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1 *****
*          GAMESS VERSION =  6 MAY 1998          *
*          FROM IOWA STATE UNIVERSITY            *
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* M.S.GORDON, J.H.JENSEN, S.KOSEKI, N.MATSUNAGA, *
* K.A.NGUYEN, S.J.SU, T.L.WINDUS,              *
* TOGETHER WITH M.DUPUIS, J.A.MONTGOMERY        *
* J.COMPUT.CHEM.  14, 1347-1363(1993)          *
*****Intel x86 (WIN32, OS/2, DOS32) VERSION*****
* PC GAMESS version 5.3, build number 1633      *
* Compiled on   Monday,   14-06-1999, 11:14:24  *
* Intel specific optimization, bug fixes,      *
* code changes, and additional functionality - *
* copyright (c) 1994, 1999 by Alex. A. Granovsky, *
* Laboratory of Chemical Cybernetics,          *
* Moscow State University, Moscow, Russia.     *
* PC GAMESS URL:                               *
* http://classic.chem.msu.su/gran/gameess/index.html *
* E-mail: gran@classic.chem.msu.su             *
* This program should not be redistributed     *
* without special permission of its developers. *
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EXECUTION OF GAMESS BEGUN 9:59:19 LT 3-JUL-1999 (Linux 2.2.5 450MHz PII)

```

ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD> $CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE
INPUT CARD> COORD=CART PLTORB=.T. $END
INPUT CARD> $SYSTEM TIMLIM=60 MEMORY=750000 $END
INPUT CARD> $BASIS GBASIS=N311 NGAUSS=6 $END
INPUT CARD> $GUESS GUESS=HUCKEL $END
INPUT CARD> $DATA
INPUT CARD> HAc(Z) generated by Kimball.exe
INPUT CARD>Cs
INPUT CARD>
INPUT CARD>C 6.0 0.72539131 9.0396177E-2 0.
INPUT CARD>C 6.0 -0.77558049 9.0396177E-2 0.
INPUT CARD>O 8.0 -1.4523747 1.1170029 0.
INPUT CARD>O 8.0 -1.7901961 -0.93979084 0.
INPUT CARD>H 1.0 1.0242143 -0.970443 0.
INPUT CARD>H 1.0 1.0242143 0.62081576 0.91871367
INPUT CARD>H 1.0 1.0242143 0.62081576 -0.91871367
INPUT CARD>H 1.0 -2.6174101 -0.45167745 0.
INPUT CARD> $END

```

750000 WORDS OF MEMORY AVAILABLE

BASIS OPTIONS

```

-----
GBASIS=N311          IGAUSS=          6          POLAR=NONE
NDFUNC=              0          DIFFSP=          F
NPFUNC=              0          DIFFS=          F

```

RUN TITLE

HAc(Z) generated by Kimball.exe

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

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THE MOMENTS OF INERTIA ARE (AMU-ANGSTROM**2)
IXX=    36.053   IYY=    66.718   IZZ=    99.368

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ATOM	ATOMIC CHARGE	X	Y	Z
------	------------------	---	---	---

C	6.0	-2.9392769666	0.6406815331	0.0000000000
C	6.0	-0.1717951261	0.0191081985	0.0000000000
O	8.0	0.6509413983	-2.1540123739	0.0000000000
O	8.0	2.1255611968	1.4983937214	0.0000000000
H	1.0	-3.0509365286	2.7203965287	0.0000000000
H	1.0	-3.7098989512	-0.2135558093	-1.7361170975
H	1.0	-3.7098989512	-0.2135558093	1.7361170975
H	1.0	3.4486383231	0.2558526508	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.5009718 *	2.4076101 *	2.7183571 *
2 C	1.5009718 *	0.0000000	1.2296226 *	1.4459357 *
3 O	2.4076101 *	1.2296226 *	0.0000000	2.0843521 *
4 O	2.7183571 *	1.4459357 *	2.0843521 *	0.0000000
5 H	1.1021229 *	2.0891723 *	3.2389695	2.8145773 *
6 H	1.1021229 *	2.0891723 *	2.6876997 *	3.3467049
7 H	1.1021229 *	2.0891723 *	2.6876997 *	3.3467049
8 H	3.3864679	1.9199427 *	1.9539871 *	0.9604883 *

	H	H	H	H
1 C	1.1021229 *	1.1021229 *	1.1021229 *	3.3864679
2 C	2.0891723 *	2.0891723 *	2.0891723 *	1.9199427 *
3 O	3.2389695	2.6876997 *	2.6876997 *	1.9539871 *
4 O	2.8145773 *	3.3467049	3.3467049	0.9604883 *
5 H	0.0000000	1.8374273 *	1.8374273 *	3.6783890
6 H	1.8374273 *	0.0000000	1.8374273 *	3.9058552
7 H	1.8374273 *	1.8374273 *	0.0000000	3.9058552
8 H	3.6783890	3.9058552	3.9058552	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
-------	------	------	----------	-------------	--------------

C

1	S	1	4563.240000	0.778202 (0.001967)	
1	S	2	682.024000	1.448695 (0.015231)	
1	S	3	154.973000	2.383089 (0.076127)	
1	S	4	44.455300	3.200089 (0.260801)	
1	S	5	13.029000	3.013004 (0.616462)	
1	S	6	1.827730	0.247599 (0.221006)	
2	L	7	20.964200	0.800629 (0.114660)	2.573592 (0.040249)
2	L	8	4.803310	2.127420 (0.919999)	2.408248 (0.237594)
2	L	9	1.459330	-0.002868 (-0.003031)	1.865281 (0.815854)
3	L	10	0.483456	0.413217 (1.000000)	0.574627 (1.000000)
4	L	11	0.145585	0.167976 (1.000000)	0.128185 (1.000000)

C

5	S	12	4563.240000	0.778202 (0.001967)
5	S	13	682.024000	1.448695 (0.015231)
5	S	14	154.973000	2.383089 (0.076127)

5	S	15	44.455300	3.200089 (0.260801)	
5	S	16	13.029000	3.013004 (0.616462)	
5	S	17	1.827730	0.247599 (0.221006)	
6	L	18	20.964200	0.800629 (0.114660)	2.573592 (0.040249)
6	L	19	4.803310	2.127420 (0.919999)	2.408248 (0.237594)
6	L	20	1.459330	-0.002868 (-0.003031)	1.865281 (0.815854)
7	L	21	0.483456	0.413217 (1.000000)	0.574627 (1.000000)
8	L	22	0.145585	0.167976 (1.000000)	0.128185 (1.000000)

O

9	S	23	8588.500000	1.205013 (0.001895)	
9	S	24	1297.230000	2.216205 (0.014386)	
9	S	25	299.296000	3.627452 (0.070732)	
9	S	26	87.377100	4.888452 (0.240001)	
9	S	27	25.678900	4.835721 (0.594797)	
9	S	28	3.740040	0.538229 (0.280802)	
10	L	29	42.117500	1.341958 (0.113889)	5.584018 (0.036511)
10	L	30	9.628370	3.587114 (0.920811)	5.733366 (0.237153)
10	L	31	2.853320	-0.005123 (-0.003274)	4.332955 (0.819702)
11	L	32	0.905661	0.661659 (1.000000)	1.259352 (1.000000)
12	L	33	0.255611	0.256209 (1.000000)	0.259068 (1.000000)

O

13	S	34	8588.500000	1.205013 (0.001895)	
13	S	35	1297.230000	2.216205 (0.014386)	
13	S	36	299.296000	3.627452 (0.070732)	
13	S	37	87.377100	4.888452 (0.240001)	
13	S	38	25.678900	4.835721 (0.594797)	
13	S	39	3.740040	0.538229 (0.280802)	
14	L	40	42.117500	1.341958 (0.113889)	5.584018 (0.036511)
14	L	41	9.628370	3.587114 (0.920811)	5.733366 (0.237153)
14	L	42	2.853320	-0.005123 (-0.003274)	4.332955 (0.819702)
15	L	43	0.905661	0.661659 (1.000000)	1.259352 (1.000000)
16	L	44	0.255611	0.256209 (1.000000)	0.259068 (1.000000)

H

17	S	45	33.865000	0.255069 (0.025494)	
17	S	46	5.094790	0.460109 (0.190373)	
17	S	47	1.158790	0.678321 (0.852161)	
18	S	48	0.325840	0.307371 (1.000000)	
19	S	49	0.102741	0.129336 (1.000000)	

H

23	S	50	33.865000	0.255069 (0.025494)	
23	S	51	5.094790	0.460109 (0.190373)	
23	S	52	1.158790	0.678321 (0.852161)	
24	S	53	0.325840	0.307371 (1.000000)	
25	S	54	0.102741	0.129336 (1.000000)	

H

26	S	55	33.865000	0.255069 (0.025494)
26	S	56	5.094790	0.460109 (0.190373)
26	S	57	1.158790	0.678321 (0.852161)
27	S	58	0.325840	0.307371 (1.000000)
28	S	59	0.102741	0.129336 (1.000000)

TOTAL NUMBER OF SHELLS = 28
TOTAL NUMBER OF BASIS FUNCTIONS = 64
NUMBER OF ELECTRONS = 32
CHARGE OF MOLECULE = 0
STATE MULTIPLICITY = 1
NUMBER OF OCCUPIED ORBITALS (ALPHA) = 16
NUMBER OF OCCUPIED ORBITALS (BETA) = 16
TOTAL NUMBER OF ATOMS = 8
THE NUCLEAR REPULSION ENERGY IS 119.1959522690

\$CONTRL OPTIONS

SCFTYP=RHF RUNTYP=OPTIMIZE EXETYP=RUN
MPLEVL= 0 LOCAL =NONE UNITS =ANGS
MULT = 1 ICHARG= 0 MAXIT = 30
NPRINT= 7 IREST = 0 COORD =CART
ECP =NONE NORMF = 0 NORMP = 0
ITOL = 20 ICUT = 9 NZVAR = 0
NOSYM = 0 INTTYP=POPLE GEOM =INPUT
PLTORB= T MOLPLT= F RPAC = F
AIMPAC= F FRIEND= CITYP =NONE

\$SYSTEM OPTIONS

KDIAG = 0 MEMORY= 750000 TIMLIM= 3600.0 SEC.
COREFL= F PTIME = F XDR = F
BALTYP=NXTVAL

PROPERTIES INPUT

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

EXTRAPOLATION 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 CUTOFF = 1.0E-09
MPTRAN = 0 DIRTRF = F
AOINTS =DUP IREST = 0

THE POINT GROUP IS CS , NAXIS= 0, ORDER= 2

DIMENSIONS OF THE SYMMETRY SUBSPACES ARE
A' = 49 A'' = 15

..... DONE SETTING UP THE RUN

CPU TIME: STEP = 0.05 , TOTAL = 0.3 SECONDS (0.0 MIN)
WALL CLOCK TIME: STEP = 0.06 , TOTAL = 0.1 SECONDS (0.0 MIN)
CPU UTILIZATION: STEP = 83.33%, TOTAL = 583.33%

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 =QA UPHESS =BFGS
NNEG = 0 NFRZ = 0
NSTEP = 20 IFOLW = 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 = 5 STPT = F
STSTEP = 1.000E-02 PROJCT= T

1NSERCH= 0

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.5553984999	0.3390340913	0.0000000000
C	6.0	-0.0909100723	0.0101116239	0.0000000000
O	8.0	0.3444633785	-1.1398543428	0.0000000000
O	8.0	1.1247986272	0.7929158677	0.0000000000
H	1.0	-1.6144861998	1.4395719519	0.0000000000
H	1.0	-1.9631941219	-0.1130088757	0.9187136700
H	1.0	1.8249409414	0.1353914019	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.5553984999	0.3390340913	0.0000000000
C	6.0	-0.0909100723	0.0101116239	0.0000000000
O	8.0	0.3444633785	-1.1398543428	0.0000000000
O	8.0	1.1247986272	0.7929158677	0.0000000000
H	1.0	-1.6144861998	1.4395719519	0.0000000000
H	1.0	-1.9631941219	-0.1130088757	-0.9187136700
H	1.0	-1.9631941219	-0.1130088757	0.9187136700
H	1.0	1.8249409414	0.1353914019	0.0000000000

1 ELECTRON INTEGRALS

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 0.4 SECONDS (0.0 MIN)
WALL CLOCK TIME: STEP = 0.04 , TOTAL = 0.1 SECONDS (0.0 MIN)

CPU UTILIZATION: STEP = 100.00%, TOTAL = 390.00%

GUESS OPTIONS

GUESS =HUCKEL

NORB = 0 NORDER= 0
TOLZ = 1.0E-08 TOLE = 1.0E-05
MIX = F PRTMO = F

INITIAL GUESS ORBITALS GENERATED BY HUCKEL ROUTINE.
HUCKEL GUESS REQUIRES 29856 WORDS.

