	-0.020173	0.312975
219	H	34	S	-0.021250	-0.022813	0.011941	-0.014509	0.074806
220	H	34	S	-0.007159	-0.019967	0.002724	-0.006850	0.161002
221	H	35	S	0.028885	0.008311	-0.061349	0.011688	0.014450
222	H	35	S	0.029566	-0.000874	-0.056755	0.014924	0.058434

61	62	63	64	65
-0.2813	-0.2647	-0.2574	-0.2475	-0.2372
A	A	A	A	A

1	CO	1	S	0.017834	0.004828	0.012382	-0.009620	0.004968
2	CO	1	X	0.000700	0.017287	0.033441	-0.070378	0.020002
3	CO	1	Y	-0.024832	0.000553	0.010019	-0.008730	-0.010100
4	CO	1	Z	-0.018570	0.023915	0.041421	-0.086783	-0.032677
5	CO	1	XX	-0.059005	0.010004	0.048495	-0.007687	-0.020737
6	CO	1	YY	0.008536	0.016648	-0.049793	0.036742	0.031927
7	CO	1	ZZ	0.050469	-0.026652	0.001298	-0.029054	-0.011190
8	CO	1	XY	-0.021795	0.021894	0.018455	0.009660	0.021706
9	CO	1	XZ	0.005417	-0.001498	-0.033129	0.001526	0.093051
10	CO	1	YZ	-0.029814	0.013725	0.015018	0.018833	-0.013325
11	CO	1	XX	-0.029095	0.005694	0.024179	-0.004102	-0.007194
12	CO	1	YY	0.004021	0.009161	-0.022862	0.016828	0.013664
13	CO	1	ZZ	0.025074	-0.014855	-0.001317	-0.012726	-0.006470
14	CO	1	XY	-0.013566	0.011840	0.012737	0.003751	0.012718
15	CO	1	XZ	0.004243	-0.003939	-0.014199	0.002687	0.037579
16	CO	1	YZ	-0.012795	0.008087	0.008472	0.008599	-0.009480
17	CO	1	S	-0.056282	-0.023357	-0.092428	0.046692	0.032687
18	CO	1	X	-0.007944	-0.071285	-0.134736	0.132315	-0.005299
19	CO	1	Y	0.070220	0.024609	0.000020	-0.020559	0.046909
20	CO	1	Z	0.050059	-0.081095	-0.135733	0.298925	0.067254
21	CO	1	S	-0.047968	-0.009781	0.236867	-0.038015	-0.600486

22	CO	1	X	0.005396	-0.087436	-0.102462	0.475038	-0.379756
23	CO	1	Y	0.126080	-0.027065	-0.060770	0.180740	-0.089647
24	CO	1	Z	0.009045	-0.035959	-0.202018	0.269906	0.553398
25	CO	1	S	0.017299	0.001825	-0.009546	-0.002171	0.034752
26	CO	1	X	-0.000220	0.003848	0.003480	0.000476	0.001433
27	CO	1	Y	-0.000724	-0.001264	-0.000732	0.002550	0.000653
28	CO	1	Z	-0.000214	0.003092	0.004412	-0.005593	-0.001487
29	CO	1	XX	0.003567	-0.005107	0.001905	0.003226	-0.064279
30	CO	1	YY	-0.011067	0.011430	0.003866	-0.002649	0.041321
31	CO	1	ZZ	0.007500	-0.006323	-0.005771	-0.000577	0.022958
32	CO	1	XY	0.002752	-0.006008	-0.019601	-0.007098	-0.012111
33	CO	1	XZ	-0.001749	0.027690	-0.015688	-0.003400	0.072264
34	CO	1	YZ	-0.015301	-0.006359	-0.005890	-0.007206	-0.012655
35	C	2	S	0.000399	0.000908	0.005058	-0.001025	0.007086
36	C	2	X	-0.008076	-0.000483	-0.006269	-0.000982	0.005773
37	C	2	Y	-0.085795	0.004731	0.002494	-0.005561	-0.008131
38	C	2	Z	0.323839	-0.018624	-0.003779	0.021744	-0.017705
39	C	2	S	-0.013609	-0.057927	-0.155534	0.158193	0.275391
40	C	2	X	-0.004634	0.025073	0.060060	-0.074884	-0.104595
41	C	2	Y	-0.068460	0.025215	0.006329	-0.099566	-0.114031
42	C	2	Z	0.262666	-0.013582	-0.010276	0.006246	-0.055633
43	C	3	S	0.002817	0.001963	0.010447	-0.010570	-0.027308
44	C	3	X	0.002012	-0.000978	-0.000625	0.015435	0.036240
45	C	3	Y	0.039931	0.005275	0.069084	0.044089	0.050335
46	C	3	Z	-0.162172	-0.023714	-0.286970	-0.129962	-0.069832
47	C	3	S	0.011101	0.065878	0.160502	-0.240656	-0.361210
48	C	3	X	-0.007788	-0.028469	-0.064313	0.110201	0.144709
49	C	3	Y	0.039373	0.012210	0.060696	0.002558	-0.009385
50	C	3	Z	-0.114434	-0.020590	-0.284425	-0.151552	-0.080362
51	C	4	S	-0.000771	-0.000182	-0.011610	0.002365	0.053626
52	C	4	X	0.020753	-0.000708	-0.002077	-0.013541	-0.021220
53	C	4	Y	0.075216	-0.011780	-0.061915	-0.020036	-0.062859
54	C	4	Z	-0.255729	0.037702	0.233634	0.090607	0.069998
55	C	4	S	-0.066408	-0.059226	-0.091995	0.330435	0.566894
56	C	4	X	0.041705	-0.007115	-0.078877	-0.052256	-0.034498
57	C	4	Y	0.065481	-0.050587	-0.150466	0.126389	0.076275
58	C	4	Z	-0.264277	0.024629	0.218738	0.162933	0.122959
59	C	5	S	0.001610	0.010346	0.037574	-0.042855	-0.040871
60	C	5	X	-0.024110	-0.010136	-0.052713	0.043630	0.097305
61	C	5	Y	-0.119639	-0.002475	-0.038668	0.032158	0.078856
62	C	5	Z	0.332742	-0.010094	0.036992	0.009676	0.005240
63	C	5	S	0.023081	0.118855	0.390991	-0.393249	-0.432296
64	C	5	X	0.033791	0.032073	-0.070314	-0.241292	-0.259654
65	C	5	Y	-0.153404	0.043142	0.153951	-0.065733	-0.093936
66	C	5	Z	0.330084	0.009015	0.105188	-0.037222	-0.026014
67	C	6	S	0.003955	0.002646	-0.005192	-0.020974	0.035534

68	C	6	X	-0.002987	-0.001202	-0.006402	0.003073	0.005654
69	C	6	Y	0.019293	0.004931	0.096451	0.072196	-0.029422
70	C	6	Z	-0.069256	-0.012791	-0.270204	-0.215356	-0.056909
71	C	6	S	0.130247	0.003089	-0.057939	0.050036	0.106075
72	C	6	X	-0.068188	-0.110774	-0.039506	0.453446	0.644248
73	C	6	Y	0.015907	0.070624	0.476076	0.037996	-0.168479
74	C	6	Z	-0.076839	-0.007567	-0.225941	-0.231647	-0.095063
75	C	7	S	0.003439	0.000723	0.005292	-0.005740	-0.015765
76	C	7	X	-0.004207	-0.001872	-0.012692	0.004725	0.028993
77	C	7	Y	-0.003348	-0.012069	-0.090584	-0.027152	-0.012958
78	C	7	Z	-0.007717	0.039907	0.312182	0.115895	0.103598
79	C	7	S	0.042809	0.040996	-0.085353	-0.313335	-0.433059
80	C	7	X	-0.005504	0.011401	0.175820	0.085681	0.053209
81	C	7	Y	-0.000202	-0.083631	-0.158458	0.205425	0.269718
82	C	7	Z	-0.006147	0.025568	0.318374	0.177742	0.198019
83	C	8	S	-0.002763	-0.002786	-0.011930	-0.001859	0.015553
84	C	8	X	0.002646	0.002509	0.004767	-0.000589	0.004332
85	C	8	Y	0.071176	-0.000698	0.008725	-0.012254	0.000926
86	C	8	Z	-0.251514	-0.001198	-0.011182	0.057596	-0.059495
87	C	8	S	-0.034768	0.071803	0.143522	-0.088618	-0.042283
88	C	8	X	0.012764	-0.008476	-0.083388	-0.049338	-0.047130
89	C	8	Y	0.064068	-0.016111	0.001991	0.028239	0.052872
90	C	8	Z	-0.196146	-0.010526	-0.022951	0.075802	-0.053550
91	C	9	S	0.002824	0.003480	0.002157	-0.008610	0.001697
92	C	9	X	-0.004740	-0.005183	-0.008988	0.006928	0.001587
93	C	9	Y	-0.040775	0.006779	0.075577	0.051358	0.011952
94	C	9	Z	0.134902	-0.036340	-0.278131	-0.158665	-0.040677
95	C	9	S	0.032596	-0.026237	-0.097408	-0.055516	-0.006856
96	C	9	X	0.002007	-0.019127	-0.073978	-0.013873	-0.058652
97	C	9	Y	-0.050497	0.040121	0.138766	0.062315	0.038853
98	C	9	Z	0.086548	-0.019255	-0.249202	-0.157084	-0.033330
99	C	10	S	-0.010705	-0.007304	-0.005082	0.010017	-0.001595
100	C	10	X	0.019575	0.012678	0.023641	-0.009289	0.002241
101	C	10	Y	-0.046954	-0.012171	-0.075455	-0.023677	-0.021735
102	C	10	Z	0.210150	0.023713	0.232209	0.077953	0.092219
103	C	10	S	-0.113637	-0.010128	0.197474	0.136604	0.235108
104	C	10	X	0.012589	0.074935	0.087836	-0.029040	-0.019653
105	C	10	Y	-0.026940	-0.055819	-0.226591	-0.049560	-0.159875
106	C	10	Z	0.212189	0.001450	0.199373	0.078503	0.071840
107	C	11	S	0.004284	0.002494	-0.012239	-0.022605	0.029657
108	C	11	X	-0.026426	-0.000670	0.008709	0.020865	0.007890
109	C	11	Y	0.074606	-0.002578	0.000324	-0.000355	0.006565
110	C	11	Z	-0.275760	0.008115	0.041486	0.062576	-0.082549
111	C	11	S	-0.022726	-0.152432	-0.401769	0.198971	0.538151
112	C	11	X	-0.092659	-0.073504	-0.114352	0.167441	0.236969
113	C	11	Y	0.155769	-0.005969	-0.177386	-0.155031	-0.378299

114	C	11	Z	-0.236751	0.022394	-0.004058	0.014271	-0.180260
115	N	12	S	0.006782	0.000375	0.016372	-0.005582	0.015693
116	N	12	X	-0.019825	0.003843	0.016470	-0.004607	-0.006285
117	N	12	Y	-0.005822	0.006581	-0.011795	0.008524	-0.012175
118	N	12	Z	0.147404	-0.007751	0.019523	-0.045123	-0.024318
119	N	12	S	0.048032	0.016298	-0.000086	-0.046696	-0.007341
120	N	12	X	-0.028154	0.001214	0.007868	0.028024	-0.076385
121	N	12	Y	0.009361	0.014412	0.055239	-0.001737	-0.027039
122	N	12	Z	0.142750	-0.050487	0.005934	-0.006716	0.002889
123	C	13	S	-0.014807	-0.011718	-0.011667	0.057178	-0.008595
124	C	13	X	-0.026218	-0.001452	-0.016794	0.010838	0.007337
125	C	13	Y	-0.004522	0.027193	0.047230	-0.050796	0.005038
126	C	13	Z	-0.055494	0.063839	0.020748	-0.132763	-0.071391
127	C	13	S	0.071783	-0.118599	0.082763	0.459459	-0.365972
128	C	13	X	-0.114152	-0.026855	-0.119510	-0.056710	0.196866
129	C	13	Y	-0.019723	0.087373	0.000357	-0.106866	0.089007
130	C	13	Z	-0.049318	0.104351	0.031180	-0.120670	-0.062544
131	C	14	S	0.003055	-0.013067	-0.025736	0.036188	-0.027196
132	C	14	X	0.005557	0.012045	-0.009578	-0.018189	0.008061
133	C	14	Y	-0.051419	-0.024740	-0.001287	0.014046	0.048989
134	C	14	Z	-0.101959	-0.119107	-0.034916	0.157378	0.002544
135	C	14	S	-0.025011	-0.113037	-0.256285	0.244502	-0.290609
136	C	14	X	-0.096422	0.160841	-0.047069	-0.375985	0.350273
137	C	14	Y	-0.138029	-0.051567	-0.001110	-0.033776	0.384391
138	C	14	Z	-0.073243	-0.158091	-0.061265	0.201526	-0.062412
139	C	15	S	-0.015593	0.005904	0.011999	-0.010167	0.049220
140	C	15	X	-0.038200	0.049288	0.020770	-0.051717	0.090904
141	C	15	Y	0.054042	-0.138379	0.029343	-0.019555	-0.049110
142	C	15	Z	0.060988	-0.300639	0.115424	-0.212836	0.012810
143	C	15	S	-0.168003	0.093413	0.087341	-0.096556	0.420788
144	C	15	X	-0.005372	-0.030167	-0.013547	0.043065	0.101579
145	C	15	Y	0.010843	-0.087900	0.106770	-0.196667	0.279542
146	C	15	Z	0.077277	-0.310808	0.095534	-0.151997	-0.122579
147	C	16	S	0.008892	-0.008323	-0.017889	0.031572	-0.035501
148	C	16	X	0.002841	-0.028629	-0.000473	-0.009854	0.005885
149	C	16	Y	0.009715	0.173436	-0.013766	-0.027536	0.030634
150	C	16	Z	0.040398	0.403962	-0.075217	0.057734	-0.050673
151	C	16	S	0.080148	-0.117627	-0.112088	0.246458	-0.190591
152	C	16	X	0.000782	-0.030507	0.046489	-0.152626	0.197932
153	C	16	Y	0.030515	0.149925	-0.074576	0.038406	-0.019734
154	C	16	Z	0.027398	0.471573	-0.068167	0.035367	0.006557
155	C	17	S	-0.008374	0.005581	0.007543	-0.020088	0.023606
156	C	17	X	0.000186	0.019713	0.011580	-0.034413	0.025542
157	C	17	Y	-0.036546	-0.067340	-0.016232	0.071118	-0.016105
158	C	17	Z	-0.114665	-0.146971	-0.013990	0.111065	0.027464
159	C	17	S	-0.063373	0.097956	0.106461	-0.287437	0.288893

160	C	17	X	-0.020909	0.051449	0.037557	-0.108272	0.086963
161	C	17	Y	-0.042268	-0.052755	-0.023067	0.094354	-0.064391
162	C	17	Z	-0.100237	-0.163622	-0.005428	0.103921	0.049452
163	C	18	S	0.001631	-0.000747	-0.001460	0.006675	-0.002682
164	C	18	X	-0.001447	0.024069	-0.004871	0.010667	0.006396
165	C	18	Y	0.014886	-0.101497	0.040162	-0.081153	0.015902
166	C	18	Z	0.041993	-0.273302	0.089048	-0.169340	0.000451
167	C	18	S	0.064804	-0.085058	-0.006586	0.139430	-0.122378
168	C	18	X	0.020492	-0.011416	-0.017969	0.095108	-0.068390
169	C	18	Y	0.005338	-0.076674	0.049254	-0.131454	0.042115
170	C	18	Z	0.045993	-0.294139	0.081304	-0.142402	-0.007786
171	C	19	S	-0.009552	0.006813	0.002218	-0.020021	0.021179
172	C	19	X	-0.017121	-0.020802	0.011006	-0.033968	0.029448
173	C	19	Y	0.032264	0.137861	-0.027826	0.037461	-0.022238
174	C	19	Z	0.075813	0.378454	-0.057519	0.031383	-0.021769
175	C	19	S	-0.065603	0.161851	0.017555	-0.350373	0.211441
176	C	19	X	0.015392	-0.022428	0.019884	-0.048446	-0.023575
177	C	19	Y	0.070503	0.089599	-0.016516	0.183783	-0.171851
178	C	19	Z	0.052320	0.451899	-0.059454	-0.044044	0.022692
179	O	20	S	0.049119	-0.051765	-0.059910	0.139294	-0.128360
180	O	20	X	0.002053	0.027000	0.017985	-0.083645	0.098340
181	O	20	Y	-0.042308	0.087102	0.031346	-0.092994	0.088894
182	O	20	Z	-0.040318	0.082304	-0.004395	0.030244	-0.114170
183	O	20	S	0.119077	-0.150446	-0.173760	0.404390	-0.367611
184	O	20	X	-0.021365	0.031232	-0.000673	-0.067354	0.138628
185	O	20	Y	-0.030580	0.098687	0.019617	-0.104182	0.113998
186	O	20	Z	-0.026995	0.071494	-0.021465	0.065240	-0.108994
187	N	21	S	0.001028	-0.008573	-0.096807	0.016354	0.258382
188	N	21	X	0.011161	0.006044	0.031021	-0.034954	-0.038822
189	N	21	Y	-0.023149	0.000860	0.011908	-0.006573	-0.050341
190	N	21	Z	-0.016850	0.014023	0.038074	-0.038471	-0.114557
191	N	21	S	-0.007752	-0.003124	-0.336673	-0.020491	0.916161
192	N	21	X	0.025260	-0.013698	0.009533	-0.005427	-0.066406
193	N	21	Y	-0.035446	0.003310	0.021495	-0.019750	-0.052262
194	N	21	Z	-0.006570	0.030886	0.067519	0.013356	-0.120737
195	H	22	S	0.000493	-0.000308	-0.001578	-0.003045	-0.009535
196	H	22	S	0.001463	-0.009834	-0.010384	0.037827	0.034123
197	H	23	S	-0.002468	-0.000456	-0.002442	0.004300	0.005738
198	H	23	S	0.001078	0.006954	0.006995	-0.020274	-0.014362
199	H	24	S	-0.002325	-0.001786	-0.019529	-0.000923	0.036020
200	H	24	S	-0.013167	-0.014756	-0.026323	0.059316	-0.032473
201	H	25	S	0.002326	0.002452	0.009003	-0.001007	-0.008426
202	H	25	S	-0.000309	0.006263	0.037977	0.010859	-0.008894
203	H	26	S	-0.001131	0.001016	0.001431	0.000098	-0.000586
204	H	26	S	0.006893	-0.013871	-0.018883	-0.001788	-0.015923
205	H	27	S	-0.001048	-0.000065	0.008944	0.008201	0.004693

206	H	27	S	0.001884	0.085533	0.088036	-0.033557	0.006419
207	H	28	S	0.012166	0.003061	0.007839	-0.027334	0.014053
208	H	28	S	-0.008773	-0.018654	-0.053257	-0.092358	-0.018413
209	H	29	S	0.010193	-0.012767	-0.011589	0.037364	-0.030398
210	H	29	S	0.002889	0.003639	0.008943	-0.072583	0.096324
211	H	30	S	0.003353	0.000986	-0.001162	0.000699	-0.001417
212	H	30	S	-0.000224	0.008463	-0.002557	-0.002133	-0.010145
213	H	31	S	-0.002449	0.002839	0.003346	-0.010358	0.008173
214	H	31	S	0.002981	-0.011594	-0.005614	0.020902	-0.012293
215	H	32	S	0.003411	-0.006399	-0.007408	0.021340	-0.018356
216	H	32	S	-0.010032	0.010347	-0.022266	-0.026793	0.028093
217	H	33	S	-0.027619	0.069124	0.046505	-0.136239	0.133861
218	H	33	S	-0.096530	0.211421	0.152253	-0.454990	0.571586
219	H	34	S	0.074297	-0.009077	0.036677	0.056986	-0.109959
220	H	34	S	0.151423	0.031674	0.173272	0.029471	-0.453587
221	H	35	S	-0.021991	0.006975	0.042612	-0.008449	-0.079933
222	H	35	S	-0.072628	0.035750	0.165934	-0.059755	-0.388404

66	67	68
-0.2302	-0.2045	-0.1942
A	A	A

1	CO	1	S	0.031799	0.013717	-0.028145
2	CO	1	X	0.030726	-0.010272	0.013750
3	CO	1	Y	0.002028	0.000902	-0.007333
4	CO	1	Z	0.025136	-0.012088	-0.008926
5	CO	1	XX	-0.033996	-0.039091	-0.003361
6	CO	1	YY	0.022148	0.020981	0.093965
7	CO	1	ZZ	0.011848	0.018110	-0.090604
8	CO	1	XY	0.000412	-0.049632	0.000516
9	CO	1	XZ	0.024529	-0.036861	-0.038021
10	CO	1	YZ	-0.045020	0.061547	-0.027812
11	CO	1	XX	-0.016904	-0.018169	-0.005738
12	CO	1	YY	0.011470	0.011359	0.043055
13	CO	1	ZZ	0.005434	0.006810	-0.037317
14	CO	1	XY	-0.001493	-0.025737	0.000013
15	CO	1	XZ	0.014375	-0.021828	-0.014584
16	CO	1	YZ	-0.019104	0.027131	-0.003037
17	CO	1	S	-0.139439	-0.018488	0.023235
18	CO	1	X	-0.029855	0.065071	0.009101
19	CO	1	Y	0.051190	0.025466	-0.005062
20	CO	1	Z	-0.080014	0.014641	0.000221
21	CO	1	S	0.019319	-0.307510	0.999872
22	CO	1	X	-0.308039	0.005019	-0.444664
23	CO	1	Y	-0.049757	-0.157337	1.037384
24	CO	1	Z	-0.167581	0.192794	-0.155980
25	CO	1	S	0.017126	0.026657	-0.067957

26 CO 1 X -0.003374 -0.003050 -0.000149
27 CO 1 Y -0.004070 -0.001653 0.000077
28 CO 1 Z 0.001128 0.000905 0.002436
29 CO 1 XX -0.004260 -0.017502 0.035222
30 CO 1 YY 0.002566 0.002237 0.001542
31 CO 1 ZZ 0.001694 0.015265 -0.036765
32 CO 1 XY 0.016392 0.003098 0.020947
33 CO 1 XZ -0.003444 0.017972 -0.024403
34 CO 1 YZ -0.006154 -0.016500 -0.018674
35 C 2 S 0.008790 0.007215 0.009516
36 C 2 X -0.006647 -0.009782 0.017100
37 C 2 Y -0.041396 -0.048366 0.002854
38 C 2 Z 0.154942 0.181327 -0.079295
39 C 2 S -0.132630 0.076016 -0.020319
40 C 2 X 0.052817 -0.055373 0.006988
41 C 2 Y 0.013867 -0.060792 0.105036
42 C 2 Z 0.195026 0.267296 -0.074630
43 C 3 S 0.009748 0.006504 0.000834
44 C 3 X -0.005302 -0.000747 0.016201
45 C 3 Y 0.004753 0.003319 -0.021780
46 C 3 Z -0.044478 -0.023430 0.080235
47 C 3 S 0.181210 -0.001387 0.123200
48 C 3 X -0.091948 0.015113 -0.073175
49 C 3 Y 0.064890 0.025625 0.113552
50 C 3 Z -0.040764 -0.048806 0.137379
51 C 4 S 0.003866 -0.000421 0.042011
52 C 4 X 0.018970 0.018884 0.035670
53 C 4 Y 0.011573 0.025530 -0.098675
54 C 4 Z -0.101411 -0.134152 -0.033860
55 C 4 S -0.284217 0.078007 -0.174327
56 C 4 X 0.101861 0.029022 0.306104
57 C 4 Y -0.132070 0.056333 -0.369910
58 C 4 Z -0.188752 -0.196552 -0.141030
59 C 5 S 0.036788 0.016018 -0.015416
60 C 5 X -0.051964 -0.026917 0.001731
61 C 5 Y -0.094626 -0.078270 -0.033854
62 C 5 Z 0.181864 0.235527 -0.020917
63 C 5 S 0.401296 0.062892 -0.079032
64 C 5 X 0.195720 -0.129450 0.444090
65 C 5 Y -0.073780 -0.170953 -0.332123
66 C 5 Z 0.248220 0.279598 -0.103689
67 C 6 S 0.022835 0.000872 0.016692
68 C 6 X -0.016725 -0.002426 0.013311
69 C 6 Y 0.040964 0.068520 -0.039906
70 C 6 Z -0.119292 -0.211212 -0.015316
71 C 6 S 0.058261 -0.086512 0.076840

72	C	6	X	-0.310452	0.164834	-0.090504
73	C	6	Y	0.085106	0.008052	-0.526883
74	C	6	Z	-0.146703	-0.287741	-0.192525
75	C	7	S	0.004091	0.001271	-0.004975
76	C	7	X	0.000238	0.003912	0.010072
77	C	7	Y	0.032062	0.068216	-0.004458
78	C	7	Z	-0.119609	-0.242267	0.006975
79	C	7	S	0.213797	-0.053532	0.352629
80	C	7	X	-0.019297	-0.026364	-0.214574
81	C	7	Y	-0.091434	0.181659	0.023180
82	C	7	Z	-0.170363	-0.279892	0.029409
83	C	8	S	0.005660	-0.011578	-0.000899
84	C	8	X	-0.008181	0.001937	0.011714
85	C	8	Y	-0.016799	-0.077871	-0.023224
86	C	8	Z	0.098370	0.294817	0.066734
87	C	8	S	0.018566	-0.031409	-0.169649
88	C	8	X	0.021104	-0.032219	0.106081
89	C	8	Y	-0.046160	-0.050473	0.039651
90	C	8	Z	0.115686	0.411747	0.094371
91	C	9	S	0.001277	-0.009094	0.015690
92	C	9	X	0.001752	0.010145	-0.019894
93	C	9	Y	-0.001248	0.042606	0.015523
94	C	9	Z	0.012910	-0.150737	-0.091630
95	C	9	S	-0.012318	-0.030268	0.267394
96	C	9	X	0.056246	-0.066648	-0.024828
97	C	9	Y	-0.034810	0.083490	-0.072844
98	C	9	Z	-0.012265	-0.188070	-0.134080
99	C	10	S	0.006856	0.018355	-0.033789
100	C	10	X	-0.036849	0.008828	0.018220
101	C	10	Y	0.058443	-0.013677	-0.003550
102	C	10	Z	-0.074271	-0.123601	0.026980
103	C	10	S	-0.121720	0.136358	-0.420507
104	C	10	X	-0.050524	0.005564	-0.111900
105	C	10	Y	0.223123	-0.142528	0.040399
106	C	10	Z	-0.063940	-0.212193	0.084885
107	C	11	S	0.014327	-0.034577	-0.014033
108	C	11	X	-0.017069	0.060222	-0.042739
109	C	11	Y	-0.048770	-0.060038	-0.014537
110	C	11	Z	0.141591	0.316839	0.004625
111	C	11	S	0.027828	-0.157447	0.066205
112	C	11	X	-0.127407	0.238907	0.212914
113	C	11	Y	0.158498	-0.234849	0.257398
114	C	11	Z	0.225026	0.346373	0.049329
115	N	12	S	-0.004343	0.031286	-0.107303
116	N	12	X	-0.017244	0.062406	0.002541
117	N	12	Y	0.044319	-0.012037	0.042620

118	N	12	Z	0.133094	-0.249766	-0.059437
119	N	12	S	-0.001288	0.117337	-0.166853
120	N	12	X	-0.049907	0.100088	-0.036858
121	N	12	Y	0.051129	-0.011385	0.110375
122	N	12	Z	0.136253	-0.264495	-0.059980
123	C	13	S	-0.008722	0.043082	-0.043372
124	C	13	X	0.024051	0.006752	0.052605
125	C	13	Y	-0.089132	0.080969	0.030173
126	C	13	Z	-0.263080	0.176109	0.057387
127	C	13	S	-0.216965	0.165355	-0.528213
128	C	13	X	0.030050	0.055701	0.065559
129	C	13	Y	-0.104567	0.108285	0.404431
130	C	13	Z	-0.356509	0.270092	-0.075434
131	C	14	S	-0.032093	0.007775	-0.017734
132	C	14	X	-0.038186	0.022902	0.004995
133	C	14	Y	0.152355	-0.042093	-0.004646
134	C	14	Z	0.332225	-0.147191	-0.011831
135	C	14	S	-0.254165	-0.034595	0.332227
136	C	14	X	0.105360	0.046508	0.452862
137	C	14	Y	0.285186	0.062964	-0.323744
138	C	14	Z	0.404158	-0.268228	0.154569
139	C	15	S	0.006799	0.012113	-0.002818
140	C	15	X	0.039192	0.006157	0.051184
141	C	15	Y	-0.067507	0.025492	-0.067219
142	C	15	Z	-0.154732	0.051424	0.041862
143	C	15	S	0.074167	0.122269	0.009869
144	C	15	X	0.016261	0.019136	-0.415694
145	C	15	Y	0.067497	0.148922	-0.385760
146	C	15	Z	-0.256555	0.028576	0.121174
147	C	16	S	-0.022531	-0.009250	0.009654
148	C	16	X	0.013272	0.001762	-0.022935
149	C	16	Y	-0.006604	0.039624	-0.042292
150	C	16	Z	-0.106370	0.044147	0.028572
151	C	16	S	-0.144065	-0.062624	-0.356707
152	C	16	X	0.124123	0.069562	-0.286303
153	C	16	Y	-0.034903	0.044333	-0.220171
154	C	16	Z	-0.098127	0.074849	0.088846
155	C	17	S	0.005913	0.006511	0.016283
156	C	17	X	-0.011495	0.016949	-0.001404
157	C	17	Y	0.100813	-0.052102	-0.025153
158	C	17	Z	0.287256	-0.138808	-0.019310
159	C	17	S	0.141397	0.066772	0.210424
160	C	17	X	0.031315	0.031773	0.087771
161	C	17	Y	0.079509	-0.099464	0.120178
162	C	17	Z	0.340979	-0.162382	-0.084695
163	C	18	S	-0.005522	-0.002708	0.001563