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

16 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'						

..... END OF INITIAL ORBITAL SELECTION

CPU TIME: STEP = 0.24 , TOTAL = 0.6 SECONDS (0.0 MIN)
WALL CLOCK TIME: STEP = 0.24 , TOTAL = 0.3 SECONDS (0.0 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 185.29%

2 ELECTRON INTEGRALS

THE -PK- OPTION IS OFF, THE INTEGRALS ARE NOT IN SUPERMATRIX FORM.
STORING 4998 INTEGRALS/RECORD ON DISK, USING 12 BYTES/INTEGRAL.
TWO ELECTRON INTEGRAL EVALUATION REQUIRES 34799 WORDS OF MEMORY.

SCHWARZ INEQUALITY OVERHEAD: 2007 INTEGRALS, T= 0.01

II,JST,KST,LST = 1	1	1	1	NREC =	1	INTLOC =	1
II,JST,KST,LST = 2	1	1	1	NREC =	1	INTLOC =	2
II,JST,KST,LST = 3	1	1	1	NREC =	1	INTLOC =	34
II,JST,KST,LST = 4	1	1	1	NREC =	1	INTLOC =	214
II,JST,KST,LST = 5	1	1	1	NREC =	1	INTLOC =	776
II,JST,KST,LST = 6	1	1	1	NREC =	1	INTLOC =	1606
II,JST,KST,LST = 7	1	1	1	NREC =	2	INTLOC =	1611
II,JST,KST,LST = 8	1	1	1	NREC =	4	INTLOC =	854
II,JST,KST,LST = 9	1	1	1	NREC =	7	INTLOC =	871
II,JST,KST,LST = 10	1	1	1	NREC =	8	INTLOC =	494
II,JST,KST,LST = 11	1	1	1	NREC =	12	INTLOC =	3416
II,JST,KST,LST = 12	1	1	1	NREC =	20	INTLOC =	1606
II,JST,KST,LST = 13	1	1	1	NREC =	31	INTLOC =	1005
II,JST,KST,LST = 14	1	1	1	NREC =	33	INTLOC =	3451
II,JST,KST,LST = 15	1	1	1	NREC =	44	INTLOC =	4664
II,JST,KST,LST = 16	1	1	1	NREC =	63	INTLOC =	2075
II,JST,KST,LST = 17	1	1	1	NREC =	89	INTLOC =	447
II,JST,KST,LST = 18	1	1	1	NREC =	94	INTLOC =	3907
II,JST,KST,LST = 19	1	1	1	NREC =	103	INTLOC =	636
II,JST,KST,LST = 20	1	1	1	NREC =	112	INTLOC =	1514
II,JST,KST,LST = 21	1	1	1	NREC =	112	INTLOC =	1514
II,JST,KST,LST = 22	1	1	1	NREC =	112	INTLOC =	1514
II,JST,KST,LST = 23	1	1	1	NREC =	112	INTLOC =	1514
II,JST,KST,LST = 24	1	1	1	NREC =	124	INTLOC =	2100
II,JST,KST,LST = 25	1	1	1	NREC =	142	INTLOC =	1313
II,JST,KST,LST = 26	1	1	1	NREC =	162	INTLOC =	4158
II,JST,KST,LST = 27	1	1	1	NREC =	173	INTLOC =	369
II,JST,KST,LST = 28	1	1	1	NREC =	185	INTLOC =	4890

SCHWARZ INEQUALITY TEST SKIPPED 8553 INTEGRAL BLOCKS.

TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 994898

200 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.17 , TOTAL = 2.8 SECONDS (0.0 MIN)

WALL CLOCK TIME: STEP = 2.19 , TOTAL = 2.5 SECONDS (0.0 MIN)
 CPU UTILIZATION: STEP = 99.09%, TOTAL = 110.67%

 RHF SCF CALCULATION

NUCLEAR ENERGY = 119.1959522690
 MAXIT = 30 NPUNCH= 2
 EXTRAP=T DAMP=F SHIFT=F RSTRCT=F DIIS=F DEM=F SOSCF=T
 DENSITY CONV= 1.00E-05
 SOSCF WILL OPTIMIZE 768 ORBITAL ROTATIONS, SOGTOL= 0.250
 MEMORY REQUIRED FOR RHF STEP= 40137 WORDS.

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
1	0	0	-227.043951244	-227.043951244	0.399747234	0.000000000
-----START SECOND ORDER SCF-----						
2	1	0	-227.623770372	-0.579819128	0.191203372	0.092957311
3	2	0	-227.650338751	-0.026568378	0.081790196	0.081291721
4	3	0	-227.714666588	-0.064327837	0.018011399	0.007126036
5	4	0	-227.715814053	-0.001147465	0.005264798	0.003792557
6	5	0	-227.715915846	-0.000101793	0.001221536	0.000691287
7	6	0	-227.715929558	-0.000013712	0.000538318	0.000390361
8	7	0	-227.715930867	-0.000001309	0.000155422	0.000092540
9	8	0	-227.715931010	-0.000000143	0.000039116	0.000019454
10	9	0	-227.715931021	-0.000000011	0.000023552	0.000006965
11	10	0	-227.715931022	-0.000000001	0.000004012	0.000001348
12	11	0	-227.715931022	0.000000000	0.000000722	0.000000310

 DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 2.6 SECONDS (0.2 SEC/ITER)
 TIME TO SOLVE SCF EQUATIONS= 0.2 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7159310223 AFTER 12 ITERATIONS

 EIGENVECTORS

				1	2	3	4	5
				-20.5870	-20.5545	-11.4215	-11.2897	-1.4732
				A'	A'	A'	A'	A'
1	C	1	S	0.000001	0.000000	0.001353	0.563339	-0.007765
2	C	1	S	0.000000	0.000007	0.001070	0.466524	-0.013291
3	C	1	X	-0.000006	-0.000002	0.000105	0.000752	0.007132
4	C	1	Y	0.000001	-0.000013	-0.000038	-0.000151	-0.003160
5	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
6	C	1	S	-0.000011	-0.000048	0.000193	0.004496	0.035133
7	C	1	X	0.000014	-0.000005	0.000228	-0.000289	0.018524
8	C	1	Y	-0.000002	0.000045	-0.000016	0.000049	-0.005406
9	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
10	C	1	S	0.000248	0.000455	0.000878	-0.001511	-0.013226
11	C	1	X	0.000075	0.000193	0.000417	-0.000023	-0.012919
12	C	1	Y	-0.000140	0.000002	-0.000107	0.000017	0.005576
13	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
14	C	2	S	-0.000003	0.000007	0.563526	-0.001458	-0.061460
15	C	2	S	-0.000028	-0.000071	0.466664	-0.001273	-0.101520
16	C	2	X	0.000040	0.000038	0.001131	-0.000184	0.042123
17	C	2	Y	0.000067	-0.000135	-0.000189	0.000057	-0.045622
18	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
19	C	2	S	0.000102	0.000289	0.003588	0.000317	0.273859
20	C	2	X	0.000084	0.000094	-0.000619	-0.000175	0.068908
21	C	2	Y	-0.000022	-0.000181	-0.000102	0.000060	-0.056966
22	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000

23	C	2	S	-0.000030	0.000026	-0.001149	0.000317	0.007519
24	C	2	X	0.000340	0.000445	0.000914	-0.000296	-0.064887
25	C	2	Y	0.000169	-0.000310	0.000034	0.000069	0.019252
26	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
27	O	3	S	-0.000435	0.551463	-0.000176	0.000004	-0.076360
28	O	3	S	-0.000367	0.471689	-0.000284	0.000008	-0.127511
29	O	3	X	-0.000009	-0.000879	-0.000106	0.000005	-0.010913
30	O	3	Y	0.000004	0.002278	0.000218	-0.000003	0.051851
31	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
32	O	3	S	-0.000024	0.005494	0.000645	-0.000028	0.358740
33	O	3	X	0.000009	0.000330	-0.000233	0.000029	-0.024559
34	O	3	Y	-0.000058	-0.000760	0.000723	-0.000016	0.092105
35	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
36	O	3	S	-0.000067	-0.000682	0.000146	0.000035	0.283263
37	O	3	X	-0.000114	-0.000112	-0.000090	0.000045	0.001070
38	O	3	Y	-0.000050	0.000051	-0.000138	0.000021	0.042377
39	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
40	O	4	S	0.551470	0.000440	-0.000062	0.000003	-0.065144
41	O	4	S	0.471674	0.000378	-0.000111	0.000005	-0.108808
42	O	4	X	-0.000332	-0.000010	-0.000084	0.000005	-0.009471
43	O	4	Y	-0.002193	-0.000001	-0.000050	0.000001	-0.032372
44	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
45	O	4	S	0.005489	0.000024	0.000282	-0.000017	0.305037
46	O	4	X	0.000134	0.000052	-0.000366	0.000018	-0.013408
47	O	4	Y	0.000793	0.000033	-0.000232	0.000012	-0.062274
48	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
49	O	4	S	-0.000434	-0.000257	0.000000	0.000031	0.272756
50	O	4	X	0.000033	-0.000080	0.000036	0.000027	-0.017557
51	O	4	Y	-0.000242	0.000143	0.000018	-0.000046	-0.048565
52	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
53	H	5	S	0.000005	-0.000006	-0.000008	0.000341	0.002932
54	H	5	S	-0.000012	-0.000046	-0.000076	0.000149	-0.001084
55	H	5	S	0.000063	0.000013	0.000033	0.000234	-0.005274
56	H	6	S	0.000000	0.000011	0.000003	0.000331	0.003684
57	H	6	S	-0.000023	-0.000054	-0.000048	0.000145	0.001537
58	H	6	S	-0.000018	0.000013	0.000082	0.000240	-0.000659
59	H	7	S	0.000000	0.000011	0.000003	0.000331	0.003684
60	H	7	S	-0.000023	-0.000054	-0.000048	0.000145	0.001537
61	H	7	S	-0.000018	0.000013	0.000082	0.000240	-0.000659
62	H	8	S	0.000206	-0.000014	-0.000024	-0.000003	0.054692
63	H	8	S	-0.000103	0.000127	-0.000063	0.000001	0.014353
64	H	8	S	0.000122	0.000011	-0.000086	0.000017	0.005459