164	C	18	X	0.022251	-0.011036	-0.017518
165	C	18	Y	-0.086149	0.059853	0.006161
166	C	18	Z	-0.242248	0.138951	0.027757
167	C	18	S	-0.093621	-0.039409	-0.212268
168	C	18	X	-0.043297	-0.036891	-0.071359
169	C	18	Y	-0.082523	0.049639	0.123549
170	C	18	Z	-0.259251	0.158032	-0.012999
171	C	19	S	0.006739	0.005574	0.019626
172	C	19	X	0.016699	0.002048	0.017947
173	C	19	Y	-0.017339	-0.001114	-0.002732
174	C	19	Z	-0.011184	-0.051907	-0.005719
175	C	19	S	0.156853	0.007390	0.536164
176	C	19	X	-0.016759	-0.063648	0.118278
177	C	19	Y	-0.126872	0.019824	-0.140258
178	C	19	Z	-0.047959	-0.005323	0.047775
179	O	20	S	-0.057489	-0.001769	-0.054072
180	O	20	X	0.056630	0.043530	0.001723
181	O	20	Y	0.101811	0.033398	-0.114214
182	O	20	Z	0.049192	-0.074224	0.029977
183	O	20	S	-0.188870	-0.020754	-0.126983
184	O	20	X	0.038421	0.056059	-0.017946
185	O	20	Y	0.107598	0.059482	-0.105214
186	O	20	Z	0.013730	-0.065928	0.053165
187	N	21	S	-0.010162	-0.011650	0.027228
188	N	21	X	0.011670	0.018789	0.113115
189	N	21	Y	-0.034222	-0.033754	-0.239601
190	N	21	Z	0.041583	-0.051826	0.084475
191	N	21	S	-0.032036	-0.056715	0.176355
192	N	21	X	0.009171	0.016634	0.173786
193	N	21	Y	-0.075591	-0.101746	-0.355481
194	N	21	Z	0.047362	-0.012271	0.084932
195	H	22	S	-0.002692	-0.005002	-0.010822
196	H	22	S	-0.039948	0.001419	-0.058436
197	H	23	S	-0.006547	-0.005459	-0.019927
198	H	23	S	0.015221	-0.017790	-0.014961
199	H	24	S	-0.005092	-0.003996	-0.005954
200	H	24	S	-0.114053	-0.043932	-0.476796
201	H	25	S	-0.002507	0.004788	0.000144
202	H	25	S	-0.016833	0.011548	-0.057662
203	H	26	S	-0.010210	0.010851	-0.006493
204	H	26	S	-0.000516	0.018115	0.000951
205	H	27	S	-0.002125	0.013460	-0.023438
206	H	27	S	-0.118020	0.117488	-0.034202
207	H	28	S	0.003670	-0.021508	-0.030128
208	H	28	S	0.046964	-0.130962	-0.257320
209	H	29	S	-0.011483	0.000421	-0.034323

210 H 29 S 0.090944 0.075347 -0.306125
211 H 30 S 0.003643 0.001420 -0.019675
212 H 30 S 0.010749 -0.003673 -0.029406
213 H 31 S 0.006579 -0.001251 -0.004709
214 H 31 S -0.007347 -0.006911 -0.066934
215 H 32 S -0.006812 -0.001919 -0.018587
216 H 32 S 0.026176 -0.041013 -0.043518
217 H 33 S 0.080690 0.027072 -0.017379
218 H 33 S 0.286566 0.203486 -0.242388
219 H 34 S 0.046637 0.073375 0.041189
220 H 34 S 0.208190 0.201245 0.354673
221 H 35 S -0.029042 -0.034442 -0.091464
222 H 35 S -0.093905 -0.144345 -0.742822

properties for the U-B3LYP density

ENERGY COMPONENTS

WAVEFUNCTION NORMALIZATION = 1.0000000000

ONE ELECTRON ENERGY = -2292.9669724318

TWO ELECTRON ENERGY = 1076.9099793933

NUCLEAR REPULSION ENERGY = 931.4200141894

TOTAL ENERGY = -284.6369788491

ELECTRON-ELECTRON POTENTIAL ENERGY = 1076.9099793933

NUCLEUS-ELECTRON POTENTIAL ENERGY = -2485.2237548798

NUCLEUS-NUCLEUS POTENTIAL ENERGY = 931.4200141894

TOTAL POTENTIAL ENERGY = -476.8937612971

TOTAL KINETIC ENERGY = 192.2567824480

VIRIAL RATIO (V/T) = 2.4805042258

MULLIKEN AND LOWDIN POPULATION ANALYSES

MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL
ALPHA ORBITALS

1 2 3 4 5

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.990371	0.998798	0.998973	0.999179	0.032428
2	0.000000	0.000000	0.000000	0.000000	-0.000002
3	-0.000002	-0.000001	0.000000	0.000000	0.000005
4	0.000014	0.000002	-0.000020	0.000006	-0.000059
5	0.000002	0.000263	-0.000176	0.000077	0.000225
6	0.001388	0.000081	0.000412	0.000012	0.000117
7	0.000020	-0.000001	0.000024	-0.000002	-0.000048
8	0.000000	0.000000	0.000000	0.000000	0.000005
9	0.000001	0.000000	-0.000001	0.000000	-0.000005
10	-0.000085	0.000001	0.000005	-0.000003	0.000062
11	-0.001321	0.000095	-0.000162	0.000002	0.000634
12	0.005030	0.000322	0.000425	0.000363	-0.001141
13	0.000599	-0.000085	0.000031	0.000301	0.025602
14	-0.000057	-0.000003	-0.000044	-0.000225	0.081554
15	0.000295	0.000078	0.000181	0.000224	0.051934
16	0.000022	0.000010	0.000027	0.000019	-0.011025
17	0.000000	0.000000	0.000000	0.000000	-0.002916
18	0.000000	0.000000	0.000000	0.000000	0.002367
19	0.000000	0.000001	-0.000001	-0.000001	-0.007312
20	0.001474	-0.000024	0.000119	0.000015	0.759769
21	0.002291	0.000541	0.000223	0.000032	0.000151
22	0.000000	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000	0.000000
24	0.000002	0.000001	0.000000	0.000000	-0.000001
25	0.000000	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000	0.000000
27	-0.000001	0.000000	0.000000	0.000000	0.000011
28	-0.000003	0.000000	0.000000	0.000005	0.000047
29	0.000000	0.000000	0.000000	0.000000	0.004502
30	0.000000	0.000000	0.000000	0.000000	0.000044
31	0.000000	0.000000	0.000000	0.000000	0.000003
32	0.000000	0.000000	0.000000	0.000000	-0.000339
33	0.000006	0.000000	-0.000021	0.000001	0.063380
34	-0.000051	-0.000045	-0.000003	0.000005	0.000000
35	0.000004	-0.000034	0.000006	-0.000010	0.000008

6 7 8 9 10

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.040682	0.061439	0.010685	0.012138	0.005150
2	-0.003109	0.014796	0.013316	0.158283	0.008241

3	0.002568	-0.013873	-0.000773	0.032494	0.134266
4	0.018004	0.055130	0.009428	0.099164	0.117600
5	0.094282	0.055709	0.015229	0.045311	0.025448
6	0.038948	0.130334	-0.042123	-0.105341	0.163122
7	-0.032978	-0.023123	0.001313	0.108314	0.124416
8	0.012903	-0.002201	0.007206	0.086361	-0.002830
9	-0.011371	-0.001243	0.002837	0.080979	0.072857
10	0.028647	-0.009177	0.032132	0.050287	0.119312
11	0.079331	0.066458	0.071118	0.238878	0.035826
12	0.362478	0.026519	0.001113	0.016183	0.006109
13	0.264107	0.040833	0.258289	0.020202	0.049368
14	0.008110	-0.005878	0.134247	0.032050	0.012979
15	0.038449	0.003383	0.046525	0.008568	0.027874
16	0.002057	-0.000229	0.127358	0.022118	0.011969
17	-0.000312	0.000164	0.092059	0.017026	0.028548
18	0.002237	0.000257	0.099309	0.016395	0.004665
19	-0.008845	-0.001415	0.074880	0.012903	0.009960
20	0.000445	0.000000	0.029161	0.003524	-0.000457
21	0.041411	0.494242	0.005124	0.030345	0.015900
22	0.000020	0.000165	0.000061	-0.000945	-0.004528
23	0.000022	-0.000152	-0.000267	-0.001173	0.006067
24	0.000136	0.008555	0.000039	0.002235	0.007184
25	0.000248	-0.000030	-0.000314	-0.003242	-0.002061
26	-0.000109	-0.000005	-0.000364	0.000636	0.003950
27	0.006635	0.001390	0.000135	-0.002787	0.005537
28	0.009538	0.002552	0.003903	0.001086	0.003590
29	-0.000003	-0.000024	0.000428	0.001449	0.000951
30	-0.000016	0.000001	0.005541	0.001492	0.002269
31	0.000082	0.000004	0.001997	0.000818	0.000144
32	0.000485	-0.000090	-0.008391	0.000130	-0.000159
33	0.000382	0.000040	0.006835	0.000419	0.000011
34	0.002348	0.045672	0.000441	0.007008	0.004512
35	0.002187	0.049797	0.001524	0.006692	0.002208

11 12 13 14 15

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.006405	0.005127	0.007248	0.003385	0.004469
2	0.019352	0.011122	0.066829	0.023258	0.098300
3	0.008533	0.004535	0.054160	0.086224	0.128715
4	0.026582	0.001744	0.009445	0.147663	0.050401
5	0.014385	0.010044	0.031888	0.107616	0.066554
6	-0.009867	0.011881	0.097678	0.112052	0.102349
7	0.071123	0.009460	0.074439	0.126691	0.099901
8	0.040144	0.012970	0.095370	0.033515	0.036771

9	0.093791	0.008432	0.033963	0.104082	0.055630
10	0.016942	0.002651	0.015568	0.140918	0.027803
11	0.065341	0.010245	0.113281	0.082090	0.066091
12	0.025497	0.002386	0.019873	0.000604	0.034870
13	0.047092	0.010708	0.016805	0.004159	0.056159
14	0.136297	0.060996	0.058206	0.000931	0.019657
15	0.095133	0.196302	0.056352	0.000256	0.012520
16	0.088313	0.120145	0.018081	0.000052	0.015723
17	0.127933	0.033626	0.079480	0.000142	0.033255
18	0.032645	0.218023	0.062837	0.000045	0.005119
19	0.056143	0.180752	0.016307	0.000045	0.016991
20	0.001534	0.062447	0.021543	0.000100	0.006145
21	0.009298	0.003027	0.021465	0.004029	0.036490
22	0.000449	0.000039	0.000620	-0.001055	-0.004976
23	0.000275	0.000090	0.001860	0.003510	0.003392
24	0.001374	0.000043	0.000257	0.008900	0.002289
25	-0.003987	-0.000070	0.003416	-0.000595	-0.001785
26	0.002338	0.000094	0.000672	0.004235	0.001831
27	0.000693	0.000053	-0.000151	0.004684	0.000973
28	0.008611	0.001354	0.000335	0.000665	0.004632
29	0.004530	0.000738	0.000233	0.000000	0.000405
30	0.007926	-0.000324	0.003284	0.000003	0.000962
31	0.000351	0.007503	0.001805	-0.000036	0.000005
32	0.000490	0.000344	-0.000023	0.000023	0.001045
33	0.000765	0.011929	0.005587	-0.000001	0.001788
34	0.001701	0.000671	0.005310	0.001216	0.009900
35	0.001866	0.000912	0.005977	0.000595	0.005625

16	17	18	19	20
----	----	----	----	----

1.000000	1.000000	1.000000	1.000000	1.000000
----------	----------	----------	----------	----------

1	0.013693	0.021539	0.021063	0.017754	0.016149
2	0.003479	0.000322	0.009503	0.072404	0.090087
3	0.004503	0.001688	0.048360	0.052714	0.076606
4	0.019731	0.007005	0.043883	0.091140	0.062719
5	0.015284	0.003489	0.022245	0.185488	0.080145
6	0.031572	-0.000090	0.012731	0.014197	0.095783
7	0.048933	0.019336	0.062912	0.112505	0.078123
8	0.065682	0.018919	0.033561	0.042859	0.025516
9	0.038384	0.007973	0.030121	0.112143	0.001710
10	0.040930	0.014742	0.057847	0.058566	0.039219
11	0.039804	0.021889	0.097485	0.060101	0.029466
12	0.075020	0.018700	0.042529	0.019407	0.034190
13	0.157388	0.024153	0.037943	0.009143	0.021429
14	0.046175	0.054551	0.062840	0.004129	0.020919

15	0.061926	0.142186	0.057539	0.002148	0.046354
16	0.055814	0.065930	0.065265	0.001165	0.029279
17	0.057416	0.094851	0.060066	0.002587	0.013851
18	0.014660	0.091847	0.055292	0.001453	0.031873
19	0.070112	0.090467	0.064541	0.001017	0.028176
20	0.067040	0.213909	0.063810	0.005776	0.044510
21	0.002968	0.000749	0.010333	0.068275	0.085207
22	-0.000297	-0.000038	-0.000124	0.003727	0.005084
23	0.000063	0.000001	0.002740	-0.000134	0.004692
24	0.002305	0.001260	0.002887	0.016697	0.000363
25	0.001357	0.001583	0.001237	-0.000490	0.001512
26	0.000555	0.000010	-0.000090	0.008230	0.000014
27	0.007039	0.001003	0.011609	0.000238	0.003404
28	0.029101	-0.000617	0.006167	0.003166	0.002831
29	0.004218	0.007319	0.000497	0.000047	0.001461
30	0.002270	0.003750	0.006300	0.000179	0.001836
31	0.000908	0.004197	0.002405	0.000254	0.002086
32	0.001204	0.002877	0.004490	0.000034	0.001629
33	0.019558	0.064430	0.000247	0.000866	0.000191
34	0.001042	0.000037	0.001674	0.000825	0.021168
35	0.000161	0.000033	0.000093	0.031391	0.002418

21	22	23	24	25
----	----	----	----	----

1.000000	1.000000	1.000000	1.000000	1.000000
----------	----------	----------	----------	----------

1	0.019923	0.071020	0.066147	0.110932	0.051340
2	0.014454	0.007974	0.021074	0.023050	0.011064
3	0.011885	0.006948	0.015788	0.038730	0.012261
4	-0.000914	-0.001247	0.018121	0.012352	0.015627
5	0.029983	0.018212	0.043490	0.032433	0.055847
6	0.026293	0.002450	0.002290	0.028493	0.033687
7	0.044011	0.026083	0.004867	0.027734	0.030412
8	0.041890	0.012616	0.027603	0.002109	0.033722
9	0.018887	0.009354	0.015245	0.025234	0.051790
10	0.027004	0.011553	0.031452	0.023961	0.015174
11	0.032782	0.013349	0.029687	0.019605	0.060481
12	0.057060	0.014757	0.029106	0.082630	0.139799
13	0.122974	0.023669	0.022257	0.041904	0.128099
14	0.054376	0.035668	0.007274	0.017127	0.021033
15	0.096909	0.016230	0.015409	0.057011	0.015392
16	0.025199	0.082161	0.004892	0.016808	0.029455
17	0.010823	0.075854	0.005228	0.048698	0.006302
18	0.006339	0.075535	0.002571	0.008465	0.012888
19	0.053896	0.076563	0.005884	0.039105	0.017684
20	0.139045	0.292850	0.031426	0.118619	0.007830

21	0.039174	0.015732	0.359014	0.136010	0.108280
22	0.004996	0.003665	0.002761	0.001277	0.002936
23	0.000865	0.000364	-0.000048	0.010878	0.002026
24	-0.000091	-0.000354	0.000373	0.000415	0.005728
25	0.007334	0.003281	0.001439	0.001069	0.000671
26	0.000119	0.000085	0.004153	0.003574	0.013806
27	0.000842	0.000807	0.005484	0.002287	0.002884
28	0.049933	0.005244	0.004680	0.001251	0.056524
29	0.008799	0.013413	0.002146	0.002445	0.015483
30	0.000594	0.000010	0.001124	0.013799	0.000244
31	0.000955	0.009382	0.000267	0.000175	0.001386
32	0.008025	0.022957	0.000323	0.001410	0.002304
33	0.035888	0.051011	0.000591	0.000206	0.001214
34	0.002631	0.000039	0.100925	0.048405	0.000509
35	0.007117	0.002765	0.116959	0.001798	0.036119

26	27	28	29	30
----	----	----	----	----

1.000000	1.000000	1.000000	1.000000	1.000000
----------	----------	----------	----------	----------

1	0.067184	0.106206	0.032281	0.367399	0.041339
2	0.040785	0.057290	0.007481	0.029778	0.080766
3	0.026096	0.058422	0.022871	0.026748	0.016878
4	0.027820	0.078615	0.057793	0.030278	0.031284
5	0.018079	0.029344	0.086097	0.013122	0.039698
6	0.007436	0.014329	0.030713	0.005532	0.142002
7	0.001572	0.033237	0.027219	0.003849	0.035148
8	0.011275	0.029021	0.072001	0.018226	0.112450
9	0.027370	0.021432	0.049899	0.015130	0.020532
10	0.018894	0.060952	0.065204	0.026971	0.052783
11	0.036924	0.064108	0.032091	0.021017	0.027786
12	0.046851	0.045061	0.025550	0.014817	0.034518
13	0.085090	0.019845	0.053058	0.005826	0.002700
14	0.039017	0.005459	0.048535	0.007850	0.008892
15	0.035832	0.005191	0.010017	0.031962	0.003906
16	0.065990	0.006905	0.044720	0.008776	0.021875
17	0.065230	0.007950	0.010128	0.003494	0.023086
18	0.083033	0.010958	0.044167	0.002178	0.031123
19	0.045234	0.004210	0.024777	0.002496	0.004518
20	0.116093	0.019920	0.024403	0.197769	0.006702
21	0.012851	0.201324	0.067705	0.084693	0.050080
22	0.002551	0.029943	0.000279	0.009683	0.032329
23	0.010255	0.009317	0.002363	0.013893	0.004151
24	0.015516	0.000524	0.038610	0.016132	0.023659
25	0.002191	0.000260	0.036258	0.003425	0.050066
26	0.008007	0.000439	0.004547	0.007415	0.002158

27	0.000144	0.043580	0.000738	0.019127	0.044831
28	0.008460	0.001083	0.020118	0.000433	0.003201
29	0.005049	0.000247	0.032461	0.000386	0.012123
30	0.023057	0.000303	0.000392	0.000876	0.007793
31	0.034343	0.003270	0.018350	0.000104	0.016717
32	0.006937	0.000034	0.000075	0.000730	0.000585
33	0.001340	0.000554	0.001121	0.000838	0.000704
34	0.003483	0.030756	0.001042	0.000759	0.000169
35	0.000013	-0.000091	0.006936	0.008288	0.013447

31 32 33 34 35

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.166029	0.085569	0.230877	0.340781	0.175573
2	0.012129	0.011983	0.032658	0.008571	0.014987
3	0.019316	0.025895	0.012278	0.007415	0.018224
4	0.034887	0.008147	0.017997	0.023049	0.006979
5	0.018558	0.023699	0.003377	0.017884	0.002954
6	0.018228	0.002234	0.008905	0.004631	0.002914
7	0.002456	0.016964	0.005833	0.007562	0.001651
8	0.010481	0.007055	0.000175	0.019963	0.001317
9	0.026847	0.004256	0.001083	0.027232	0.001078
10	0.029651	0.010603	0.000485	0.012845	0.006920
11	0.015246	0.012166	0.003750	0.017869	0.006348
12	0.066788	0.029126	0.032632	0.140890	0.007597
13	0.031082	0.036084	0.036800	0.053205	0.025294
14	0.048164	0.045260	0.020489	0.018593	0.092763
15	0.069815	0.093369	0.043104	0.025198	0.085349
16	0.079184	0.030073	0.042148	0.009423	0.081058
17	0.068487	0.021226	0.113788	0.021193	0.071277
18	0.049788	0.023608	0.081867	0.028429	0.071951
19	0.030947	0.027038	0.081949	0.029287	0.102500
20	0.031467	0.297586	0.014861	0.048524	0.066744
21	0.006181	0.125583	0.015396	0.014473	0.029773
22	0.000204	0.000799	0.020869	-0.000049	0.002759
23	0.005289	0.015009	0.003749	-0.000015	0.013742
24	0.019023	0.000447	0.008386	0.016836	0.001204
25	0.000619	0.002860	0.000387	-0.000472	0.000824
26	0.015456	0.000284	0.000626	0.018665	0.000068
27	0.008675	0.007995	0.000354	0.002080	0.002203
28	0.002116	0.024963	0.000174	0.014702	0.048924
29	0.046599	0.001432	0.011000	0.007471	0.021493
30	0.027994	0.003662	0.067936	0.012367	0.000500
31	0.022658	0.002111	0.017012	0.013146	0.000114
32	0.003927	0.000217	0.065022	0.031805	0.026326

33	0.007385	0.000124	0.000149	0.000325	0.004576
34	0.000794	0.002011	0.003886	0.001317	0.000480
35	0.003530	0.000561	-0.000001	0.004805	0.003532

36 37 38 39 40

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.129481	0.265354	0.217209	0.111689	0.204663
2	0.082670	0.028311	0.027443	0.045739	0.015815
3	0.041038	0.020683	0.045024	0.040938	0.035612
4	0.028382	0.008938	0.057239	0.082561	0.019320
5	0.026972	0.014490	0.041629	0.097467	0.054505
6	0.005245	0.010162	0.062097	0.085802	0.081246
7	0.025287	0.012785	0.069407	0.025680	0.029674
8	0.067684	0.038271	0.063726	0.055041	0.010010
9	0.043593	0.016978	0.080320	0.068880	0.008275
10	0.019877	0.016219	0.078873	0.092607	0.022883
11	0.021012	0.040458	0.022096	0.086549	0.092979
12	0.012958	0.054634	0.010228	0.005437	0.088506
13	0.029701	0.063365	0.002442	0.008199	0.072834
14	0.023055	0.048402	0.008536	0.002338	0.051133
15	0.044786	0.016978	0.020757	0.001985	0.010823
16	0.063649	0.067557	0.006729	0.001037	0.013365
17	0.008635	0.030511	0.001930	0.000424	0.017890
18	0.009663	0.012936	0.002369	0.000599	0.005554
19	0.063501	0.066660	0.002392	0.000798	0.017558
20	0.030088	0.015473	0.043547	0.001358	0.001314
21	0.024771	0.008188	0.014430	0.013765	0.046847
22	0.019611	0.004157	0.001461	0.020083	0.000422
23	0.013920	0.012703	0.016901	0.004845	0.024596
24	-0.000003	0.000071	0.029933	0.049727	0.000106
25	0.012754	0.010526	0.006018	0.022022	0.003071
26	0.023067	0.005353	0.033427	0.021051	0.001130
27	0.000553	-0.000059	0.024471	0.044056	0.014877
28	0.011828	0.007319	0.000252	0.003355	0.026722
29	0.063871	0.061587	0.000618	0.000293	0.006178
30	0.000471	0.008771	0.000494	0.000135	0.013806
31	0.000144	0.000174	0.001558	0.000429	0.001175
32	0.051648	0.031470	0.001155	0.000208	0.004145
33	0.000190	0.000418	0.000346	0.000067	0.000005
34	-0.000003	0.000021	0.000120	0.000253	0.000043
35	-0.000099	0.000136	0.004824	0.004582	0.002916

41 42 43 44 45

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.507763	0.851817	0.439364	0.132458	0.046951
2	0.031853	0.011935	0.025737	0.038128	0.031568
3	0.021218	0.002607	0.031245	0.077091	0.015047
4	0.024154	0.007153	0.028794	0.048316	0.015879
5	0.022482	0.008738	0.004519	0.061743	0.019377
6	0.021740	0.004379	0.012972	0.041948	0.087119
7	0.026772	0.007118	0.019969	0.024236	0.072878
8	0.008145	0.005973	0.027384	0.027166	0.030761
9	0.010313	0.001035	0.038930	0.065794	0.031545
10	0.018282	0.004850	0.025051	0.036086	0.036599
11	0.008198	0.007477	0.017821	0.032823	0.059143
12	0.043185	0.004522	0.069352	0.028042	0.003350
13	0.026813	0.003131	0.045137	0.040382	0.023866
14	0.012930	0.002948	0.013606	0.015200	0.118751
15	0.015016	0.001823	0.003220	0.000517	0.053056
16	0.005326	0.001732	0.001118	0.000231	0.046513
17	0.004701	0.001321	0.002057	0.000531	0.041404
18	0.016568	0.001245	0.004446	0.001970	0.044845
19	0.007732	0.001313	0.005799	0.005476	0.071676
20	0.069869	0.014456	0.043853	0.035930	0.059681
21	0.042697	0.020790	0.015875	0.037442	0.061639
22	0.007697	0.004751	0.002965	0.006877	0.006497
23	0.000109	0.000399	0.019552	0.076731	0.000873
24	0.010465	0.000035	0.037081	0.041273	0.004920
25	0.001579	0.002206	0.000320	0.003895	0.000289
26	0.001450	0.000007	0.030662	0.073552	0.009718
27	0.012604	0.003926	0.023677	0.037582	0.000421
28	0.005385	0.001950	0.001192	0.001408	0.000169
29	0.001265	0.000303	0.000051	0.000037	0.000065
30	0.000079	0.000001	0.002437	0.000219	0.001040
31	0.011597	0.000292	0.003433	0.000879	0.000514
32	0.000169	-0.000021	0.000261	0.000044	0.000143
33	0.001230	0.006104	0.000107	0.000007	0.000029
34	0.000207	0.008581	0.000798	0.001117	0.003048
35	0.000406	0.005102	0.001215	0.004871	0.000629

46 47 48 49 50

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.026121	0.007517	0.011201	0.057641	0.052616
2	0.005497	0.009510	0.076891	0.046797	0.080169
3	0.006915	0.009037	0.070632	0.034588	0.083027
4	0.005123	0.008596	0.069768	0.032516	0.054357

5	0.004801	0.000422	0.005359	0.031370	0.034459
6	0.006669	0.004081	0.015922	0.051531	0.053324
7	0.005511	0.005336	0.029878	0.084028	0.076017
8	0.001442	0.016615	0.078858	0.061947	0.105752
9	0.000584	0.010497	0.064379	0.033895	0.058519
10	0.001149	0.009768	0.071513	0.033187	0.020501
11	0.001099	0.001323	0.001405	0.009054	0.011450
12	0.017710	0.002850	0.006606	0.114507	0.036124
13	0.030259	0.001681	0.004901	0.032515	0.010307
14	0.042950	0.050718	0.026611	0.022355	0.002594
15	0.032913	0.032594	0.016499	0.030758	0.003490
16	0.084030	0.066472	0.020652	0.048459	0.009740
17	0.124246	0.149612	0.031197	0.047243	0.011903
18	0.152640	0.158471	0.032163	0.041113	0.010410
19	0.118189	0.080449	0.026874	0.034890	0.007077
20	0.021806	0.005995	0.020266	0.036407	0.010599
21	0.002990	0.000994	0.003742	0.014404	0.047608
22	0.003106	0.009453	0.079897	0.005707	0.076495
23	0.006057	0.003605	0.025001	0.000393	0.003635
24	0.000089	0.003914	0.026089	0.000223	0.043479
25	0.000158	0.018159	0.083853	0.052942	0.023781
26	0.000125	0.003458	0.016254	0.001749	0.061362
27	0.000462	0.005976	0.032969	0.015335	0.006338
28	0.002608	0.001736	0.002115	0.011835	0.002332
29	-0.000124	0.075943	0.011981	0.001088	0.000174
30	0.149036	0.036769	0.007809	0.005694	0.000057
31	0.141167	0.083393	0.008604	0.001963	0.000103
32	0.004079	0.121492	0.017977	0.000674	0.000238
33	0.000342	0.003451	0.001076	0.001432	0.000264
34	0.000070	0.000067	0.001144	0.001803	0.000591
35	0.000182	0.000045	-0.000087	-0.000042	0.001107

51 52 53 54 55

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.034465	0.061494	0.141737	0.011923	0.004737
2	0.116640	0.023722	0.033054	0.063527	0.054283
3	0.077880	0.055065	0.074731	0.007611	0.026303
4	0.048250	0.089336	0.082131	0.016237	0.000914
5	0.024684	0.069911	0.031808	0.065083	0.035563
6	0.058375	0.011706	0.005864	0.031695	0.029435
7	0.094964	0.018258	0.005101	0.090044	0.016826
8	0.055637	0.049526	0.042803	0.124191	0.010486
9	0.059837	0.081683	0.092224	0.050629	0.000253
10	0.032837	0.104398	0.105120	0.003414	0.008386

11	0.045605	0.085065	0.034423	0.066784	0.012831
12	0.049158	0.089950	0.167014	0.034973	0.034346
13	0.008771	0.056140	0.014774	0.040863	0.001726
14	0.008854	0.012588	0.006797	0.117213	0.033793
15	0.002357	0.005127	0.002180	0.000148	0.100903
16	0.005288	0.030752	0.002112	0.096285	0.220926
17	0.003864	0.035687	0.000302	0.124012	0.011304
18	0.005302	0.020248	0.000909	0.028160	0.112202
19	0.004724	0.002797	0.003063	0.017195	0.251954
20	0.009781	0.011623	0.011722	0.000750	0.027028
21	0.013132	0.013318	0.096195	0.004175	0.003895
22	0.042080	0.001020	0.000417	0.000000	0.000013
23	0.094371	0.005805	0.004936	0.000002	0.000033
24	0.004694	0.003221	0.000511	0.000042	-0.000004
25	0.049299	0.005298	0.000999	0.000026	0.000002
26	0.003887	0.032280	0.009940	0.000777	0.000065
27	0.031803	0.003016	0.000855	0.000148	-0.000053
28	0.006129	0.012027	0.020110	0.000817	0.000448
29	0.000172	0.000259	0.000189	0.000005	0.000000
30	0.002769	0.000551	0.000201	0.000005	0.000015
31	0.003389	0.000275	0.000195	0.000013	0.000001
32	0.000089	0.000305	0.000076	0.000008	0.000006
33	0.000747	0.001166	0.001740	0.000107	0.000019
34	0.000069	0.001411	0.001687	0.002311	0.001319
35	0.000096	0.004972	0.004082	0.000828	0.000043

56 57 58

1.000000 1.000000 1.000000

1	0.012857	0.002309	0.009280
2	0.074584	0.000652	0.142187
3	0.036524	0.122830	0.091486
4	0.002263	0.191888	0.029067
5	0.052738	0.001753	0.134780
6	0.050276	0.183891	0.000121
7	0.018667	0.163074	0.000339
8	0.013909	0.000095	0.172014
9	0.000684	0.136245	0.095060
10	0.010453	0.190789	0.041399
11	0.016045	0.001878	0.160030
12	0.064393	0.001019	0.015523
13	0.000589	0.001213	0.036159
14	0.104630	0.000345	0.009638
15	0.145087	0.000247	0.009106
16	0.002226	0.000120	0.004691