				6	7	8	9	10
				-1.3304	-1.0540	-0.8005	-0.6853	-0.6726
				A'	A'	A'	A'	A'
1	C	1	S	0.004744	-0.095294	0.033614	-0.014341	0.011243
2	C	1	S	0.007720	-0.160849	0.056743	-0.024646	0.019682
3	C	1	X	-0.003780	0.024344	0.062253	-0.063584	0.068793
4	C	1	Y	0.005816	-0.004056	0.003093	0.092266	-0.004337
5	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
6	C	1	S	-0.019297	0.416103	-0.142353	0.053773	-0.041792
7	C	1	X	-0.004594	0.049111	0.115182	-0.098202	0.092900
8	C	1	Y	0.006278	-0.008390	0.003707	0.155581	-0.000029
9	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
10	C	1	S	-0.038688	0.344180	-0.235198	0.213460	-0.201880
11	C	1	X	-0.009813	0.020955	-0.007979	0.009859	0.017713
12	C	1	Y	0.018230	0.004098	0.016992	0.073521	-0.009829
13	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
14	C	2	S	0.016569	-0.041536	-0.066972	0.029277	0.010383
15	C	2	S	0.026837	-0.070685	-0.116369	0.050315	0.019040
16	C	2	X	0.014433	-0.076277	0.030289	0.088853	-0.099784
17	C	2	Y	0.082473	0.039428	0.041073	0.085802	0.054480
18	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
19	C	2	S	-0.076323	0.207618	0.348688	-0.157763	-0.077383
20	C	2	X	0.029490	-0.122057	0.069277	0.173820	-0.192240

21	C	2	Y	0.110772	0.059441	0.074045	0.164378	0.104216
22	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
23	C	2	S	-0.003663	0.047851	0.257099	-0.155330	0.093793
24	C	2	X	-0.045558	-0.013529	-0.077149	0.165180	-0.129560
25	C	2	Y	-0.033567	0.001529	0.040876	0.009007	0.042566
26	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
27	O	3	S	0.071854	0.025665	0.032931	-0.031053	-0.032046
28	O	3	S	0.120587	0.043197	0.055590	-0.052354	-0.054217
29	O	3	X	0.020842	-0.018289	-0.015531	0.118741	-0.055091
30	O	3	Y	-0.029950	-0.001590	0.069561	-0.068667	-0.148743
31	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
32	O	3	S	-0.343458	-0.123922	-0.161668	0.152954	0.159650
33	O	3	X	0.035961	-0.027539	-0.025324	0.183707	-0.087940
34	O	3	Y	-0.065630	-0.005708	0.101152	-0.100874	-0.215454
35	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
36	O	3	S	-0.281176	-0.120981	-0.199115	0.209554	0.241241
37	O	3	X	0.022843	-0.012716	-0.006279	0.123001	-0.081940
38	O	3	Y	-0.026394	-0.001643	0.064428	-0.066741	-0.161941
39	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
40	O	4	S	-0.091412	0.005846	0.013439	0.001784	-0.030888
41	O	4	S	-0.153110	0.009909	0.022969	0.002960	-0.052306
42	O	4	X	0.005935	-0.020453	-0.149587	-0.109885	-0.010544
43	O	4	Y	-0.024252	0.010043	0.006974	0.010525	0.155873
44	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
45	O	4	S	0.431737	-0.030767	-0.071964	-0.005122	0.156836
46	O	4	X	0.011429	-0.038334	-0.252499	-0.177914	-0.023225
47	O	4	Y	-0.058861	0.016257	0.016749	0.020635	0.238021
48	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
49	O	4	S	0.413281	-0.012758	-0.044163	-0.047740	0.204682
50	O	4	X	-0.017336	-0.017475	-0.154822	-0.129819	-0.012591
51	O	4	Y	-0.046916	0.002454	-0.010049	0.027832	0.198412
52	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
53	H	5	S	-0.000160	0.070820	-0.035610	0.096845	-0.021177
54	H	5	S	-0.001190	0.055663	-0.037003	0.128970	-0.010217
55	H	5	S	0.002589	-0.013658	-0.010491	0.032297	0.010514
56	H	6	S	-0.003178	0.070055	-0.053188	0.007394	-0.033528
57	H	6	S	-0.001518	0.059935	-0.059938	-0.003905	-0.039159
58	H	6	S	-0.000518	-0.011668	-0.015153	0.007295	-0.004616
59	H	7	S	-0.003178	0.070055	-0.053188	0.007394	-0.033528
60	H	7	S	-0.001518	0.059935	-0.059938	-0.003905	-0.039159
61	H	7	S	-0.000518	-0.011668	-0.015153	0.007295	-0.004616
62	H	8	S	0.079166	-0.021711	-0.111963	-0.072480	-0.059905
63	H	8	S	0.025360	-0.026026	-0.127401	-0.075498	-0.076557
64	H	8	S	0.004790	-0.001816	-0.023144	-0.017547	0.021364

				11	12	13	14	15
				-0.6540	-0.6093	-0.5709	-0.5633	-0.4624
				A''	A'	A''	A'	A''
1	C	1	S	0.000000	0.004030	0.000000	-0.000230	0.000000
2	C	1	S	0.000000	0.007025	0.000000	-0.000603	0.000000
3	C	1	X	0.000000	0.106815	0.000000	0.050395	0.000000
4	C	1	Y	0.000000	0.127712	0.000000	-0.105303	0.000000
5	C	1	Z	0.145643	0.000000	-0.117788	0.000000	0.034440
6	C	1	S	0.000000	-0.018089	0.000000	0.001215	0.000000
7	C	1	X	0.000000	0.190453	0.000000	0.100321	0.000000
8	C	1	Y	0.000000	0.226064	0.000000	-0.188695	0.000000
9	C	1	Z	0.258579	0.000000	-0.206209	0.000000	0.055168
10	C	1	S	0.000000	-0.009170	0.000000	0.058639	0.000000
11	C	1	X	0.000000	0.102585	0.000000	0.072343	0.000000
12	C	1	Y	0.000000	0.143312	0.000000	-0.083203	0.000000
13	C	1	Z	0.134805	0.000000	-0.166942	0.000000	0.078429
14	C	2	S	0.000000	-0.015676	0.000000	-0.007716	0.000000
15	C	2	S	0.000000	-0.026421	0.000000	-0.013239	0.000000
16	C	2	X	0.000000	-0.068638	0.000000	-0.044206	0.000000
17	C	2	Y	0.000000	0.027824	0.000000	0.124118	0.000000
18	C	2	Z	0.099064	0.000000	0.072832	0.000000	-0.072134

19	C	2	S	0.000000	0.077192	0.000000	0.026504	0.000000
20	C	2	X	0.000000	-0.133019	0.000000	-0.078200	0.000000
21	C	2	Y	0.000000	0.052297	0.000000	0.205967	0.000000
22	C	2	Z	0.177878	0.000000	0.130218	0.000000	-0.131871
23	C	2	S	0.000000	0.042945	0.000000	0.055425	0.000000
24	C	2	X	0.000000	-0.040359	0.000000	0.007985	0.000000
25	C	2	Y	0.000000	0.011005	0.000000	-0.029997	0.000000
26	C	2	Z	0.105462	0.000000	0.114409	0.000000	-0.098270
27	O	3	S	0.000000	-0.000792	0.000000	-0.012419	0.000000
28	O	3	S	0.000000	-0.001149	0.000000	-0.020479	0.000000
29	O	3	X	0.000000	0.015330	0.000000	0.103415	0.000000
30	O	3	Y	0.000000	-0.018889	0.000000	-0.121172	0.000000
31	O	3	Z	0.089549	0.000000	0.093063	0.000000	-0.195954
32	O	3	S	0.000000	-0.000251	0.000000	0.059144	0.000000
33	O	3	X	0.000000	0.021525	0.000000	0.158459	0.000000
34	O	3	Y	0.000000	-0.024904	0.000000	-0.194563	0.000000
35	O	3	Z	0.142346	0.000000	0.147447	0.000000	-0.306381
36	O	3	S	0.000000	0.037064	0.000000	0.077552	0.000000
37	O	3	X	0.000000	0.027351	0.000000	0.152141	0.000000
38	O	3	Y	0.000000	-0.004580	0.000000	-0.138327	0.000000
39	O	3	Z	0.118820	0.000000	0.133117	0.000000	-0.326205
40	O	4	S	0.000000	0.018071	0.000000	0.019930	0.000000
41	O	4	S	0.000000	0.030503	0.000000	0.033808	0.000000
42	O	4	X	0.000000	0.081106	0.000000	-0.021167	0.000000
43	O	4	Y	0.000000	-0.085025	0.000000	-0.132568	0.000000
44	O	4	Z	0.092293	0.000000	0.183928	0.000000	0.197939
45	O	4	S	0.000000	-0.089939	0.000000	-0.105725	0.000000
46	O	4	X	0.000000	0.135885	0.000000	-0.033300	0.000000
47	O	4	Y	0.000000	-0.129721	0.000000	-0.204224	0.000000
48	O	4	Z	0.145411	0.000000	0.282391	0.000000	0.297161
49	O	4	S	0.000000	-0.130615	0.000000	-0.119908	0.000000
50	O	4	X	0.000000	0.101073	0.000000	-0.052443	0.000000
51	O	4	Y	0.000000	-0.118499	0.000000	-0.198182	0.000000
52	O	4	Z	0.126130	0.000000	0.284804	0.000000	0.349804
53	H	5	S	0.000000	0.099158	0.000000	-0.106296	0.000000
54	H	5	S	0.000000	0.145257	0.000000	-0.181737	0.000000
55	H	5	S	0.000000	0.027210	0.000000	-0.076999	0.000000
56	H	6	S	-0.103731	-0.090133	0.092239	0.021224	-0.029948
57	H	6	S	-0.153684	-0.139625	0.135382	0.028136	-0.042098
58	H	6	S	-0.039621	-0.038437	0.033653	0.011715	0.003675
59	H	7	S	0.103731	-0.090133	-0.092239	0.021224	0.029948
60	H	7	S	0.153684	-0.139625	-0.135382	0.028136	0.042098
61	H	7	S	0.039621	-0.038437	-0.033653	0.011715	-0.003675
62	H	8	S	0.000000	0.086354	0.000000	0.046532	0.000000
63	H	8	S	0.000000	0.109783	0.000000	0.058511	0.000000
64	H	8	S	0.000000	0.024221	0.000000	0.016950	0.000000

				16	17	18	19	20
				-0.4426	0.1328	0.1375	0.1881	0.2005
				A'	A''	A'	A'	A'
1	C	1	S	-0.007145	0.000000	-0.047946	-0.010212	0.001036
2	C	1	S	-0.012898	0.000000	-0.079455	-0.016668	0.001397
3	C	1	X	0.051414	0.000000	-0.025042	-0.062750	-0.010843
4	C	1	Y	-0.028595	0.000000	-0.002552	0.019418	-0.129358
5	C	1	Z	0.000000	0.029293	0.000000	0.000000	0.000000
6	C	1	S	0.036849	0.000000	0.116489	0.032948	0.003667
7	C	1	X	0.112936	0.000000	0.004058	-0.114252	-0.005273
8	C	1	Y	-0.056093	0.000000	-0.005685	0.032601	-0.144223
9	C	1	Z	0.000000	0.030721	0.000000	0.000000	0.000000
10	C	1	S	0.145043	0.000000	1.865371	-0.043243	-0.125945
11	C	1	X	0.085125	0.000000	-0.230751	-0.664327	-0.154217
12	C	1	Y	-0.035751	0.000000	-0.093331	0.242975	-1.142813
13	C	1	Z	0.000000	0.494043	0.000000	0.000000	0.000000
14	C	2	S	-0.005608	0.000000	0.009571	-0.014987	0.006860
15	C	2	S	-0.009143	0.000000	0.016863	-0.025363	0.011611
16	C	2	X	-0.047530	0.000000	-0.006908	0.013784	-0.013515

17	C	2	Y	-0.017599	0.000000	-0.024082	0.032178	-0.025522
18	C	2	Z	0.000000	0.199920	0.000000	0.000000	0.000000
19	C	2	S	0.033223	0.000000	-0.034403	0.052514	-0.021503
20	C	2	X	-0.083279	0.000000	0.000193	0.070901	-0.027113
21	C	2	Y	-0.019639	0.000000	-0.039586	0.054376	-0.047463
22	C	2	Z	0.000000	0.351894	0.000000	0.000000	0.000000
23	C	2	S	-0.008170	0.000000	-0.210109	0.451713	-0.257399
24	C	2	X	0.085665	0.000000	0.034242	-0.827605	-0.096608
25	C	2	Y	0.069834	0.000000	-0.057432	0.239439	-0.067568
26	C	2	Z	0.000000	0.564293	0.000000	0.000000	0.000000
27	O	3	S	-0.000632	0.000000	-0.008538	0.005989	0.002894
28	O	3	S	-0.001263	0.000000	-0.014345	0.010449	0.005082
29	O	3	X	0.223390	0.000000	0.003990	-0.050487	0.009662
30	O	3	Y	0.115070	0.000000	-0.000974	-0.006960	-0.006000
31	O	3	Z	0.000000	-0.145591	0.000000	0.000000	0.000000
32	O	3	S	0.002404	0.000000	0.037930	-0.036971	-0.016091
33	O	3	X	0.347201	0.000000	0.003758	-0.070533	0.013405
34	O	3	Y	0.186134	0.000000	-0.003713	-0.008566	-0.014196
35	O	3	Z	0.000000	-0.198596	0.000000	0.000000	0.000000
36	O	3	S	0.032784	0.000000	0.146263	0.055265	-0.016661
37	O	3	X	0.347651	0.000000	0.016572	-0.114925	0.036168
38	O	3	Y	0.187700	0.000000	0.026873	0.016381	-0.008799
39	O	3	Z	0.000000	-0.429714	0.000000	0.000000	0.000000
40	O	4	S	-0.001199	0.000000	-0.018762	0.028079	0.001419
41	O	4	S	-0.002083	0.000000	-0.031578	0.047517	0.002540
42	O	4	X	0.059550	0.000000	-0.008222	-0.048339	-0.037622
43	O	4	Y	0.141826	0.000000	-0.020600	0.045716	-0.014744
44	O	4	Z	0.000000	-0.078306	0.000000	0.000000	0.000000
45	O	4	S	0.018184	0.000000	0.080132	-0.125773	-0.011960
46	O	4	X	0.096797	0.000000	-0.018498	-0.051464	-0.052933
47	O	4	Y	0.232417	0.000000	-0.038024	0.089065	-0.021814
48	O	4	Z	0.000000	-0.106262	0.000000	0.000000	0.000000
49	O	4	S	-0.096164	0.000000	0.362885	-0.473153	0.009879
50	O	4	X	0.131405	0.000000	-0.010467	-0.233240	-0.152027
51	O	4	Y	0.239067	0.000000	-0.069695	0.038689	-0.052369
52	O	4	Z	0.000000	-0.217491	0.000000	0.000000	0.000000
53	H	5	S	-0.026464	0.000000	-0.005872	-0.020708	0.032694
54	H	5	S	-0.067929	0.000000	0.060357	0.002828	-0.005961
55	H	5	S	-0.028971	0.000000	-0.686479	-0.590055	2.124834
56	H	6	S	-0.004265	0.050369	-0.018959	-0.005338	-0.013062
57	H	6	S	-0.005782	0.182750	-0.008534	0.048256	0.004063
58	H	6	S	-0.025271	0.715456	-0.966064	-0.362758	-0.937638
59	H	7	S	-0.004265	-0.050369	-0.018959	-0.005338	-0.013062
60	H	7	S	-0.005782	-0.182750	-0.008534	0.048256	0.004063
61	H	7	S	-0.025271	-0.715456	-0.966064	-0.362758	-0.937638
62	H	8	S	-0.020167	0.000000	-0.032978	0.054220	0.010129
63	H	8	S	-0.010792	0.000000	0.007457	-0.104651	-0.001153
64	H	8	S	0.037560	0.000000	-0.494953	1.535948	0.256325

				21	22	23	24	25
				0.2167	0.3028	0.3683	0.4205	0.4536
				A''	A'	A'	A'	A''
1	C	1	S	0.000000	0.016883	0.001712	-0.005706	0.000000
2	C	1	S	0.000000	0.026310	0.009072	-0.013439	0.000000
3	C	1	X	0.000000	-0.109642	-0.014414	0.065215	0.000000
4	C	1	Y	0.000000	-0.005427	-0.013823	-0.007420	0.000000
5	C	1	Z	0.131636	0.000000	0.000000	0.000000	0.035400
6	C	1	S	0.000000	0.019786	-0.158398	0.092014	0.000000
7	C	1	X	0.000000	-0.088642	-0.153880	0.242258	0.000000
8	C	1	Y	0.000000	0.002592	0.047704	0.005038	0.000000
9	C	1	Z	0.141161	0.000000	0.000000	0.000000	-0.013047
10	C	1	S	0.000000	-1.377772	1.369914	-0.903308	0.000000
11	C	1	X	0.000000	-1.870746	1.403917	-0.641775	0.000000
12	C	1	Y	0.000000	0.234934	-0.382741	-0.554961	0.000000
13	C	1	Z	1.064496	0.000000	0.000000	0.000000	1.997021
14	C	2	S	0.000000	-0.056561	0.004301	0.014748	0.000000

15	C	2	S	0.000000	-0.100906	0.010829	0.019893	0.000000
16	C	2	X	0.000000	-0.034415	0.118396	-0.039272	0.000000
17	C	2	Y	0.000000	0.093124	0.083340	0.020312	0.000000
18	C	2	Z	-0.079249	0.000000	0.000000	0.000000	-0.084861
19	C	2	S	0.000000	0.270773	-0.092268	0.178531	0.000000
20	C	2	X	0.000000	-0.096796	0.299691	-0.128820	0.000000
21	C	2	Y	0.000000	0.185743	0.131852	0.113763	0.000000
22	C	2	Z	-0.130207	0.000000	0.000000	0.000000	-0.213998
23	C	2	S	0.000000	2.500270	-0.958281	-2.400726	0.000000
24	C	2	X	0.000000	-0.873206	1.545237	-1.637786	0.000000
25	C	2	Y	0.000000	0.668256	0.925855	1.851653	0.000000
26	C	2	Z	-0.398902	0.000000	0.000000	0.000000	-0.651018
27	O	3	S	0.000000	-0.004594	-0.016220	-0.039012	0.000000
28	O	3	S	0.000000	-0.007481	-0.027409	-0.062406	0.000000
29	O	3	X	0.000000	0.005032	-0.066092	-0.024927	0.000000
30	O	3	Y	0.000000	-0.025396	0.008663	0.054733	0.000000
31	O	3	Z	0.081489	0.000000	0.000000	0.000000	0.043440
32	O	3	S	0.000000	0.013579	0.066232	0.059038	0.000000
33	O	3	X	0.000000	-0.004621	-0.076311	-0.046779	0.000000
34	O	3	Y	0.000000	-0.038082	0.021797	0.073538	0.000000
35	O	3	Z	0.110241	0.000000	0.000000	0.000000	0.064990
36	O	3	S	0.000000	0.167399	0.507942	2.406601	0.000000
37	O	3	X	0.000000	0.095565	-0.412893	-0.193661	0.000000
38	O	3	Y	0.000000	-0.014561	0.065992	0.882836	0.000000
39	O	3	Z	0.258257	0.000000	0.000000	0.000000	0.176336
40	O	4	S	0.000000	0.015266	0.027209	-0.005978	0.000000
41	O	4	S	0.000000	0.026377	0.045385	-0.009082	0.000000
42	O	4	X	0.000000	0.111924	0.095567	-0.061782	0.000000
43	O	4	Y	0.000000	0.014065	0.016410	-0.030025	0.000000
44	O	4	Z	0.035913	0.000000	0.000000	0.000000	0.023860
45	O	4	S	0.000000	-0.078799	-0.095132	-0.005712	0.000000
46	O	4	X	0.000000	0.141632	0.122958	-0.101517	0.000000
47	O	4	Y	0.000000	0.031784	0.009342	-0.020870	0.000000
48	O	4	Z	0.047644	0.000000	0.000000	0.000000	0.012306
49	O	4	S	0.000000	-0.206247	-0.904249	0.498503	0.000000
50	O	4	X	0.000000	0.500626	0.509832	-0.368439	0.000000
51	O	4	Y	0.000000	0.016327	0.282118	-0.390928	0.000000
52	O	4	Z	0.116764	0.000000	0.000000	0.000000	0.157907
53	H	5	S	0.000000	-0.048646	-0.032082	-0.027187	0.000000
54	H	5	S	0.000000	-0.360069	-0.294649	0.129090	0.000000
55	H	5	S	0.000000	0.307626	0.331616	0.039399	0.000000
56	H	6	S	-0.000698	-0.014360	0.047149	0.010708	0.042279
57	H	6	S	-0.160246	-0.046786	0.399142	-0.164105	1.206550
58	H	6	S	1.694735	-0.356668	-0.231530	0.186557	-0.038690
59	H	7	S	0.000698	-0.014360	0.047149	0.010708	-0.042279
60	H	7	S	0.160246	-0.046786	0.399142	-0.164105	-1.206550
61	H	7	S	-1.694735	-0.356668	-0.231530	0.186557	0.038690
62	H	8	S	0.000000	0.007949	0.028301	0.031541	0.000000
63	H	8	S	0.000000	0.089533	0.188778	0.301842	0.000000
64	H	8	S	0.000000	-0.508208	-0.457330	0.373022	0.000000

				26	27	28	29	30
				0.4548	0.5638	0.6039	0.6164	0.6992
				A'	A'	A''	A'	A'
1	C	1	S	-0.005872	0.003476	0.000000	-0.046077	-0.063848
2	C	1	S	-0.013133	0.011306	0.000000	-0.087782	-0.125893
3	C	1	X	0.042566	-0.073173	0.000000	0.037585	0.092171
4	C	1	Y	0.023081	0.015851	0.000000	0.003583	0.009582
5	C	1	Z	0.000000	0.000000	0.007806	0.000000	0.000000
6	C	1	S	0.106388	-0.147485	0.000000	0.249621	0.440797
7	C	1	X	0.091990	-0.274327	0.000000	0.111174	0.307945
8	C	1	Y	-0.051934	0.036637	0.000000	0.024408	0.120064
9	C	1	Z	0.000000	0.000000	-0.005483	0.000000	0.000000
10	C	1	S	-0.823197	1.574892	0.000000	3.211336	2.608445
11	C	1	X	0.011140	0.665516	0.000000	0.816937	0.833383
12	C	1	Y	2.329190	-0.073677	0.000000	-0.738588	-0.230039