17	0.127570	0.000474	0.019032
18	0.191166	0.000125	0.000621
19	0.018702	0.000139	0.013143
20	0.038318	0.000015	0.000364
21	0.015548	0.000232	0.009742
22	0.000054	-0.000006	0.000005
23	0.000164	0.000013	0.000019
24	-0.000007	0.000009	0.000051
25	0.000007	0.000017	0.000010
26	0.000291	0.000055	0.000003
27	0.000008	-0.000002	-0.000052
28	0.000052	0.000294	0.001151
29	0.000020	0.000002	0.000003
30	0.000000	0.000000	0.000001
31	0.000005	0.000000	0.000000
32	0.000024	-0.000011	0.000021
33	0.000283	-0.000003	0.000083
34	0.001824	0.000205	0.004891
35	0.000046	0.000095	0.000035

MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL
BETA ORBITALS

	1	2	3	4	5
	1.000000	1.000000	1.000000	1.000000	1.000000
1	0.995125	0.999459	0.999087	0.998568	0.031337
2	0.000000	0.000000	-0.000001	0.000000	-0.000001
3	-0.000001	0.000000	0.000001	-0.000001	0.000005
4	0.000005	0.000005	-0.000036	0.000019	-0.000059
5	0.000103	-0.000004	-0.000416	0.000394	0.000209
6	0.000633	-0.000015	0.000569	0.000099	0.000148
7	0.000010	-0.000004	0.000028	-0.000001	-0.000045
8	0.000000	0.000000	0.000001	0.000000	0.000005
9	0.000000	0.000000	-0.000001	0.000000	-0.000005
10	-0.000037	-0.000001	0.000013	0.000006	0.000047
11	-0.000543	-0.000025	-0.000317	0.000164	0.000635
12	0.002341	0.000261	0.000367	0.000253	-0.001081
13	0.000345	0.000202	0.000062	-0.000015	0.026249
14	-0.000108	-0.000158	-0.000032	-0.000133	0.083520
15	0.000280	0.000109	0.000169	0.000235	0.054318
16	0.000018	0.000013	0.000033	0.000030	-0.012203
17	0.000000	0.000000	0.000000	0.000000	-0.002943
18	0.000000	0.000000	0.000000	0.000000	0.002415
19	-0.000001	-0.000001	0.000000	0.000001	-0.007437

20	0.000687	-0.000024	0.000112	0.000063	0.756270
21	0.001174	0.000183	0.000379	0.000400	0.000169
22	0.000000	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000	0.000000
24	0.000001	0.000000	0.000000	0.000002	-0.000001
25	0.000000	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000001	0.000001	0.000011
28	-0.000001	0.000003	0.000002	0.000003	0.000046
29	0.000000	0.000000	0.000000	0.000000	0.004555
30	0.000000	0.000000	0.000000	0.000000	0.000048
31	0.000000	0.000000	0.000000	0.000000	0.000003
32	0.000000	0.000000	0.000000	0.000000	-0.000350
33	-0.000001	0.000000	-0.000034	0.000002	0.064128
34	-0.000029	-0.000008	0.000002	-0.000038	-0.000001
35	-0.000001	0.000004	0.000011	-0.000050	0.000009

6 7 8 9 10

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.038629	0.057029	0.010276	0.011455	0.004983
2	-0.002709	0.014922	0.013066	0.155634	0.003688
3	0.002538	-0.014309	-0.000647	0.035474	0.139826
4	0.021354	0.053313	0.008976	0.095372	0.112837
5	0.099678	0.053358	0.015691	0.047771	0.028343
6	0.031951	0.141741	-0.042314	-0.114815	0.157026
7	-0.034242	-0.023085	0.001880	0.117065	0.128955
8	0.012827	-0.002011	0.006932	0.085207	-0.004458
9	-0.010727	-0.001749	0.003152	0.083715	0.074702
10	0.028637	-0.010151	0.031942	0.048198	0.115417
11	0.088147	0.065897	0.071202	0.239987	0.038831
12	0.340463	0.033141	0.001473	0.016435	0.005746
13	0.266074	0.050429	0.255411	0.021754	0.050219
14	0.007182	-0.006951	0.131691	0.030868	0.013495
15	0.038224	0.004567	0.048794	0.009203	0.028497
16	0.002235	-0.000191	0.125835	0.021613	0.012172
17	-0.000351	0.000184	0.094486	0.017592	0.029408
18	0.002479	0.000352	0.097732	0.015875	0.004717
19	-0.008831	-0.001761	0.077978	0.013282	0.010199
20	0.000581	0.000018	0.029480	0.003488	-0.000459
21	0.052255	0.477464	0.005216	0.030984	0.016230
22	0.000030	0.000164	0.000054	-0.001177	-0.004817
23	0.000022	-0.000147	-0.000258	-0.001045	0.006400
24	0.000307	0.008672	0.000032	0.002062	0.006879
25	0.000253	-0.000030	-0.000333	-0.003438	-0.002090

26	-0.000089	-0.000007	-0.000344	0.000731	0.004090
27	0.006386	0.001701	0.000140	-0.002857	0.005308
28	0.009464	0.003124	0.003771	0.001221	0.003686
29	-0.000003	-0.000026	0.000326	0.001426	0.000956
30	-0.000018	0.000000	0.005664	0.001529	0.002329
31	0.000088	0.000007	0.001923	0.000802	0.000139
32	0.000473	-0.000099	-0.008213	0.000157	-0.000169
33	0.000395	0.000061	0.006975	0.000418	0.000011
34	0.003240	0.045059	0.000454	0.007172	0.004617
35	0.003057	0.049312	0.001558	0.006841	0.002289

11	12	13	14	15
----	----	----	----	----

1.000000	1.000000	1.000000	1.000000	1.000000
----------	----------	----------	----------	----------

1	0.005680	0.004146	0.006952	0.002888	0.004074
2	0.019369	0.009035	0.065434	0.023966	0.096486
3	0.009309	0.003565	0.054714	0.087929	0.129450
4	0.026867	0.001487	0.009788	0.146408	0.051755
5	0.015223	0.008645	0.032986	0.106346	0.067355
6	-0.010999	0.009635	0.098134	0.110831	0.103168
7	0.073877	0.008055	0.077019	0.129036	0.099663
8	0.038263	0.010587	0.096398	0.034330	0.035831
9	0.096706	0.007319	0.035187	0.105167	0.056003
10	0.016307	0.002234	0.016230	0.140751	0.027175
11	0.066409	0.008461	0.117643	0.080065	0.065866
12	0.025466	0.001897	0.020603	0.000619	0.033731
13	0.045651	0.009745	0.019181	0.003922	0.056396
14	0.134714	0.060651	0.057694	0.000903	0.019345
15	0.094631	0.201161	0.052082	0.000343	0.012536
16	0.087475	0.120558	0.018613	0.000074	0.015628
17	0.128078	0.035167	0.078711	0.000204	0.033134
18	0.032486	0.224447	0.056019	0.000082	0.005028
19	0.056462	0.182458	0.015786	0.000028	0.017036
20	0.001430	0.064334	0.019366	0.000101	0.006101
21	0.009662	0.002468	0.022134	0.003960	0.037333
22	0.000460	0.000021	0.000619	-0.001063	-0.005123
23	0.000310	0.000071	0.001957	0.003615	0.003537
24	0.001362	0.000037	0.000247	0.008765	0.002363
25	-0.004198	-0.000103	0.003494	-0.000624	-0.001808
26	0.002477	0.000081	0.000740	0.004281	0.001840
27	0.000621	0.000051	-0.000150	0.004671	0.000953
28	0.008175	0.001332	0.000391	0.000609	0.004698
29	0.004462	0.000638	0.000274	0.000001	0.000407
30	0.007924	-0.000326	0.003310	0.000004	0.000965
31	0.000346	0.007681	0.001560	-0.000037	0.000005

32	0.000504	0.000346	0.000017	0.000027	0.001059
33	0.000748	0.012809	0.005100	-0.000003	0.001787
34	0.001787	0.000550	0.005540	0.001232	0.010325
35	0.001957	0.000756	0.006227	0.000568	0.005897

16 17 18 19 20

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.009910	0.016172	0.012331	0.015772	0.006915
2	0.003560	0.000314	0.009953	0.074620	0.087631
3	0.004834	0.001821	0.050577	0.055597	0.074577
4	0.019596	0.007500	0.051728	0.087425	0.059780
5	0.015113	0.003324	0.027993	0.185797	0.076974
6	0.029981	-0.000074	0.012115	0.015831	0.095097
7	0.049092	0.020747	0.073671	0.108326	0.076614
8	0.064834	0.020035	0.032111	0.048800	0.022545
9	0.037740	0.008500	0.032917	0.113066	0.000557
10	0.042238	0.015354	0.066510	0.055803	0.035617
11	0.039827	0.023451	0.097997	0.066058	0.026750
12	0.071998	0.019243	0.038789	0.018056	0.035638
13	0.156021	0.023958	0.034602	0.009932	0.024975
14	0.046935	0.056878	0.061726	0.003465	0.026863
15	0.063447	0.143702	0.053062	0.002234	0.052965
16	0.056467	0.068686	0.063558	0.000657	0.035367
17	0.057853	0.097914	0.058811	0.001555	0.016051
18	0.016068	0.094126	0.051523	0.001535	0.036147
19	0.071811	0.091815	0.062592	0.000449	0.033757
20	0.070228	0.202628	0.051466	0.006493	0.043157
21	0.003104	0.000731	0.012658	0.065139	0.079730
22	-0.000310	-0.000040	-0.000049	0.003493	0.005516
23	0.000069	0.000001	0.002862	0.000122	0.004543
24	0.002327	0.001290	0.004364	0.015426	0.000400
25	0.001414	0.001707	0.001092	-0.000247	0.001693
26	0.000577	0.000010	0.000079	0.008399	-0.000010
27	0.006980	0.001061	0.013081	-0.000131	0.003051
28	0.027534	-0.000603	0.005501	0.003489	0.004459
29	0.004323	0.007483	0.000596	0.000027	0.002071
30	0.002327	0.003939	0.006352	0.000066	0.002298
31	0.001032	0.004317	0.002030	0.000317	0.002299
32	0.001143	0.003382	0.004547	0.000059	0.002493
33	0.020628	0.060543	0.000309	0.000936	0.000910
34	0.001109	0.000076	0.001931	0.001390	0.019631
35	0.000192	0.000010	0.000615	0.030044	0.002941

21 22 23 24 25

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.005584	0.036288	0.024006	0.031353	0.026452
2	0.018249	0.006397	0.026212	0.016215	0.020549
3	0.011581	0.008626	0.018057	0.049501	0.003384
4	-0.000585	-0.001336	0.020116	0.010793	0.021956
5	0.031775	0.019167	0.049311	0.054855	0.033427
6	0.029533	0.001567	0.008998	0.039241	0.014275
7	0.044554	0.028907	0.004819	0.048946	0.006464
8	0.040149	0.012529	0.026801	0.014436	0.028685
9	0.017380	0.012244	0.009834	0.067088	0.018258
10	0.025106	0.015655	0.032162	0.032870	0.016747
11	0.032279	0.011833	0.030741	0.051051	0.031687
12	0.052959	0.020538	0.006293	0.089198	0.131158
13	0.127007	0.025210	0.008420	0.042261	0.176430
14	0.054492	0.035264	0.001945	0.010273	0.042273
15	0.106176	0.025038	0.001172	0.027999	0.037576
16	0.023998	0.095495	0.002437	0.008382	0.039264
17	0.014537	0.084846	0.000100	0.038280	0.015779
18	0.005625	0.075609	0.001965	0.017654	0.021027
19	0.055983	0.088949	0.000801	0.025773	0.019665
20	0.142250	0.257512	0.004737	0.130747	0.080464
21	0.039516	0.016540	0.436146	0.118587	0.048076
22	0.005890	0.003184	0.003412	0.001634	0.002738
23	0.000635	0.000987	0.000674	0.014283	0.000214
24	-0.000110	-0.000249	0.000450	-0.000004	0.009966
25	0.007395	0.003431	0.000864	0.001168	0.003670
26	0.000149	0.000466	0.002960	0.016738	0.002305
27	0.000695	0.000795	0.008055	0.000955	0.004239
28	0.046311	0.007585	0.002728	0.001129	0.081125
29	0.008876	0.014963	0.000498	0.000366	0.022943
30	0.001215	0.001032	0.000013	0.009487	0.004183
31	0.001113	0.011164	0.000273	0.000266	0.004643
32	0.007448	0.025175	0.000009	-0.000316	0.002167
33	0.032744	0.051102	0.000462	0.002917	0.006853
34	0.003558	0.000145	0.140102	0.011381	0.003026
35	0.005933	0.003341	0.124428	0.014492	0.018328

26 27 28 29 30

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.023694	0.040545	0.005817	0.003739	0.021171
2	0.047269	0.051845	0.019933	0.091514	0.003346
3	0.035009	0.070007	0.013390	0.024628	0.003196

4	0.034581	0.091712	0.064321	0.050865	0.011329
5	0.021013	0.029805	0.081693	0.043608	0.022890
6	0.007920	0.013845	0.040299	0.156910	-0.000153
7	0.003953	0.046981	0.010231	0.032057	0.008576
8	0.011993	0.035967	0.072085	0.116477	0.013494
9	0.021167	0.040249	0.041817	0.028241	0.019673
10	0.012673	0.080407	0.069939	0.058472	0.008680
11	0.046970	0.060689	0.040072	0.025511	0.005767
12	0.020492	0.058774	0.022636	0.031598	0.055412
13	0.061212	0.031995	0.056695	0.011059	0.029269
14	0.030012	0.003758	0.052454	0.007939	0.078043
15	0.036520	0.005586	0.008441	0.005433	0.140511
16	0.048477	0.012737	0.050495	0.011199	0.072503
17	0.069221	0.010547	0.010283	0.010222	0.051612
18	0.062781	0.015082	0.051038	0.016082	0.054238
19	0.047788	0.005962	0.024022	0.005620	0.045479
20	0.193289	0.001606	0.014472	0.012290	0.232699
21	0.024297	0.158794	0.056353	0.049113	0.013076
22	0.009569	0.026321	0.005590	0.036327	-0.000015
23	0.014501	0.011697	-0.000205	0.004859	0.000090
24	0.014591	0.001272	0.046625	0.039374	0.009978
25	0.000354	0.002234	0.035678	0.050391	0.006422
26	0.008798	-0.000036	0.006085	0.007426	0.012331
27	0.002737	0.049609	0.006952	0.043372	0.000982
28	0.010569	0.005933	0.019202	0.000630	0.012027
29	0.004562	0.000114	0.036744	0.001232	0.024826
30	0.031762	0.000688	0.000264	0.000011	0.011885
31	0.025032	0.006001	0.023846	0.007149	0.018803
32	0.006656	0.000981	0.000044	0.000240	0.006228
33	0.004064	-0.000096	0.001278	0.000577	0.003961
34	0.006631	0.028507	0.000025	0.000144	-0.000020
35	-0.000155	-0.000118	0.011389	0.015691	0.001692