13	C	1	Z	0.000000	0.000000	-0.562688	0.000000	0.000000
14	C	2	S	0.016903	0.022188	0.000000	0.054639	0.003287
15	C	2	S	0.029239	0.049649	0.000000	0.106736	-0.001917
16	C	2	X	-0.047879	-0.092833	0.000000	-0.042988	0.194282
17	C	2	Y	-0.055887	-0.033153	0.000000	-0.081009	0.106942
18	C	2	Z	0.000000	0.000000	-0.190729	0.000000	0.000000
19	C	2	S	-0.064066	-0.379811	0.000000	-0.512291	0.240625
20	C	2	X	-0.095733	-0.332713	0.000000	-0.359005	0.455445
21	C	2	Y	-0.143092	-0.103400	0.000000	-0.381855	0.544189
22	C	2	Z	0.000000	0.000000	-0.918828	0.000000	0.000000
23	C	2	S	0.119612	0.184020	0.000000	-0.980974	-1.887587
24	C	2	X	-1.246031	1.627172	0.000000	3.280431	1.600377
25	C	2	Y	-1.364820	-0.413163	0.000000	0.873881	-1.208469
26	C	2	Z	0.000000	0.000000	1.678825	0.000000	0.000000
27	O	3	S	-0.004927	0.008786	0.000000	-0.004855	0.003186
28	O	3	S	-0.011310	0.015508	0.000000	-0.009115	0.004901
29	O	3	X	-0.019058	-0.009674	0.000000	-0.038442	-0.054040
30	O	3	Y	0.012451	0.016301	0.000000	0.012896	0.024085
31	O	3	Z	0.000000	0.000000	-0.026908	0.000000	0.000000
32	O	3	S	0.097228	-0.054603	0.000000	0.049681	-0.016311
33	O	3	X	-0.062560	-0.034337	0.000000	-0.021250	-0.076443
34	O	3	Y	0.004981	0.032910	0.000000	0.016594	0.090623
35	O	3	Z	0.000000	0.000000	-0.059150	0.000000	0.000000
36	O	3	S	-0.542094	-0.472916	0.000000	-0.144955	-0.351042
37	O	3	X	0.265168	0.004919	0.000000	-0.520458	-0.253449
38	O	3	Y	-0.006874	-0.102929	0.000000	-0.203048	0.022621
39	O	3	Z	0.000000	0.000000	-0.175168	0.000000	0.000000
40	O	4	S	-0.018583	0.013399	0.000000	-0.004277	0.016673
41	O	4	S	-0.030388	0.022066	0.000000	-0.010293	0.029822
42	O	4	X	-0.062851	-0.098359	0.000000	-0.018850	0.018640
43	O	4	Y	-0.017060	0.068994	0.000000	-0.079102	0.100479
44	O	4	Z	0.000000	0.000000	-0.046009	0.000000	0.000000
45	O	4	S	0.047267	-0.019586	0.000000	0.091003	-0.096344
46	O	4	X	-0.070311	-0.128652	0.000000	-0.033088	0.001838
47	O	4	Y	-0.025165	0.110450	0.000000	-0.164427	0.181697
48	O	4	Z	0.000000	0.000000	-0.092418	0.000000	0.000000
49	O	4	S	0.900996	-1.055759	0.000000	-1.018794	-0.236415
50	O	4	X	-0.523356	-0.664922	0.000000	0.460511	-0.021724
51	O	4	Y	-0.161945	0.759724	0.000000	0.023815	0.400410
52	O	4	Z	0.000000	0.000000	-0.185626	0.000000	0.000000
53	H	5	S	-0.037335	-0.008287	0.000000	-0.041273	-0.039686
54	H	5	S	-1.351762	-0.151854	0.000000	-0.673482	-0.942064
55	H	5	S	-0.003498	-0.159861	0.000000	0.220907	0.693456
56	H	6	S	0.014031	-0.012215	-0.004834	-0.021975	-0.018576
57	H	6	S	0.677189	-0.237637	-0.223580	-0.732498	-0.674760
58	H	6	S	0.029999	0.085563	0.278514	0.182920	0.097509
59	H	7	S	0.014031	-0.012215	0.004834	-0.021975	-0.018576
60	H	7	S	0.677189	-0.237637	0.223580	-0.732498	-0.674760
61	H	7	S	0.029999	0.085563	-0.278514	0.182920	0.097509
62	H	8	S	-0.003207	0.104756	0.000000	-0.021157	0.000156
63	H	8	S	0.003544	1.875942	0.000000	-0.803163	0.520424
64	H	8	S	0.301272	-1.200039	0.000000	-0.019776	-0.414832

				31	32	33	34	35
				0.7391	0.7537	0.7604	0.8368	0.8674
				A'	A''	A'	A'	A'
1	C	1	S	0.030106	0.000000	0.007674	-0.004320	0.036570
2	C	1	S	0.058873	0.000000	0.015704	-0.005443	0.087896
3	C	1	X	0.166113	0.000000	-0.053913	0.093037	0.113003
4	C	1	Y	0.043465	0.000000	0.241065	0.045651	-0.024564
5	C	1	Z	0.000000	-0.244484	0.000000	0.000000	0.000000
6	C	1	S	-0.181420	0.000000	-0.080450	-0.091130	-0.707329
7	C	1	X	0.805319	0.000000	-0.184490	0.326395	0.289053
8	C	1	Y	0.226551	0.000000	1.081618	0.182846	-0.047900
9	C	1	Z	0.000000	-1.143774	0.000000	0.000000	0.000000
10	C	1	S	0.532655	0.000000	-0.329394	-0.545569	-0.865403

11	C	1	X	-0.629846	0.000000	-0.040527	-1.041790	-1.936378
12	C	1	Y	-0.700948	0.000000	-1.563034	-0.340033	0.468715
13	C	1	Z	0.000000	1.871489	0.000000	0.000000	0.000000
14	C	2	S	0.005269	0.000000	-0.001532	-0.029054	0.094610
15	C	2	S	0.010025	0.000000	-0.000405	-0.063986	0.213095
16	C	2	X	0.003546	0.000000	-0.094565	0.160854	0.037371
17	C	2	Y	0.009168	0.000000	-0.007164	-0.220832	0.053002
18	C	2	Z	0.000000	0.017487	0.000000	0.000000	0.000000
19	C	2	S	-0.052457	0.000000	-0.050297	0.416744	-1.651668
20	C	2	X	-0.255927	0.000000	-0.152124	0.689206	0.464507
21	C	2	Y	0.075531	0.000000	0.110796	-0.918848	0.171364
22	C	2	Z	0.000000	-0.001660	0.000000	0.000000	0.000000
23	C	2	S	1.051475	0.000000	-0.317711	1.679963	3.527297
24	C	2	X	2.133985	0.000000	-0.570093	-1.251298	-2.538642
25	C	2	Y	-0.054185	0.000000	0.081431	0.800048	0.198289
26	C	2	Z	0.000000	-0.251861	0.000000	0.000000	0.000000
27	O	3	S	0.002713	0.000000	0.002671	0.033641	-0.016770
28	O	3	S	0.003739	0.000000	0.005622	0.060905	-0.029841
29	O	3	X	-0.071433	0.000000	0.054574	0.038814	0.035139
30	O	3	Y	-0.013993	0.000000	0.023085	-0.093885	0.068506
31	O	3	Z	0.000000	0.012720	0.000000	0.000000	0.000000
32	O	3	S	0.009636	0.000000	-0.048358	-0.201006	0.103874
33	O	3	X	-0.132855	0.000000	0.086978	0.042232	0.117399
34	O	3	Y	-0.023546	0.000000	0.055342	-0.108460	0.057990
35	O	3	Z	0.000000	0.035758	0.000000	0.000000	0.000000
36	O	3	S	-0.590970	0.000000	0.268702	-0.323615	0.021967
37	O	3	X	-0.225730	0.000000	0.077556	0.498642	0.049495
38	O	3	Y	-0.176935	0.000000	0.144176	-0.956117	0.349994
39	O	3	Z	0.000000	0.018562	0.000000	0.000000	0.000000
40	O	4	S	0.011515	0.000000	-0.011739	0.011789	-0.003335
41	O	4	S	0.018912	0.000000	-0.021300	0.021516	-0.006565
42	O	4	X	-0.024096	0.000000	-0.007957	-0.012563	-0.016687
43	O	4	Y	0.047165	0.000000	-0.043375	0.019709	-0.044338
44	O	4	Z	0.000000	-0.006340	0.000000	0.000000	0.000000
45	O	4	S	-0.021943	0.000000	0.079922	-0.084077	0.047146
46	O	4	X	-0.073860	0.000000	0.002239	-0.057751	-0.024950
47	O	4	Y	0.092514	0.000000	-0.083200	0.023755	-0.090893
48	O	4	Z	0.000000	-0.030231	0.000000	0.000000	0.000000
49	O	4	S	-0.991276	0.000000	0.285710	-0.146682	0.108052
50	O	4	X	0.261533	0.000000	-0.056875	0.065327	0.124419
51	O	4	Y	0.334895	0.000000	-0.154444	0.069563	0.028700
52	O	4	Z	0.000000	0.074692	0.000000	0.000000	0.000000
53	H	5	S	0.018956	0.000000	-0.057911	-0.004198	-0.009553
54	H	5	S	0.505972	0.000000	-0.631159	-0.183147	-0.004218
55	H	5	S	0.284227	0.000000	1.619936	0.093668	-0.527386
56	H	6	S	0.055157	-0.049804	0.013834	-0.001746	-0.016089
57	H	6	S	0.741519	-0.493365	0.201152	-0.094472	0.007414
58	H	6	S	-0.667548	1.467740	-0.658468	-0.323376	-0.636796
59	H	7	S	0.055157	0.049804	0.013834	-0.001746	-0.016089
60	H	7	S	0.741519	0.493365	0.201152	-0.094472	0.007414
61	H	7	S	-0.667548	-1.467740	-0.658468	-0.323376	-0.636796
62	H	8	S	0.006898	0.000000	-0.008406	0.017820	0.003453
63	H	8	S	0.226272	0.000000	-0.243695	0.545594	0.094173
64	H	8	S	-0.529405	0.000000	0.232599	-0.204524	0.159413

				36	37	38	39	40
				1.0389	1.0620	1.0724	1.1279	1.1417
				A'	A''	A'	A'	A''
1	C	1	S	0.060426	0.000000	0.063577	0.036603	0.000000
2	C	1	S	0.146791	0.000000	0.155425	0.086451	0.000000
3	C	1	X	-0.001596	0.000000	-0.026899	-0.023198	0.000000
4	C	1	Y	-0.027096	0.000000	0.025417	-0.012350	0.000000
5	C	1	Z	0.000000	0.020224	0.000000	0.000000	-0.009089
6	C	1	S	-1.413838	0.000000	-1.590169	-0.887843	0.000000
7	C	1	X	-0.002455	0.000000	-0.039286	0.076412	0.000000
8	C	1	Y	-0.024084	0.000000	-0.020122	-0.128217	0.000000

9	C	1	Z	0.000000	0.050641	0.000000	0.000000	-0.050669
10	C	1	S	5.233517	0.000000	6.752780	5.088939	0.000000
11	C	1	X	1.215885	0.000000	1.963243	1.634636	0.000000
12	C	1	Y	-0.334168	0.000000	-0.267667	0.061677	0.000000
13	C	1	Z	0.000000	0.094936	0.000000	0.000000	0.667040
14	C	2	S	-0.004061	0.000000	-0.038346	-0.023403	0.000000
15	C	2	S	-0.009854	0.000000	-0.077108	-0.066913	0.000000
16	C	2	X	-0.029719	0.000000	0.001828	-0.112319	0.000000
17	C	2	Y	0.066454	0.000000	-0.064933	0.017180	0.000000
18	C	2	Z	0.000000	0.026173	0.000000	0.000000	0.077246
19	C	2	S	0.378940	0.000000	0.484805	0.816056	0.000000
20	C	2	X	-0.139200	0.000000	-0.050916	0.006534	0.000000
21	C	2	Y	0.020181	0.000000	-0.048917	0.205040	0.000000
22	C	2	Z	0.000000	0.057062	0.000000	0.000000	0.059705
23	C	2	S	-3.130985	0.000000	-4.654623	-2.734232	0.000000
24	C	2	X	1.727384	0.000000	2.633932	3.251336	0.000000
25	C	2	Y	-0.323112	0.000000	-0.211453	-0.806718	0.000000
26	C	2	Z	0.000000	-0.480773	0.000000	0.000000	-1.001154
27	O	3	S	0.019018	0.000000	0.000991	0.009045	0.000000
28	O	3	S	0.036061	0.000000	0.004055	0.018172	0.000000
29	O	3	X	-0.058273	0.000000	0.033510	0.059933	0.000000
30	O	3	Y	0.131447	0.000000	-0.182844	0.084491	0.000000
31	O	3	Z	0.000000	0.067490	0.000000	0.000000	-0.227988
32	O	3	S	-0.191168	0.000000	-0.061534	-0.108554	0.000000
33	O	3	X	-0.175095	0.000000	0.160683	0.220467	0.000000
34	O	3	Y	0.522282	0.000000	-0.587064	0.277548	0.000000
35	O	3	Z	0.000000	0.236098	0.000000	0.000000	-0.840840
36	O	3	S	0.194850	0.000000	0.449596	-0.237530	0.000000
37	O	3	X	-0.036084	0.000000	-0.622262	-0.639812	0.000000
38	O	3	Y	-0.767014	0.000000	0.870644	-0.444724	0.000000
39	O	3	Z	0.000000	-0.247981	0.000000	0.000000	1.434884
40	O	4	S	-0.024373	0.000000	0.006548	0.033351	0.000000
41	O	4	S	-0.046199	0.000000	0.013746	0.064283	0.000000
42	O	4	X	0.092168	0.000000	-0.014202	-0.099899	0.000000
43	O	4	Y	0.036933	0.000000	0.079931	-0.135430	0.000000
44	O	4	Z	0.000000	-0.226200	0.000000	0.000000	-0.061597
45	O	4	S	0.228752	0.000000	-0.098833	-0.335820	0.000000
46	O	4	X	0.385036	0.000000	-0.070488	-0.361486	0.000000
47	O	4	Y	0.194030	0.000000	0.201741	-0.544807	0.000000
48	O	4	Z	0.000000	-0.815710	0.000000	0.000000	-0.235191
49	O	4	S	-0.071754	0.000000	0.059329	-0.327942	0.000000
50	O	4	X	-0.748010	0.000000	0.074835	0.535571	0.000000
51	O	4	Y	-0.416374	0.000000	-0.185470	1.279220	0.000000
52	O	4	Z	0.000000	1.275111	0.000000	0.000000	0.506872
53	H	5	S	-0.025329	0.000000	-0.008768	0.004597	0.000000
54	H	5	S	-0.425559	0.000000	-0.784064	-0.407463	0.000000
55	H	5	S	-0.320058	0.000000	-0.321419	-0.400031	0.000000
56	H	6	S	0.012303	-0.013205	-0.020696	0.008621	0.004364
57	H	6	S	-0.510778	0.087179	-0.632881	-0.318939	0.111393
58	H	6	S	-0.303698	-0.140853	-0.182587	-0.049519	0.199217
59	H	7	S	0.012303	0.013205	-0.020696	0.008621	-0.004364
60	H	7	S	-0.510778	-0.087179	-0.632881	-0.318939	-0.111393
61	H	7	S	-0.303698	0.140853	-0.182587	-0.049519	-0.199217
62	H	8	S	-0.021848	0.000000	-0.042019	0.022266	0.000000
63	H	8	S	-0.236477	0.000000	-0.276833	0.348596	0.000000
64	H	8	S	0.267604	0.000000	-0.051245	-0.640032	0.000000

41	42	43	44	45
1.2010	1.2672	1.7143	1.7904	2.4991
A'	A'	A'	A'	A'

1	C	1	S	0.005762	0.014884	-0.009467	0.005008	0.001981
2	C	1	S	0.017905	0.034568	-0.022892	0.013578	-0.002945
3	C	1	X	0.023991	-0.044915	-0.014703	0.000294	-0.017151
4	C	1	Y	0.000397	-0.009344	0.000148	0.042093	-0.031928
5	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
6	C	1	S	-0.248737	-0.267741	0.352147	-0.107089	0.061499

7	C	1	X	0.015181	-0.238853	-0.098195	-0.124770	0.050629
8	C	1	Y	0.046066	0.089235	-0.048463	0.089709	0.050625
9	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
10	C	1	S	0.718733	-0.992605	-3.278909	-1.099462	0.031891
11	C	1	X	0.111493	-0.477830	-1.037247	-0.290829	-0.102686
12	C	1	Y	0.091436	-0.438330	0.340764	0.557499	0.095404
13	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
14	C	2	S	-0.005860	0.019896	0.022582	0.014506	0.003051
15	C	2	S	-0.010535	0.033733	0.070212	0.031972	0.000898
16	C	2	X	0.066395	-0.074150	0.043459	0.043342	-0.154619
17	C	2	Y	0.028291	0.031165	-0.061752	0.147446	0.014291
18	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
19	C	2	S	0.043246	-0.178944	-0.710272	-0.093641	0.037942
20	C	2	X	0.106945	0.151279	-0.323241	-0.253607	0.236152
21	C	2	Y	0.077489	0.077026	0.256228	-0.469659	-0.139826
22	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
23	C	2	S	-0.648632	1.915552	-0.860456	0.304995	0.721393
24	C	2	X	-0.525349	-1.228215	-3.371340	-2.000691	0.029024
25	C	2	Y	-0.910846	0.545120	1.454985	-1.299668	-0.286402
26	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
27	O	3	S	0.009389	-0.009854	0.097274	-0.059356	-0.014318
28	O	3	S	0.020788	-0.020522	0.210389	-0.127666	-0.031462
29	O	3	X	-0.124572	-0.153248	-0.016451	-0.039996	-0.014321
30	O	3	Y	-0.065903	0.037658	-0.018924	0.033756	0.005146
31	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
32	O	3	S	-0.158760	0.138238	-1.716113	1.028064	0.298543
33	O	3	X	-0.518906	-0.596212	-0.049275	-0.122714	0.032324
34	O	3	Y	-0.304791	0.096839	-0.048340	0.120724	0.033604
35	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
36	O	3	S	0.049631	-0.059630	4.091601	-1.870921	-0.770084
37	O	3	X	1.055668	1.228713	0.037895	0.752303	0.043818
38	O	3	Y	0.693811	-0.137020	1.252077	-0.631255	-0.377082
39	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
40	O	4	S	0.002103	-0.008295	0.054948	0.097441	-0.001571
41	O	4	S	0.001406	-0.016442	0.121795	0.211798	0.004013
42	O	4	X	0.103185	-0.150399	0.001467	0.030112	0.121557
43	O	4	Y	-0.108690	0.031230	0.033960	0.037384	-0.119994
44	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
45	O	4	S	0.032862	0.095035	-1.049128	-1.743928	-0.139284
46	O	4	X	0.370493	-0.627397	-0.015043	0.201607	0.008367
47	O	4	Y	-0.531419	0.136579	0.142557	0.166917	0.013150
48	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
49	O	4	S	0.114056	0.201088	2.753090	3.690674	-0.308407
50	O	4	X	-0.954062	1.548418	-0.016185	-0.890851	-0.249378
51	O	4	Y	1.194778	-0.431940	-1.184097	-1.083518	0.325999
52	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
53	H	5	S	0.011886	-0.006246	-0.042682	0.050886	0.291194
54	H	5	S	-0.081576	0.090760	0.234433	-0.146922	-0.437570
55	H	5	S	-0.140181	0.247290	-0.129348	0.018614	0.135582
56	H	6	S	-0.017385	-0.022855	0.034456	-0.063401	0.095807
57	H	6	S	-0.177651	-0.141198	0.223065	0.109770	-0.140898
58	H	6	S	-0.006449	-0.119087	0.149264	-0.021935	-0.008608
59	H	7	S	-0.017385	-0.022855	0.034456	-0.063401	0.095807
60	H	7	S	-0.177651	-0.141198	0.223065	0.109770	-0.140898
61	H	7	S	-0.006449	-0.119087	0.149264	-0.021935	-0.008608
62	H	8	S	0.010178	-0.051291	-0.132594	0.110756	-1.506935
63	H	8	S	0.480420	-0.447919	-0.697316	-0.789242	2.309495
64	H	8	S	0.124295	-0.487930	0.230164	0.229961	-0.869749

46	47	48	49	50
2.5106	2.5267	2.5467	2.8862	3.0073
A''	A'	A'	A''	A'

1	C	1	S	0.000000	-0.002593	0.030468	0.000000	0.003138
2	C	1	S	0.000000	-0.002386	0.031660	0.000000	0.006375
3	C	1	X	0.000000	0.088089	0.166749	0.000000	-0.039619
4	C	1	Y	0.000000	0.480328	0.036828	0.000000	-0.603219