31 32 33 34 35

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.024858	0.049479	0.014140	0.008159	0.010029
2	0.001363	0.082515	0.026543	0.003933	0.017681
3	0.007033	0.108861	0.007059	0.010141	0.003629
4	0.004968	0.038240	0.008389	0.031052	0.023356
5	0.005595	0.031191	0.017010	0.007219	0.048531
6	0.002714	0.009668	0.002216	0.011744	0.017666
7	0.002338	0.035574	0.006960	0.013855	0.033507
8	0.000569	0.034151	0.008952	0.020868	0.075901
9	0.003128	0.019204	0.014721	0.023880	0.085745

10	0.005006	0.042324	0.005136	0.012945	0.053591
11	0.011145	0.046636	0.001058	0.013794	0.028241
12	0.047052	0.037796	0.010836	0.037736	0.079778
13	0.036773	0.018891	0.016251	0.022649	0.057757
14	0.060433	0.004535	0.020590	0.094465	0.027902
15	0.130764	0.003489	0.083705	0.047451	0.023891
16	0.055631	0.003226	0.075450	0.118544	0.057989
17	0.063681	0.011886	0.114243	0.079493	0.008564
18	0.045202	0.003407	0.109705	0.069729	0.006722
19	0.013263	0.006916	0.126537	0.140336	0.059941
20	0.363132	0.012069	0.077800	0.028243	0.024466
21	0.014920	0.270633	0.014504	0.002074	0.058298
22	-0.000015	-0.000237	0.010189	0.006157	0.003866
23	0.004552	0.061099	0.001527	0.004255	0.001575
24	0.002488	0.001010	-0.000057	0.024353	0.015186
25	0.000151	0.000174	0.000000	0.002078	0.006986
26	0.002052	0.002822	0.009973	0.011546	0.049439
27	0.001306	0.030968	0.000663	0.000022	0.002482
28	0.000381	0.001733	0.000878	0.021396	0.009620
29	0.023901	0.001919	0.031669	0.074996	0.060227
30	0.035279	0.009844	0.056539	0.002215	0.000453
31	0.023727	0.000074	0.025118	0.000341	0.000086
32	0.003612	0.006111	0.099647	0.049383	0.045350
33	0.002664	0.000687	0.000720	0.004408	0.000107
34	-0.000038	0.006623	0.000633	0.000104	-0.000079
35	0.000370	0.006481	0.000699	0.000436	0.001519

36 37 38 39 40

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.037170	0.043871	0.037942	0.052371	0.043128
2	0.079030	0.077572	0.013327	0.036285	0.044030
3	0.032774	0.073263	0.034623	0.042218	0.070571
4	0.047677	0.071097	0.038670	0.060190	0.021672
5	0.058358	0.095139	0.018163	0.047481	0.020215
6	0.051051	0.085909	0.094537	0.019180	0.060619
7	0.011105	0.070144	0.036456	0.035492	0.054395
8	0.054124	0.025667	0.028070	0.059743	0.042710
9	0.033497	0.031714	0.033097	0.107636	0.023825
10	0.029540	0.080098	0.041387	0.024467	0.057670
11	0.072419	0.015154	0.121936	0.014439	0.073635
12	0.104839	0.034345	0.169159	0.099826	0.071147
13	0.037050	0.013269	0.111165	0.033962	0.056685
14	0.009107	0.008784	0.051662	0.014426	0.042668
15	0.006904	0.003669	0.002921	0.003320	0.010373

16	0.007062	0.003209	0.006498	0.002271	0.008538
17	0.006413	0.002129	0.014927	0.007822	0.017939
18	0.006352	0.003171	0.003610	0.003461	0.015431
19	0.007784	0.004729	0.012331	0.007420	0.027992
20	0.045218	0.006823	0.033157	0.000032	0.023300
21	0.109231	0.109991	0.006395	0.048337	0.018745
22	0.054080	0.001531	0.004316	0.005492	0.000607
23	0.010464	0.002394	0.022040	0.044842	0.064356
24	0.032260	0.001135	0.031649	0.061759	0.017157
25	0.028371	0.017949	0.001222	0.001140	0.010647
26	0.013131	0.006879	0.001078	0.098194	0.014518
27	0.009342	0.080058	0.001638	0.016710	0.040326
28	0.001481	0.010688	0.007385	0.035113	0.028683
29	0.000592	0.001034	0.002981	0.000658	-0.000072
30	0.000228	0.001685	0.011755	0.007547	0.011742
31	0.000144	0.000870	0.000328	0.000205	0.000460
32	-0.000029	0.001156	0.001725	0.002507	0.004286
33	0.000744	0.000793	0.000019	0.000101	0.000061
34	0.000509	0.000164	0.001141	0.000075	0.001866
35	0.001979	0.013915	0.002690	0.005277	0.000075

41 42 43 44 45

1.000000 1.000000 1.000000 1.000000 1.000000

1	0.038973	0.016460	0.013360	0.046137	0.122336
2	0.030535	0.000483	0.001448	0.085745	0.057505
3	0.028115	0.001079	0.003200	0.077115	0.049155
4	0.022515	0.000426	0.000588	0.078463	0.047191
5	0.029709	0.000961	0.001149	0.026993	0.020192
6	0.069063	0.005947	0.003390	0.031735	0.030056
7	0.059421	0.006316	0.005373	0.039428	0.050262
8	0.026461	0.014942	0.010721	0.044653	0.065901
9	0.021501	0.005136	0.002770	0.041099	0.053421
10	0.029958	0.008676	0.010221	0.035371	0.046868
11	0.031836	0.007427	0.006480	0.005244	0.002041
12	0.047475	0.015214	0.019853	0.061186	0.061198
13	0.034050	0.016616	0.029266	0.007671	0.009040
14	0.069731	0.083709	0.051530	0.033632	0.025286
15	0.025382	0.014695	0.068891	0.026460	0.029217
16	0.031348	0.102186	0.056858	0.033412	0.041430
17	0.059850	0.107366	0.142902	0.031002	0.040711
18	0.065894	0.169403	0.128229	0.030844	0.036415
19	0.080973	0.080622	0.093716	0.032121	0.036821
20	0.052614	0.029749	0.018225	0.022784	0.029815
21	0.012572	0.003359	0.000506	0.003835	0.023508

22	0.003902	0.000238	0.000228	0.078247	0.027133
23	0.012077	0.000831	0.003445	0.013481	0.001194
24	0.007571	0.000106	0.000890	0.030595	0.014336
25	0.001023	0.015722	0.009661	0.039448	0.050076
26	0.006716	0.000046	0.000062	0.011423	0.002375
27	0.006616	0.004289	0.004020	0.015511	0.022575
28	0.009620	0.001627	0.018628	0.007523	0.001253
29	0.001291	0.018058	0.070599	0.000544	0.000194
30	0.052298	0.030557	0.102153	0.003257	0.000078
31	0.021203	0.212360	0.008927	0.002875	0.000406
32	0.007959	0.024127	0.108280	0.000429	0.000007
33	-0.000080	0.000876	0.004388	0.000631	0.000023
34	0.001824	0.000019	-0.000008	0.001156	0.001337
35	0.000002	0.000372	0.000051	-0.000053	0.000645

46	47	48	49	50
----	----	----	----	----

1.000000	1.000000	1.000000	1.000000	1.000000
----------	----------	----------	----------	----------

1	0.832013	0.601636	0.212675	0.053289	0.011136
2	0.016745	0.025949	0.046240	0.098842	0.041147
3	0.018758	0.013835	0.039014	0.076781	0.116756
4	0.019970	0.007839	0.035612	0.037345	0.163985
5	0.003879	0.005768	0.016573	0.051712	0.089814
6	0.007379	0.017129	0.089441	0.027360	0.000469
7	0.008524	0.019477	0.088128	0.077912	0.001684
8	0.005966	0.028477	0.054008	0.094557	0.058958
9	0.001509	0.038441	0.037918	0.082057	0.133382
10	0.000818	0.035714	0.032501	0.046984	0.161546
11	0.004575	0.017595	0.015497	0.061080	0.077139
12	0.002412	0.044211	0.029877	0.023112	0.010116
13	0.000829	0.022616	0.017023	0.020010	0.036882
14	0.002399	0.002587	0.005614	0.001594	0.010472
15	0.000962	0.007069	0.005029	0.002959	0.001950
16	0.001214	0.009632	0.008889	0.008023	0.023449
17	0.001432	0.006714	0.006261	0.007082	0.027008
18	0.000618	0.002951	0.005278	0.003530	0.012305
19	0.000993	0.000662	0.004088	0.000546	0.000185
20	0.003047	0.004772	0.004965	0.000473	0.000818
21	0.010706	0.003480	0.021760	0.006480	0.014629
22	0.023891	0.008665	0.084162	0.000816	0.000917
23	0.002461	0.018269	0.010476	0.077205	0.000821
24	0.007624	0.001805	0.010351	0.020929	0.000001
25	0.002831	0.034776	0.073393	0.000152	0.000370
26	0.001444	0.000722	0.032917	0.084384	0.000148
27	0.000297	0.015147	0.001860	0.028786	-0.000111

28	0.001559	0.003230	0.000846	0.002836	0.000318
29	0.000035	0.000129	0.000028	0.000095	-0.000003
30	0.001139	0.000074	0.002565	0.000063	0.000016
31	0.000861	0.000051	0.003022	0.000136	0.000001
32	0.000059	0.000028	0.000028	0.000064	0.000018
33	0.003707	0.000063	0.000088	0.000008	0.000010
34	0.007187	0.000263	-0.000269	0.000170	0.003615
35	0.002158	0.000223	0.004144	0.002630	0.000051

51	52	53	54	55
----	----	----	----	----

1.000000	1.000000	1.000000	1.000000	1.000000
----------	----------	----------	----------	----------

1	0.024819	0.027853	0.028858	0.002617	0.024887
2	0.068006	0.101569	0.022287	0.000640	0.131098
3	0.008447	0.055176	0.015503	0.125479	0.095491
4	0.016363	0.000790	0.000055	0.188510	0.022665
5	0.072351	0.067562	0.013381	0.001832	0.136155
6	0.034981	0.051248	0.009269	0.180705	0.000074
7	0.102805	0.031469	0.004170	0.166594	0.000367
8	0.140227	0.016078	0.000629	0.000048	0.162115
9	0.059992	0.000491	0.000852	0.140807	0.097287
10	0.001714	0.016539	0.003354	0.188255	0.035318
11	0.075635	0.022557	0.001859	0.001357	0.162697
12	0.024666	0.071138	0.019642	0.000484	0.011451
13	0.035081	0.001068	0.000722	0.000988	0.040809
14	0.099756	0.094170	0.045758	0.000155	0.013243
15	0.000270	0.014487	0.230569	0.000178	0.012973
16	0.085604	0.174800	0.048868	0.000057	0.003386
17	0.100713	0.072218	0.087982	0.000289	0.022964
18	0.018630	0.010297	0.300378	0.000094	0.002023
19	0.018823	0.153202	0.120308	0.000063	0.012911
20	0.000003	0.009269	0.044478	0.000084	0.002594
21	0.007105	0.004669	0.000111	0.000186	0.003646
22	0.000006	0.000038	0.000006	-0.000005	0.000004
23	0.000003	0.000058	0.000001	0.000015	0.000009
24	0.000023	-0.000009	0.000001	0.000005	0.000021
25	0.000001	0.000008	0.000002	0.000023	0.000024
26	0.000305	0.000194	0.000072	0.000030	0.000029
27	0.000101	-0.000069	0.000033	-0.000004	-0.000107
28	0.000213	0.000462	0.000084	0.000261	0.000209
29	0.000002	0.000001	0.000002	0.000003	0.000003
30	0.000009	0.000004	0.000016	0.000000	0.000001
31	-0.000001	0.000000	0.000001	0.000001	-0.000001
32	0.000002	0.000012	0.000016	-0.000007	-0.000010
33	0.000004	0.000028	0.000215	0.000006	-0.000003

34	0.003074	0.002642	0.000572	0.000188	0.005546
35	0.000266	-0.000021	-0.000053	0.000065	0.000117

ATOMIC SPIN POPULATION (ALPHA MINUS BETA)

ATOM	MULL.POP.	LOW.POP.
1 CO	2.712285	2.718518
2 C	0.039921	0.025976
3 C	-0.019101	-0.007962
4 C	0.026053	0.018244
5 C	-0.008420	0.000444
6 C	0.036242	0.021839
7 C	-0.032094	-0.010349
8 C	0.024746	0.015426
9 C	-0.015506	-0.006922
10 C	0.024056	0.015146
11 C	-0.019176	-0.008267
12 N	0.122997	0.108405
13 C	-0.013916	-0.002972
14 C	0.014711	0.010121
15 C	-0.009299	-0.005685
16 C	0.010566	0.006909
17 C	-0.006482	-0.003083
18 C	0.009839	0.006334
19 C	-0.006039	-0.003201
20 O	0.041405	0.044879
21 N	0.059237	0.048811
22 H	-0.000699	-0.000862
23 H	0.000242	0.000422
24 H	-0.000765	-0.000602
25 H	-0.000390	-0.000501
26 H	0.000483	0.000565
27 H	-0.000316	-0.000521
28 H	0.009836	0.007474
29 H	-0.000242	-0.000198
30 H	0.000064	0.000090
31 H	-0.000174	-0.000168
32 H	-0.000141	0.000144
33 H	0.001795	0.001757
34 H	-0.003638	-0.002427
35 H	0.001923	0.002215

***** ALL ELECTRONS *****

----- POPULATIONS IN EACH AO -----
MULLIKEN LOWDIN

1	CO	1	S	1.54032	0.73852
2	CO	1	X	1.67521	1.52632
3	CO	1	Y	1.67516	1.52634
4	CO	1	Z	1.66940	1.51709
5	CO	1	XX	0.66284	0.92680
6	CO	1	YY	0.55482	0.80987
7	CO	1	ZZ	0.60943	0.86159
8	CO	1	XY	1.10294	1.06243
9	CO	1	XZ	0.98595	0.94966
10	CO	1	YZ	1.19163	1.14889
11	CO	1	XX	0.24485	0.31303
12	CO	1	YY	0.21147	0.30104
13	CO	1	ZZ	0.21944	0.29932
14	CO	1	XY	0.40095	0.44165
15	CO	1	XZ	0.37013	0.40880
16	CO	1	YZ	0.43544	0.47404
17	CO	1	S	0.48410	0.17162
18	CO	1	X	0.10839	0.18063
19	CO	1	Y	0.11170	0.18984
20	CO	1	Z	0.07921	0.11815
21	CO	1	S	0.04351	0.07516
22	CO	1	X	0.03491	0.06620
23	CO	1	Y	0.02204	0.05922
24	CO	1	Z	0.01893	0.04209
25	CO	1	S	0.44763	0.35365
26	CO	1	X	0.34442	0.47932
27	CO	1	Y	0.34469	0.48281
28	CO	1	Z	0.33972	0.47855
29	CO	1	XX	0.05878	0.19971
30	CO	1	YY	0.03537	0.17126
31	CO	1	ZZ	0.05657	0.12266
32	CO	1	XY	0.11007	0.14990
33	CO	1	XZ	0.09175	0.17115
34	CO	1	YZ	0.08578	0.13011
35	C	2	S	1.14918	0.73176
36	C	2	X	0.92180	0.83643
37	C	2	Y	0.92337	0.84665
38	C	2	Z	0.71514	0.64165
39	C	2	S	-0.23234	0.21887
40	C	2	X	0.21997	0.23649
41	C	2	Y	0.11253	0.24174
42	C	2	Z	0.20430	0.29281
43	C	3	S	1.14362	0.72568
44	C	3	X	0.93596	0.84491
45	C	3	Y	0.90176	0.83664
46	C	3	Z	0.73602	0.66037