5	C	1	Z	-0.465227	0.000000	0.000000	-0.389259	0.000000
6	C	1	S	0.000000	0.012203	-0.156999	0.000000	-0.045574
7	C	1	X	0.000000	-0.123179	-0.249022	0.000000	-0.009572
8	C	1	Y	0.000000	-0.617950	-0.032365	0.000000	0.693346
9	C	1	Z	0.615681	0.000000	0.000000	0.425142	0.000000
10	C	1	S	0.000000	-0.316416	2.135665	0.000000	0.100930
11	C	1	X	0.000000	-0.084969	0.438730	0.000000	0.038058
12	C	1	Y	0.000000	0.067307	-0.065720	0.000000	-0.392366
13	C	1	Z	0.006247	0.000000	0.000000	-0.198509	0.000000
14	C	2	S	0.000000	0.001664	-0.003733	0.000000	0.007482
15	C	2	S	0.000000	0.002016	-0.004916	0.000000	0.016059
16	C	2	X	0.000000	-0.014683	-0.081851	0.000000	-0.171589
17	C	2	Y	0.000000	-0.113373	0.041667	0.000000	-1.172306
18	C	2	Z	0.179176	0.000000	0.000000	-1.260673	0.000000
19	C	2	S	0.000000	-0.002978	0.052663	0.000000	-0.095499
20	C	2	X	0.000000	0.030785	0.140116	0.000000	0.104004
21	C	2	Y	0.000000	0.106679	-0.053808	0.000000	1.512511
22	C	2	Z	-0.184071	0.000000	0.000000	1.379563	0.000000
23	C	2	S	0.000000	0.439930	-1.179406	0.000000	-0.169507
24	C	2	X	0.000000	-0.106095	0.273618	0.000000	-0.143854
25	C	2	Y	0.000000	-0.162439	-0.147217	0.000000	-0.856048
26	C	2	Z	-0.033817	0.000000	0.000000	-0.672562	0.000000
27	O	3	S	0.000000	-0.010534	-0.001602	0.000000	-0.016874
28	O	3	S	0.000000	-0.023342	-0.003132	0.000000	-0.041492
29	O	3	X	0.000000	-0.009614	-0.005992	0.000000	0.001788
30	O	3	Y	0.000000	-0.011917	-0.007636	0.000000	-0.094239
31	O	3	Z	0.000675	0.000000	0.000000	-0.047694	0.000000
32	O	3	S	0.000000	0.205963	0.029240	0.000000	0.347865
33	O	3	X	0.000000	-0.035710	-0.032628	0.000000	-0.133075
34	O	3	Y	0.000000	0.029143	-0.033079	0.000000	0.239514
35	O	3	Z	0.007242	0.000000	0.000000	-0.061512	0.000000
36	O	3	S	0.000000	-0.420066	-0.018782	0.000000	-0.300710
37	O	3	X	0.000000	0.140427	0.100002	0.000000	0.085651
38	O	3	Y	0.000000	-0.101526	0.066922	0.000000	0.138366
39	O	3	Z	0.004562	0.000000	0.000000	0.088842	0.000000
40	O	4	S	0.000000	0.003273	0.003058	0.000000	0.015823
41	O	4	S	0.000000	0.007689	0.005280	0.000000	0.031704
42	O	4	X	0.000000	0.015564	-0.022992	0.000000	0.034347
43	O	4	Y	0.000000	-0.023356	0.028679	0.000000	-0.022085
44	O	4	Z	0.010026	0.000000	0.000000	-0.053423	0.000000
45	O	4	S	0.000000	-0.071150	-0.027738	0.000000	-0.218890
46	O	4	X	0.000000	0.017875	0.004436	0.000000	0.103770
47	O	4	Y	0.000000	-0.006984	0.007705	0.000000	0.052586
48	O	4	Z	0.004103	0.000000	0.000000	-0.016577	0.000000
49	O	4	S	0.000000	0.037382	0.234499	0.000000	0.406024
50	O	4	X	0.000000	-0.068984	0.007950	0.000000	-0.055391
51	O	4	Y	0.000000	0.101357	-0.089294	0.000000	0.012251
52	O	4	Z	0.003009	0.000000	0.000000	0.092154	0.000000
53	H	5	S	0.000000	-1.233067	0.764288	0.000000	-0.147538
54	H	5	S	0.000000	1.863341	-1.349684	0.000000	0.046988
55	H	5	S	0.000000	-0.896815	0.199594	0.000000	0.359527
56	H	6	S	-1.011445	0.488053	0.955427	-0.016950	0.099872
57	H	6	S	1.501828	-0.708358	-1.641119	0.106202	-0.093125
58	H	6	S	-0.753226	0.401271	0.358599	-0.276812	-0.134313
59	H	7	S	1.011445	0.488053	0.955427	0.016950	0.099872
60	H	7	S	-1.501828	-0.708358	-1.641119	-0.106202	-0.093125
61	H	7	S	0.753226	0.401271	0.358599	0.276812	-0.134313
62	H	8	S	0.000000	-0.176322	0.268600	0.000000	0.060213
63	H	8	S	0.000000	0.304095	-0.454846	0.000000	-0.147303
64	H	8	S	0.000000	-0.119242	0.148152	0.000000	0.041943

51	52	53	54	55
3.1621	3.2662	3.3025	3.3979	5.3042
A'	A'	A''	A'	A'

1	C	1	S	-0.004316	-0.024981	0.000000	-0.004628	-0.002933
2	C	1	S	-0.012201	-0.047337	0.000000	-0.008924	-0.003400

3	C	1	X	-1.311508	0.291533	0.000000	-0.144528	-0.003945
4	C	1	Y	0.198605	0.102319	0.000000	-1.112055	0.022220
5	C	1	Z	0.000000	0.000000	-1.228826	0.000000	0.000000
6	C	1	S	0.025906	0.264931	0.000000	0.074310	0.039335
7	C	1	X	1.728235	0.015816	0.000000	0.241105	0.034262
8	C	1	Y	-0.274914	-0.210280	0.000000	1.428095	-0.037610
9	C	1	Z	0.000000	0.000000	1.540599	0.000000	0.000000
10	C	1	S	0.485302	-0.847991	0.000000	-0.556538	-0.180720
11	C	1	X	-0.856241	-0.374759	0.000000	-0.430157	-0.085572
12	C	1	Y	0.119298	0.226790	0.000000	-0.989555	0.067112
13	C	1	Z	0.000000	0.000000	-1.177279	0.000000	0.000000
14	C	2	S	0.018465	-0.003651	0.000000	-0.006489	-0.005151
15	C	2	S	0.039329	-0.008423	0.000000	-0.012492	0.007772
16	C	2	X	-0.304813	-1.321825	0.000000	-0.080182	-0.062868
17	C	2	Y	0.004777	0.133787	0.000000	0.654301	0.089986
18	C	2	Z	0.000000	0.000000	0.357500	0.000000	0.000000
19	C	2	S	-0.258407	-0.007586	0.000000	0.060712	-0.042542
20	C	2	X	0.786216	1.761583	0.000000	0.142795	0.062610
21	C	2	Y	-0.125221	-0.255699	0.000000	-1.025830	-0.023196
22	C	2	Z	0.000000	0.000000	-0.467573	0.000000	0.000000
23	C	2	S	0.670704	0.778132	0.000000	0.618589	-0.054933
24	C	2	X	0.061478	-1.294679	0.000000	-0.423805	-0.211457
25	C	2	Y	-0.032665	0.144741	0.000000	0.398180	0.023624
26	C	2	Z	0.000000	0.000000	0.406539	0.000000	0.000000
27	O	3	S	0.000267	0.009176	0.000000	0.003808	-0.000133
28	O	3	S	0.001759	0.021971	0.000000	0.009813	-0.002396
29	O	3	X	-0.038169	-0.073928	0.000000	0.008646	-0.444364
30	O	3	Y	0.003597	0.000511	0.000000	0.013353	-0.774790
31	O	3	Z	0.000000	0.000000	0.042367	0.000000	0.000000
32	O	3	S	-0.009546	-0.173770	0.000000	-0.035981	0.033467
33	O	3	X	0.028169	0.027051	0.000000	0.044465	0.496872
34	O	3	Y	-0.053251	-0.171405	0.000000	-0.156998	0.839383
35	O	3	Z	0.000000	0.000000	0.010480	0.000000	0.000000
36	O	3	S	-0.242139	0.027897	0.000000	-0.328244	-0.054685
37	O	3	X	-0.102582	0.125427	0.000000	0.227364	-0.274800
38	O	3	Y	-0.118505	-0.044503	0.000000	-0.218309	-0.395182
39	O	3	Z	0.000000	0.000000	-0.062539	0.000000	0.000000
40	O	4	S	0.001277	0.010735	0.000000	-0.001799	0.002662
41	O	4	S	0.000430	0.017883	0.000000	-0.002653	0.008156
42	O	4	X	0.021312	0.053361	0.000000	-0.028975	-0.456103
43	O	4	Y	0.026241	0.092382	0.000000	0.019068	-0.790223
44	O	4	Z	0.000000	0.000000	0.012557	0.000000	0.000000
45	O	4	S	0.063423	-0.030908	0.000000	-0.010986	-0.098287
46	O	4	X	0.067815	0.118611	0.000000	-0.003310	0.516381
47	O	4	Y	-0.011293	0.030497	0.000000	-0.021666	0.882653
48	O	4	Z	0.000000	0.000000	-0.004259	0.000000	0.000000
49	O	4	S	-0.422841	-0.106362	0.000000	0.061182	0.293339
50	O	4	X	-0.065069	-0.001555	0.000000	-0.125991	-0.291508
51	O	4	Y	0.266343	0.120873	0.000000	-0.048435	-0.542106
52	O	4	Z	0.000000	0.000000	-0.027081	0.000000	0.000000
53	H	5	S	0.080507	-0.025442	0.000000	-0.620323	0.020194
54	H	5	S	-0.091478	0.028002	0.000000	0.565111	-0.024539
55	H	5	S	-0.148823	-0.116115	0.000000	0.263910	0.010753
56	H	6	S	0.141781	-0.136118	0.534315	0.280992	-0.022017
57	H	6	S	-0.143433	0.101520	-0.468162	-0.229252	0.060671
58	H	6	S	-0.178822	-0.063222	-0.286098	-0.149387	-0.031416
59	H	7	S	0.141781	-0.136118	-0.534315	0.280992	-0.022017
60	H	7	S	-0.143433	0.101520	0.468162	-0.229252	0.060671
61	H	7	S	-0.178822	-0.063222	0.286098	-0.149387	-0.031416
62	H	8	S	0.088281	0.159490	0.000000	-0.031951	0.073832
63	H	8	S	0.108198	-0.002838	0.000000	0.098675	-0.174359
64	H	8	S	0.038067	0.231857	0.000000	0.018990	0.173016

56
5.3168
A''

57
5.4080
A''

58
5.4788
A'

59
5.5591
A'

60
5.6152
A'

1	C	1	S	0.000000	0.000000	0.003528	-0.000740	-0.006364
2	C	1	S	0.000000	0.000000	0.002869	-0.000877	-0.006918
3	C	1	X	0.000000	0.000000	0.020936	0.007794	-0.019692
4	C	1	Y	0.000000	0.000000	-0.039777	-0.015909	-0.003787
5	C	1	Z	0.015968	-0.028415	0.000000	0.000000	0.000000
6	C	1	S	0.000000	0.000000	-0.010814	0.006560	0.047465
7	C	1	X	0.000000	0.000000	-0.037093	-0.030405	0.094046
8	C	1	Y	0.000000	0.000000	0.055850	0.032554	-0.001151
9	C	1	Z	-0.028990	0.052825	0.000000	0.000000	0.000000
10	C	1	S	0.000000	0.000000	0.454814	-0.350541	-0.168531
11	C	1	X	0.000000	0.000000	0.230172	-0.122293	-0.098561
12	C	1	Y	0.000000	0.000000	-0.021136	-0.146954	0.076801
13	C	1	Z	0.019964	-0.212309	0.000000	0.000000	0.000000
14	C	2	S	0.000000	0.000000	-0.014529	0.003421	-0.026234
15	C	2	S	0.000000	0.000000	-0.027449	0.000691	-0.026760
16	C	2	X	0.000000	0.000000	0.116368	-0.041216	-0.135861
17	C	2	Y	0.000000	0.000000	-0.061247	0.044303	-0.112194
18	C	2	Z	0.029755	0.102068	0.000000	0.000000	0.000000
19	C	2	S	0.000000	0.000000	0.142318	-0.063537	0.059238
20	C	2	X	0.000000	0.000000	-0.161613	0.075007	0.362912
21	C	2	Y	0.000000	0.000000	-0.107571	-0.113233	0.020464
22	C	2	Z	-0.033264	-0.192719	0.000000	0.000000	0.000000
23	C	2	S	0.000000	0.000000	-0.486409	0.188344	-0.379667
24	C	2	X	0.000000	0.000000	0.653723	-0.353546	-0.589213
25	C	2	Y	0.000000	0.000000	0.188535	0.454980	-0.172261
26	C	2	Z	0.074187	0.402920	0.000000	0.000000	0.000000
27	O	3	S	0.000000	0.000000	0.004123	0.007004	0.003425
28	O	3	S	0.000000	0.000000	0.009799	0.013103	0.007357
29	O	3	X	0.000000	0.000000	-1.150324	0.284448	0.196692
30	O	3	Y	0.000000	0.000000	0.521962	0.297076	0.830896
31	O	3	Z	0.600586	-1.127931	0.000000	0.000000	0.000000
32	O	3	S	0.000000	0.000000	-0.085925	-0.123813	-0.045763
33	O	3	X	0.000000	0.000000	1.328235	-0.331574	-0.234014
34	O	3	Y	0.000000	0.000000	-0.593406	-0.367455	-0.986310
35	O	3	Z	-0.652912	1.264864	0.000000	0.000000	0.000000
36	O	3	S	0.000000	0.000000	0.167210	0.351067	0.072727
37	O	3	X	0.000000	0.000000	-0.725568	0.169653	0.140157
38	O	3	Y	0.000000	0.000000	0.231827	0.187120	0.429306
39	O	3	Z	0.268465	-0.618859	0.000000	0.000000	0.000000
40	O	4	S	0.000000	0.000000	-0.005583	0.002973	0.007566
41	O	4	S	0.000000	0.000000	-0.010340	0.006286	0.014200
42	O	4	X	0.000000	0.000000	0.225806	0.812035	-0.865724
43	O	4	Y	0.000000	0.000000	0.006488	-0.904785	-0.434084
44	O	4	Z	-1.123599	-0.600118	0.000000	0.000000	0.000000
45	O	4	S	0.000000	0.000000	0.106947	-0.035453	-0.117348
46	O	4	X	0.000000	0.000000	-0.268439	-0.959059	1.061752
47	O	4	Y	0.000000	0.000000	-0.016673	1.059440	0.518264
48	O	4	Z	1.236333	0.677575	0.000000	0.000000	0.000000
49	O	4	S	0.000000	0.000000	-0.357627	0.217799	0.312977
50	O	4	X	0.000000	0.000000	0.131257	0.675052	-0.649257
51	O	4	Y	0.000000	0.000000	0.067275	-0.642722	-0.216715
52	O	4	Z	-0.531043	-0.343168	0.000000	0.000000	0.000000
53	H	5	S	0.000000	0.000000	-0.009108	-0.001401	-0.000808
54	H	5	S	0.000000	0.000000	-0.041766	0.000102	-0.025935
55	H	5	S	0.000000	0.000000	-0.016126	0.103220	-0.008309
56	H	6	S	-0.010847	0.019277	0.001890	0.011792	0.008063
57	H	6	S	0.004813	-0.047632	0.031544	-0.036218	-0.033226
58	H	6	S	0.041965	-0.044533	0.018922	-0.004027	0.004053
59	H	7	S	0.010847	-0.019277	0.001890	0.011792	0.008063
60	H	7	S	-0.004813	0.047632	0.031544	-0.036218	-0.033226
61	H	7	S	-0.041965	0.044533	0.018922	-0.004027	0.004053
62	H	8	S	0.000000	0.000000	0.042274	0.343921	-0.051461
63	H	8	S	0.000000	0.000000	0.021670	-0.593686	0.032378
64	H	8	S	0.000000	0.000000	0.017322	-0.013290	0.240011