47	C	3	S	-0.06462	0.22156
48	C	3	X	0.00702	0.23908
49	C	3	Y	0.08493	0.24233
50	C	3	Z	0.20963	0.30361
51	C	4	S	1.14467	0.72956
52	C	4	X	0.90345	0.84267
53	C	4	Y	0.91991	0.82632
54	C	4	Z	0.75053	0.67647
55	C	4	S	-0.04172	0.21963
56	C	4	X	0.14890	0.22981
57	C	4	Y	0.06970	0.25458
58	C	4	Z	0.22163	0.30730
59	C	5	S	1.11950	0.68528
60	C	5	X	0.83130	0.75945
61	C	5	Y	0.85038	0.78267
62	C	5	Z	0.85892	0.77915
63	C	5	S	-0.53723	0.20139
64	C	5	X	0.20523	0.21751
65	C	5	Y	0.54038	0.24061
66	C	5	Z	0.24182	0.30985
67	C	6	S	1.12682	0.69763
68	C	6	X	0.90590	0.83383
69	C	6	Y	0.87786	0.80635
70	C	6	Z	0.79921	0.72048
71	C	6	S	-0.63853	0.19726
72	C	6	X	0.12468	0.22314
73	C	6	Y	0.34285	0.23375
74	C	6	Z	0.22691	0.30896
75	C	7	S	1.13012	0.70717
76	C	7	X	0.90327	0.83276
77	C	7	Y	0.90591	0.83293
78	C	7	Z	0.76573	0.68226
79	C	7	S	-0.20987	0.19649
80	C	7	X	0.17036	0.23155
81	C	7	Y	0.27203	0.23633
82	C	7	Z	0.23818	0.30116
83	C	8	S	1.14976	0.73226
84	C	8	X	0.95398	0.86586
85	C	8	Y	0.89483	0.82010
86	C	8	Z	0.71008	0.63675
87	C	8	S	-0.30153	0.21893
88	C	8	X	0.03488	0.24057
89	C	8	Y	0.26596	0.23756
90	C	8	Z	0.21548	0.29153
91	C	9	S	1.14377	0.72528
92	C	9	X	0.89973	0.84376

93	C	9	Y	0.93618	0.83937
94	C	9	Z	0.73834	0.65965
95	C	9	S	-0.02673	0.22105
96	C	9	X	0.04768	0.23580
97	C	9	Y	0.04649	0.24521
98	C	9	Z	0.22165	0.30543
99	C	10	S	1.14500	0.72806
100	C	10	X	0.94509	0.85361
101	C	10	Y	0.88320	0.81644
102	C	10	Z	0.74623	0.67334
103	C	10	S	-0.13804	0.21996
104	C	10	X	0.00272	0.24854
105	C	10	Y	0.20439	0.23272
106	C	10	Z	0.21747	0.30824
107	C	11	S	1.11987	0.67742
108	C	11	X	0.80906	0.74026
109	C	11	Y	0.89255	0.81327
110	C	11	Z	0.85650	0.77312
111	C	11	S	-0.08687	0.20066
112	C	11	X	0.51267	0.21316
113	C	11	Y	0.28425	0.23269
114	C	11	Z	0.24196	0.30782
115	N	12	S	1.23114	0.85138
116	N	12	X	0.97350	0.88618
117	N	12	Y	1.10193	1.01689
118	N	12	Z	0.96870	0.89171
119	N	12	S	-0.04753	0.30564
120	N	12	X	-0.14783	0.31039
121	N	12	Y	0.21869	0.37298
122	N	12	Z	0.40249	0.42026
123	C	13	S	1.15482	0.70737
124	C	13	X	0.87986	0.80159
125	C	13	Y	0.93444	0.82485
126	C	13	Z	0.69320	0.62062
127	C	13	S	0.32881	0.22231
128	C	13	X	0.29972	0.21022
129	C	13	Y	0.14411	0.23922
130	C	13	Z	0.15470	0.24590
131	C	14	S	1.12155	0.69823
132	C	14	X	0.90265	0.83233
133	C	14	Y	0.87541	0.80868
134	C	14	Z	0.83749	0.75610
135	C	14	S	-0.42325	0.19760
136	C	14	X	0.26211	0.22797
137	C	14	Y	0.06335	0.24560
138	C	14	Z	0.21381	0.31105

139	C	15	S	1.12204	0.69263
140	C	15	X	0.79408	0.72425
141	C	15	Y	0.84226	0.77299
142	C	15	Z	0.83991	0.75376
143	C	15	S	-0.32551	0.19805
144	C	15	X	0.13901	0.20053
145	C	15	Y	0.37054	0.22686
146	C	15	Z	0.23354	0.28132
147	C	16	S	1.13886	0.72461
148	C	16	X	0.88454	0.83118
149	C	16	Y	0.91916	0.82661
150	C	16	Z	0.79076	0.71464
151	C	16	S	-0.26086	0.21993
152	C	16	X	0.12564	0.22626
153	C	16	Y	0.08796	0.25586
154	C	16	Z	0.22291	0.30800
155	C	17	S	1.14984	0.73469
156	C	17	X	0.94526	0.85337
157	C	17	Y	0.88561	0.81911
158	C	17	Z	0.70586	0.63179
159	C	17	S	-0.06204	0.22359
160	C	17	X	0.08537	0.23782
161	C	17	Y	0.08447	0.24426
162	C	17	Z	0.18488	0.28045
163	C	18	S	1.14407	0.72834
164	C	18	X	0.93146	0.85040
165	C	18	Y	0.89210	0.82242
166	C	18	Z	0.74632	0.66846
167	C	18	S	-0.04540	0.22246
168	C	18	X	0.11803	0.23820
169	C	18	Y	0.06590	0.24659
170	C	18	Z	0.18899	0.29514
171	C	19	S	1.14935	0.73151
172	C	19	X	0.90807	0.84560
173	C	19	Y	0.90960	0.81859
174	C	19	Z	0.72715	0.65219
175	C	19	S	-0.22533	0.21915
176	C	19	X	0.25859	0.23471
177	C	19	Y	0.02835	0.24936
178	C	19	Z	0.19608	0.29199
179	O	20	S	1.37552	1.05516
180	O	20	X	1.18248	1.09711
181	O	20	Y	1.15645	1.06580
182	O	20	Z	1.31734	1.24288
183	O	20	S	0.27854	0.39379
184	O	20	X	0.36638	0.42762

185	O	20	Y	0.26124	0.40871
186	O	20	Z	0.43050	0.48873
187	N	21	S	1.22339	0.85253
188	N	21	X	1.06701	0.98015
189	N	21	Y	0.98666	0.89086
190	N	21	Z	1.04938	0.95732
191	N	21	S	0.07368	0.32393
192	N	21	X	0.27709	0.38849
193	N	21	Y	0.14580	0.35006
194	N	21	Z	0.33932	0.39780
195	H	22	S	0.71426	0.61903
196	H	22	S	0.09836	0.21697
197	H	23	S	0.70949	0.61685
198	H	23	S	0.14524	0.21734
199	H	24	S	0.72081	0.62262
200	H	24	S	0.19366	0.22509
201	H	25	S	0.71423	0.61897
202	H	25	S	0.09462	0.21697
203	H	26	S	0.71069	0.61791
204	H	26	S	0.15095	0.21801
205	H	27	S	0.72541	0.62597
206	H	27	S	0.15773	0.22255
207	H	28	S	0.71719	0.62209
208	H	28	S	0.15298	0.21293
209	H	29	S	0.71193	0.61429
210	H	29	S	0.15088	0.22214
211	H	30	S	0.70579	0.61482
212	H	30	S	0.14721	0.21333
213	H	31	S	0.70645	0.61497
214	H	31	S	0.13736	0.21458
215	H	32	S	0.71490	0.62019
216	H	32	S	0.10249	0.21712
217	H	33	S	0.62098	0.50491
218	H	33	S	-0.01948	0.11579
219	H	34	S	0.67036	0.56251
220	H	34	S	-0.00230	0.14434
221	H	35	S	0.67295	0.56323
222	H	35	S	0.03156	0.15006

----- MULLIKEN ATOMIC OVERLAP POPULATIONS -----
(OFF-DIAGONAL ELEMENTS NEED TO BE MULTIPLIED BY 2)

1	2	3	4	5
---	---	---	---	---

1	15.7893687			
2	0.0029156	4.9841387		

3	-0.0018472	-0.2847758	3.2733260		
4	0.0205447	0.2132918	0.2573416	3.8595976	
5	-0.0024944	-0.6313690	0.2659863	-0.1967668	7.0917477
6	-0.0525183	0.1852628	-0.2580024	0.0961068	-1.6237692
7	0.0029811	-0.5656555	0.5364682	-0.3436667	0.1511887
8	0.0036579	-0.5180645	0.0966572	0.0018271	0.3067522
9	-0.0003799	0.1100769	-0.0032661	-0.0062556	-0.0313164
10	0.0182808	-0.0080786	-0.0056803	0.0084796	0.1229244
11	0.0426724	0.3076800	-0.0349190	0.1451276	-1.2401462
12	0.2114459	-0.0020357	0.0005424	-0.0027586	-0.0234884
13	-0.0410827	0.0001853	-0.0000057	-0.0004811	-0.0272338
14	0.0208133	0.0000029	-0.0000023	0.0000438	0.0000168
15	-0.0211936	-0.0000013	0.0000007	-0.0000178	-0.0005965
16	-0.0013516	0.0000000	0.0000000	-0.0000001	-0.0000089
17	-0.0015138	0.0000000	0.0000000	0.0000000	0.0000000
18	0.0033673	0.0000000	0.0000000	0.0000000	-0.0000037
19	0.0072092	0.0000001	0.0000000	-0.0000003	-0.0000066
20	0.1212148	-0.0000006	0.0000008	0.0000038	0.0001915
21	0.2441337	0.0148185	-0.0076784	-0.0614289	-0.0687167
22	0.0000636	0.2672077	-0.1063719	0.0138587	0.0068426
23	-0.0001227	-0.0112652	0.2157939	-0.0241910	0.0171161
24	0.0015200	0.0103509	0.0002493	0.1826484	-0.0198984
25	0.0001451	-0.0586403	0.0072231	0.0004376	-0.0007760
26	-0.0001381	-0.0014615	0.0001787	-0.0000800	0.0002506
27	0.0001688	0.0001463	-0.0000563	0.0000759	-0.0017901
28	0.0007571	-0.0000001	0.0000010	-0.0000190	-0.0009303
29	0.0008114	0.0000000	0.0000000	0.0000000	0.0000002
30	-0.0001871	0.0000000	0.0000000	0.0000000	0.0000000
31	0.0001688	0.0000000	0.0000000	0.0000000	0.0000000
32	-0.0006215	0.0000000	0.0000000	0.0000000	0.0000059
33	0.0012356	0.0000000	0.0000000	0.0000059	0.0000567
34	0.0005154	0.0000553	0.0001433	0.0039089	0.0022048
35	-0.0029791	-0.0008353	0.0030143	-0.0505786	0.0143292

6 7 8 9 10

6	8.5623158				
7	-1.2839522	5.6958130			
8	0.3506375	-0.7164061	4.9501490		
9	-0.3413731	0.5833209	-0.3180910	3.3665535	
10	0.1063146	-0.3019068	0.2003697	0.2989707	3.4736598
11	-2.0758090	0.4869659	-0.6461477	0.2392990	-0.0171319
12	-0.0328987	-0.0099308	0.0126177	-0.0058625	-0.0213090
13	-0.0043413	0.0095859	-0.0025197	0.0060501	-0.0184150
14	-0.0072617	0.0000590	-0.0000519	-0.0000065	0.0077859
15	0.0017349	0.0000160	0.0000097	-0.0000299	-0.0012243

16	0.0000439	0.0000003	0.0000001	-0.0000006	-0.0000388
17	-0.0000025	0.0000000	0.0000000	0.0000001	0.0000055
18	-0.0000003	0.0000003	0.0000000	0.0000013	0.0000506
19	-0.0002329	0.0000148	-0.0000078	0.0000331	0.0009174
20	-0.0002411	-0.0000022	0.0000010	-0.0000013	0.0000977
21	0.0148343	-0.0122344	-0.0026893	0.0004400	-0.0006575
22	0.0291138	-0.0430824	-0.0533013	0.0069971	0.0004924
23	0.0132798	0.0056181	-0.0017474	0.0001670	-0.0000704
24	0.0309551	0.0099733	0.0001503	-0.0000528	0.0000681
25	0.0381452	-0.0512377	0.2683476	-0.1152569	0.0174678
26	0.0105222	0.0082991	-0.0177668	0.2176358	-0.0212443
27	0.0224162	0.0104996	0.0089819	-0.0031306	0.1475505
28	0.0042307	0.0004927	0.0000443	0.0026183	-0.0013588
29	0.0000002	0.0000000	0.0000000	0.0000000	-0.0000001
30	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
31	0.0000000	0.0000000	0.0000000	0.0000000	-0.0000005
32	0.0000267	-0.0000018	0.0000004	-0.0000069	-0.0002272
33	-0.0000675	-0.0000006	0.0000000	0.0000000	0.0000022
34	-0.0296477	-0.0002677	-0.0000264	-0.0000177	-0.0000184
35	0.0098823	0.0027606	0.0000574	-0.0000039	-0.0000119

11 12 13 14 15

11	7.3704640				
12	0.0760409	4.4764336			
13	-0.0060253	0.2157305	5.1255674		
14	-0.0303325	-0.0330779	-0.8469334	4.7212828	
15	-0.0056063	-0.0285924	-0.3604421	-0.4244054	4.8370909
16	-0.0000774	-0.0011778	0.0492621	-0.0537796	0.1804967
17	0.0000342	0.0001069	0.0177268	0.0238427	0.0043654
18	-0.0003648	-0.0010464	0.0425170	0.2013617	-0.1870563
19	0.0016103	0.0036250	0.1944069	0.1918125	-0.1100070
20	-0.0001136	-0.0292276	0.0070670	0.0532713	0.0218200
21	0.0106233	-0.0420236	0.0041882	-0.0008016	0.0005313
22	-0.0011188	0.0000006	0.0000003	0.0000000	0.0000000
23	0.0003054	0.0000009	0.0000001	0.0000000	0.0000000
24	-0.0009728	-0.0000335	0.0000057	-0.0000001	0.0000004
25	0.0035229	0.0000776	-0.0000185	-0.0000002	0.0000000
26	0.0179267	-0.0006700	-0.0000470	-0.0000101	-0.0000006
27	-0.0006441	-0.0116216	0.0112106	0.0031205	0.0003340
28	-0.0087529	-0.0520183	0.2941037	0.0220773	0.0257309
29	0.0000010	0.0000008	-0.0019355	0.0161044	-0.0164018
30	-0.0000001	0.0000001	0.0000570	0.0056430	0.0252849
31	0.0000003	0.0000063	-0.0021549	0.0132620	0.0104904
32	0.0006450	0.0007109	-0.0714191	-0.0359435	0.0479536
33	0.0000476	0.0008073	-0.0029177	0.0046143	0.0157333

34 0.0021149 -0.0007873 -0.0021081 0.0006495 -0.0001079
35 -0.0069293 0.0015037 0.0000890 -0.0000335 -0.0000311

16 17 18 19 20

16 3.2050171
17 0.4832104 2.7311016
18 0.0862208 0.4459473 3.1213333
19 -0.1096675 0.0282500 0.1741739 3.3718776
20 -0.0381012 -0.0095510 0.0078795 -0.0104821 6.0120787
21 0.0000470 -0.0000007 0.0000012 -0.0000365 -0.0053312
22 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
23 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
24 0.0000000 0.0000000 0.0000000 0.0000000 -0.0000008
25 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
26 0.0000000 0.0000000 0.0000000 0.0000013 0.0000000
27 -0.0000009 -0.0000026 0.0000064 -0.0001871 0.0000006
28 -0.0011024 0.0002582 0.0031048 -0.0175109 -0.0001848
29 0.1594762 0.0123176 0.0097641 0.0110177 0.0018559
30 -0.0519250 0.2750805 -0.0462286 0.0190129 -0.0003419
31 0.0160858 -0.0462204 0.2509511 -0.0239686 0.0000294
32 0.0044936 0.0136128 -0.0702157 0.2192276 -0.0003800
33 -0.0181435 0.0006849 -0.0003018 0.0007800 0.2371350
34 -0.0000128 0.0000004 -0.0000015 -0.0000032 -0.0000503
35 -0.0000019 0.0000000 0.0000000 0.0000006 -0.0001992

21 22 23 24 25

21 4.4929444
22 0.0000962 0.6994603
23 -0.0007212 -0.0064654 0.6565010
24 -0.0092933 -0.0008812 -0.0094190 0.7118435
25 0.0000002 -0.0002395 -0.0000299 0.0000053 0.7078719
26 0.0000008 -0.0000494 0.0000006 -0.0000001 -0.0073700
27 -0.0000108 0.0000062 -0.0000001 0.0000004 -0.0008290
28 0.0000350 0.0000000 0.0000000 0.0000000 -0.0000025
29 0.0000010 0.0000000 0.0000000 0.0000000 0.0000000
30 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
31 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
32 -0.0000013 0.0000000 0.0000000 0.0000000 0.0000000
33 -0.0001306 0.0000000 0.0000000 0.0000001 0.0000000
34 0.2852879 0.0000002 -0.0000045 0.0003604 0.0000000
35 0.3061095 -0.0000040 -0.0000095 0.0068889 -0.0000003

26 27 28 29 30

26	0.6663757				
27	-0.0107153	0.6896795			
28	-0.0000028	0.0177638	0.5669735		
29	0.0000000	0.0000001	-0.0000031	0.6765422	
30	0.0000000	0.0000000	0.0000013	-0.0135040	0.6526674
31	0.0000000	0.0000007	0.0000655	-0.0006337	-0.0119563
32	0.0000002	0.0001666	0.0137531	0.0000861	-0.0005869
33	0.0000000	0.0000005	0.0000258	0.0073068	-0.0000199
34	0.0000002	-0.0000015	0.0000199	-0.0000004	0.0000000
35	0.0000000	0.0000002	0.0000028	0.0000000	0.0000000

31	32	33	34	35
----	----	----	----	----

31	0.6474645				
32	-0.0097757	0.7058581			
33	-0.0000024	0.0000282	0.3546328		
34	0.0000000	0.0000007	0.0000157	0.4298752	
35	0.0000000	0.0000000	-0.0000253	-0.0240368	0.4455534

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 CO	16.367561	0.632439	16.947425	0.052575
2 C	4.013949	-0.013949	4.046402	-0.046402
3 C	3.954321	0.045679	4.074174	-0.074174
4 C	4.117055	-0.117055	4.086333	-0.086333
5 C	4.110302	-0.110302	3.975904	0.024096
6 C	3.765705	0.234295	4.021399	-0.021399
7 C	4.175712	-0.175712	4.020656	-0.020656
8 C	3.923441	0.076559	4.043556	-0.043556
9 C	4.007112	-0.007112	4.075555	-0.075555
10 C	4.006064	-0.006064	4.080918	-0.080918
11 C	4.629989	-0.629989	3.958408	0.041592
12 N	4.701091	0.298909	5.055440	-0.055440
13 C	4.589673	-0.589673	3.872065	0.127935
14 C	3.853124	0.146876	4.077544	-0.077544
15 C	4.015879	-0.015879	3.850394	0.149606
16 C	3.908964	0.091036	4.107092	-0.107092
17 C	3.979254	0.020746	4.025078	-0.025078
18 C	4.041461	-0.041461	4.072025	-0.072025
19 C	3.951860	0.048140	4.043111	-0.043111
20 O	6.368438	-0.368438	6.179794	-0.179794
21 N	5.162336	-0.162336	5.141131	-0.141131
22 H	0.812626	0.187374	0.835999	0.164001
23 H	0.854736	0.145264	0.834193	0.165807
24 H	0.914468	0.085532	0.847717	0.152283
25 H	0.808844	0.191156	0.835933	0.164067

26 H	0.861636	0.138364	0.835920	0.164080
27 H	0.883139	0.116861	0.848523	0.151477
28 H	0.870174	0.129826	0.835022	0.164978
29 H	0.862807	0.137193	0.836432	0.163568
30 H	0.852997	0.147003	0.828159	0.171841
31 H	0.843812	0.156188	0.829556	0.170444
32 H	0.817390	0.182610	0.837306	0.162694
33 H	0.601504	0.398496	0.620697	0.379303
34 H	0.668060	0.331940	0.706846	0.293154
35 H	0.704512	0.295488	0.713292	0.286708

 BOND ORDER AND VALENCE ANALYSIS BOND ORDER
 THRESHOLD=0.050

BOND		BOND		BOND	
ATOM PAIR	DIST	ORDER	ATOM PAIR	DIST	ORDER
1 4	3.998	0.058	1 5	2.806	0.109
1 12	1.941	0.642	1 13	2.860	0.084
1 21	1.977	0.707	1 11	2.896	0.094
2 6	2.531	-0.261	2 3	1.402	1.499
2 9	3.779	0.142	2 4	2.442	0.126
3 4	1.432	1.410	2 7	1.444	1.584
3 7	2.480	0.172	2 8	2.486	0.113
3 11	4.384	-0.156	2 11	3.835	0.288
4 9	5.179	0.070	3 5	2.472	0.112
4 21	2.475	-0.058	3 6	2.923	0.147
5 7	2.475	-0.054	3 8	3.780	0.102
5 10	3.886	0.303	3 10	5.185	0.051
5 21	1.509	0.875	3 23	1.104	0.802
6 7	1.467	1.593	4 5	1.408	1.451
6 13	3.732	-0.063	4 10	5.007	-0.078
6 27	3.505	0.055	4 11	3.893	0.607
7 10	2.850	0.052	4 24	1.108	0.743
8 10	2.445	0.088	5 6	1.458	1.356
9 11	2.483	0.147	5 7	2.475	-0.054
10 13	2.931	0.109	5 8	3.815	0.115
11 13	2.447	0.243	5 11	2.625	-0.242
13 14	1.467	0.818	5 24	2.183	0.055
13 19	2.470	0.125	6 8	2.527	-0.092
14 16	2.501	0.065	6 11	1.466	1.120
15 16	1.406	1.415	6 21	2.592	-0.051
15 29	2.194	0.066	7 8	1.444	1.530
16 18	2.472	0.100	7 11	2.497	-0.098
			8 9	1.402	1.474
			9 10	1.430	1.441
			10 11	1.415	1.632
			10 27	1.104	0.742
			11 12	1.454	0.838
			12 13	1.332	1.305
			13 16	3.886	0.200
			13 18	3.794	0.238
			14 15	1.438	1.364
			14 17	2.883	0.181
			14 19	1.443	1.668
			15 17	2.441	0.074
			15 20	1.466	0.769
			16 17	1.428	1.614
			16 29	1.107	0.746
			17 18	1.423	1.553

17	30	1.105	0.829	18	19	1.416	1.509	18	31	1.104	0.815
19	32	1.106	0.805	20	33	0.992	0.752	21	34	1.044	0.806
21	35	1.039	0.834								

ATOM	TOTAL VALENCE	BONDED VALENCE	FREE VALENCE
1 CO	4.779	2.342	2.437
2 C	4.319	4.318	0.001
3 C	4.152	4.152	0.000
4 C	4.315	4.315	0.000
5 C	4.095	4.095	0.000
6 C	3.979	3.978	0.001
7 C	5.015	5.015	0.000
8 C	4.191	4.191	0.000
9 C	4.233	4.232	0.000
10 C	4.315	4.315	0.000
11 C	4.532	4.532	0.000
12 N	2.717	2.707	0.010
13 C	3.963	3.963	0.000
14 C	4.247	4.246	0.000
15 C	3.854	3.854	0.000
16 C	4.197	4.197	0.000
17 C	4.344	4.344	0.000
18 C	4.262	4.262	0.000
19 C	4.275	4.275	0.000
20 O	1.981	1.980	0.001
21 N	3.102	3.099	0.003
22 H	0.844	0.844	0.000
23 H	0.897	0.897	0.000
24 H	0.932	0.932	0.000
25 H	0.840	0.840	0.000
26 H	0.898	0.898	0.000
27 H	0.919	0.919	0.000
28 H	0.986	0.986	0.000
29 H	0.900	0.900	0.000
30 H	0.905	0.905	0.000
31 H	0.892	0.892	0.000
32 H	0.841	0.841	0.000
33 H	0.816	0.816	0.000
34 H	0.836	0.836	0.000
35 H	0.874	0.874	0.000

ATOMIC SPIN DENSITY AT THE NUCLEUS (A.U.)

1 CO	17.0	-0.0000082
------	------	------------

2 C	4.0	0.0000003
3 C	4.0	0.0000003
4 C	4.0	-0.0000001
5 C	4.0	-0.0000004
6 C	4.0	0.0000003
7 C	4.0	0.0000005
8 C	4.0	0.0000000
9 C	4.0	0.0000001
10 C	4.0	-0.0000005
11 C	4.0	0.0000002
12 N	5.0	-0.0000037
13 C	4.0	0.0000007
14 C	4.0	-0.0000004
15 C	4.0	0.0000005
16 C	4.0	-0.0000001
17 C	4.0	0.0000002
18 C	4.0	0.0000000
19 C	4.0	0.0000001
20 O	6.0	-0.0000118
21 N	5.0	-0.0000037
22 H	1.0	-0.0004671
23 H	1.0	0.0002214
24 H	1.0	-0.0003483
25 H	1.0	-0.0002682
26 H	1.0	0.0002910
27 H	1.0	-0.0002985
28 H	1.0	0.0034649
29 H	1.0	-0.0001242
30 H	1.0	0.0000519
31 H	1.0	-0.0000970
32 H	1.0	0.0000442
33 H	1.0	0.0014521
34 H	1.0	-0.0012248
35 H	1.0	0.0014814

ELECTROSTATIC MOMENTS

POINT	1	X	Y	Z (BOHR)	CHARGE
		0.000000	0.000000	0.000000	2.00 (A.U.)
		DX	DY	DZ	/D/ (DEBYE)
		-0.864445	-7.431417	5.516268	9.295291

..... END OF PROPERTY EVALUATION

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.73 , TOTAL = 9376.8 SECONDS (156.3 MIN)
WALL CLOCK TIME: STEP = 0.79 , TOTAL = 8678.0 SECONDS (144.6 MIN)
CPU UTILIZATION: STEP = 91.99% , TOTAL = 100.00%
.....END OF NBO ANALYSIS.....

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.51 , TOTAL = 9377.3 SECONDS (156.3 MIN)
WALL CLOCK TIME: STEP = 0.52 , TOTAL = 8678.5 SECONDS (144.6 MIN)
CPU UTILIZATION: STEP = 98.78% , TOTAL = 100.00%

\$VIB

IVIB= 0 IATOM= 0 ICOORD= 0 E= -284.6369788491
-2.303160993E-06-1.239383611E-05-2.196699747E-05-1.540587035E-05-
9.362265933E-06
-3.820066080E-07-1.435160666E-05 5.497239257E-06 1.170191226E-05
1.170500510E-05
1.761434679E-06-5.350580078E-05 1.398911240E-05-3.291792099E-06-
1.766734743E-05
5.133083330E-06 6.490159923E-06 4.337636893E-05 3.569282235E-06
1.489161310E-05
-2.047292422E-08 2.653916237E-05 8.570390337E-07-3.426435172E-05-
7.915517191E-06
1.852255679E-05-4.858304430E-05-2.682663207E-05 1.076563110E-05
2.294923009E-05
-9.860067849E-06 8.746138525E-06 3.927894239E-05 1.416126478E-05
1.186856886E-05
8.246745022E-06 3.982780727E-05-3.000759358E-06 1.464290540E-06
1.740324705E-06
-1.654264691E-05-1.292333725E-05-6.975946707E-07-7.484168418E-06-
2.433296996E-05
3.651844169E-06-1.680927922E-05-5.284530114E-06-1.626105631E-05-
1.783920486E-06
1.561908043E-05 1.217801891E-05-4.280053275E-05 2.794218685E-05
2.344107851E-05
-2.326582237E-05-2.294081766E-05-1.081178886E-05-3.044246551E-05-
2.059435736E-05
-6.791838640E-06 2.772742157E-05-2.428844882E-06-1.149082262E-05
4.769915443E-06
-4.090937259E-05-8.219322931E-06-1.499941379E-05 2.718740728E-05
1.344135986E-05
-2.292002308E-05 8.487504599E-05 3.578803525E-05-3.151715153E-05
4.928600594E-05
3.200959921E-05 2.459018900E-05 3.523082552E-05-4.276733243E-06
7.132138455E-05

-3.218628107E-05 4.174330579E-08-1.472402470E-05-4.853040956E-06
1.056697631E-05
-1.231881089E-05 1.799617508E-05-5.979901819E-05 4.252615357E-06
2.327759900E-05
1.261866687E-05-2.896823980E-05 2.226561283E-05-1.112055667E-05
1.207681138E-05
3.718059485E-06-2.730670364E-05 5.710687562E-05-3.811838452E-05
2.850834593E-05
1.436640222E-05-3.823063939E-05-5.547241964E-05-2.986843431E-06-
1.522289064E-05
-8.644451461E-01-7.431416952E+00 5.516268216E+00
.....END OF GEOMETRY SEARCH.....

TIMING STATISTICS ON NODE 0:

CPU TIME: STEP = 0.03 , TOTAL = 9377.3 SECONDS (156.3 MIN)
WALL CLOCK TIME: STEP = 0.03 , TOTAL = 8678.5 SECONDS (144.6
MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 100.00%

OVERALL TIMING STATISTICS:

GLOBAL CPU TIME ELAPSED = 414812.0 SECONDS (6913.5 MIN)
NODE 0 WALL CLOCK TIME = 8678.5 SECONDS (144.6 MIN)
JOB CPU UTILIZATION: TOTAL = 4779.76% , PER NODE AVERAGE =
99.58%

2174173 WORDS OF DYNAMIC MEMORY USED

**WARNING! YOU ARE USING OUTDATED VERSION OF THE PC GAMESS!
PLEASE CHECK PC GAMESS HOMEPAGE FOR INFORMATION ON UPDATES!**

EXECUTION OF PC GAMESS TERMINATED NORMALLY 6:59:45 LT 1-SEP-
2009