				24.3642	24.5943	51.4969	51.5483
				A'	A'	A'	A'
1	C	1	S	-0.987174	-1.771905	0.001734	0.002796
2	C	1	S	1.053150	1.907824	-0.002967	-0.004767
3	C	1	X	-0.022437	0.017246	0.001440	-0.000586
4	C	1	Y	0.006897	-0.004144	-0.000911	0.002253
5	C	1	Z	0.000000	0.000000	0.000000	0.000000
6	C	1	S	-0.215703	-0.485100	0.012263	0.014147
7	C	1	X	0.041984	-0.050288	-0.006086	0.007770
8	C	1	Y	-0.013230	0.011082	0.001264	-0.009021
9	C	1	Z	0.000000	0.000000	0.000000	0.000000
10	C	1	S	0.050075	1.144719	-0.203585	-0.044608
11	C	1	X	-0.155722	0.319421	-0.064425	-0.024055
12	C	1	Y	0.036048	-0.063000	0.052963	-0.031252
13	C	1	Z	0.000000	0.000000	0.000000	0.000000
14	C	2	S	-1.770571	0.989794	-0.001699	0.007055
15	C	2	S	1.898882	-1.071294	0.003036	-0.011260
16	C	2	X	0.018503	0.030284	-0.009765	-0.002323
17	C	2	Y	-0.012509	-0.003233	-0.002428	0.014200
18	C	2	Z	0.000000	0.000000	0.000000	0.000000
19	C	2	S	-0.404825	0.281224	-0.024912	-0.008500
20	C	2	X	-0.045733	-0.071784	-0.000779	0.009643
21	C	2	Y	0.050374	-0.001588	-0.003507	-0.010581
22	C	2	Z	0.000000	0.000000	0.000000	0.000000
23	C	2	S	0.289908	-0.652010	-0.089206	-0.112242
24	C	2	X	-0.234354	0.502211	-0.295326	-0.024993
25	C	2	Y	0.033794	-0.107149	0.008883	0.194329
26	C	2	Z	0.000000	0.000000	0.000000	0.000000
27	O	3	S	-0.006597	0.000533	-0.812286	-2.095234
28	O	3	S	0.000275	-0.000259	0.843603	2.178605
29	O	3	X	0.013346	-0.009234	0.003298	-0.003632
30	O	3	Y	-0.026795	0.012126	0.002482	0.006957
31	O	3	Z	0.000000	0.000000	0.000000	0.000000
32	O	3	S	0.007053	0.018534	-0.100627	-0.277369
33	O	3	X	-0.038411	0.022027	-0.009142	0.012961
34	O	3	Y	0.072018	-0.025847	-0.006446	-0.027925
35	O	3	Z	0.000000	0.000000	0.000000	0.000000
36	O	3	S	0.085795	-0.080358	0.174205	0.388661
37	O	3	X	0.036581	-0.045405	0.031927	-0.048567
38	O	3	Y	0.050122	-0.035082	0.047801	0.102821
39	O	3	Z	0.000000	0.000000	0.000000	0.000000
40	O	4	S	0.001982	-0.001814	-2.095102	0.812516
41	O	4	S	0.000011	0.000031	2.177502	-0.845481
42	O	4	X	0.020753	-0.005357	-0.003798	0.004280
43	O	4	Y	0.009510	-0.000715	-0.007319	-0.000669
44	O	4	Z	0.000000	0.000000	0.000000	0.000000
45	O	4	S	-0.037230	0.019105	-0.271635	0.112479
46	O	4	X	-0.038723	0.005219	0.014070	-0.015064
47	O	4	Y	-0.010289	-0.006181	0.024396	-0.002879
48	O	4	Z	0.000000	0.000000	0.000000	0.000000
49	O	4	S	0.143071	-0.077513	0.402023	-0.133132
50	O	4	X	0.011787	-0.008127	-0.049890	0.048390
51	O	4	Y	-0.078860	0.057938	-0.112893	0.011610
52	O	4	Z	0.000000	0.000000	0.000000	0.000000
53	H	5	S	0.014763	0.023096	-0.000229	0.001665
54	H	5	S	-0.008548	-0.083108	0.000280	0.009290
55	H	5	S	-0.065901	-0.061755	-0.012021	-0.008627
56	H	6	S	0.013096	0.023105	-0.000650	-0.003460
57	H	6	S	-0.008506	-0.079387	0.013618	0.009189
58	H	6	S	-0.071895	-0.052566	0.007449	0.002922
59	H	7	S	0.013096	0.023105	-0.000650	-0.003460
60	H	7	S	-0.008506	-0.079387	0.013618	0.009189
61	H	7	S	-0.071895	-0.052566	0.007449	0.002922
62	H	8	S	0.000399	0.002792	0.006821	0.007683
63	H	8	S	-0.061966	0.006106	-0.072537	-0.008283
64	H	8	S	0.005334	-0.028659	0.016725	0.014200

..... END OF RHF CALCULATION

CPU TIME: STEP = 2.96 , TOTAL = 5.8 SECONDS (0.1 MIN)
WALL CLOCK TIME: STEP = 2.96 , TOTAL = 5.5 SECONDS (0.1 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 104.92%

ENERGY COMPONENTS

WAVEFUNCTION NORMALIZATION = 1.0000000000

ONE ELECTRON ENERGY = -547.4815567661
TWO ELECTRON ENERGY = 200.5696734747
NUCLEAR REPULSION ENERGY = 119.1959522690

TOTAL ENERGY = -227.7159310223

ELECTRON-ELECTRON POTENTIAL ENERGY = 200.5696734747
NUCLEUS-ELECTRON POTENTIAL ENERGY = -775.0992604757
NUCLEUS-NUCLEUS POTENTIAL ENERGY = 119.1959522690

TOTAL POTENTIAL ENERGY = -455.3336347320
TOTAL KINETIC ENERGY = 227.6177037096
VIRIAL RATIO (V/T) = 2.0004315451

MULLIKEN AND LOWDIN POPULATION ANALYSES

MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL

	1	2	3	4	5
	2.000000	2.000000	2.000000	2.000000	2.000000
1	0.000002	0.000012	0.000241	1.999629	-0.004965
2	0.000065	0.000129	1.999692	0.000146	0.355536
3	-0.000002	1.999862	0.000063	0.000000	0.906394
4	1.999927	-0.000004	0.000002	0.000000	0.701674
5	0.000001	0.000000	0.000001	0.000075	-0.001333
6	0.000000	0.000000	0.000005	0.000075	0.000075
7	0.000000	0.000000	0.000005	0.000075	0.000075
8	0.000007	0.000001	-0.000007	0.000000	0.042545
	6	7	8	9	10
	2.000000	2.000000	2.000000	2.000000	2.000000
1	0.015038	1.265098	0.265874	0.402454	0.133639
2	0.121589	0.385269	0.497279	0.471523	0.316150
3	0.667463	0.077702	0.263705	0.562884	0.727170
4	1.121659	0.021916	0.644787	0.302941	0.730293
5	0.000059	0.077142	0.024431	0.197137	0.003410
6	0.000278	0.081939	0.059024	0.000872	0.019648
7	0.000278	0.081939	0.059024	0.000872	0.019648
8	0.073638	0.008993	0.185875	0.061316	0.050040
	11	12	13	14	15
	2.000000	2.000000	2.000000	2.000000	2.000000
1	0.686509	0.849380	0.422830	0.378473	0.030483
2	0.382850	0.129886	0.177745	0.267483	0.128829
3	0.233474	0.015197	0.238686	0.560943	0.971836
4	0.226349	0.354491	0.833101	0.479241	0.842410

5	0.000000	0.193948	0.000000	0.266921	0.000000
6	0.235409	0.176196	0.163819	0.007593	0.013221
7	0.235409	0.176196	0.163819	0.007593	0.013221
8	0.000000	0.104705	0.000000	0.031752	0.000000

16

2.000000

1	0.093872
2	0.069289
3	1.322965
4	0.471817
5	0.021386
6	0.003758
7	0.003758
8	0.013156

----- POPULATIONS IN EACH AO -----

				MULLIKEN	LOWDIN
1	C	1	S	1.10329	1.04653
2	C	1	S	0.89079	0.92839
3	C	1	X	0.17336	0.17635
4	C	1	Y	0.20794	0.21309
5	C	1	Z	0.20566	0.21009
6	C	1	S	0.73985	0.57645
7	C	1	X	0.50779	0.50471
8	C	1	Y	0.59111	0.54522
9	C	1	Z	0.58989	0.54444
10	C	1	S	0.76689	0.37989
11	C	1	X	0.12115	0.33184
12	C	1	Y	0.29657	0.36290
13	C	1	Z	0.34427	0.37931
14	C	2	S	1.10410	1.04748
15	C	2	S	0.88990	0.92710
16	C	2	X	0.20308	0.21188
17	C	2	Y	0.21465	0.22272
18	C	2	Z	0.11392	0.11608
19	C	2	S	0.84571	0.60285
20	C	2	X	0.58660	0.55230
21	C	2	Y	0.50430	0.49879
22	C	2	Z	0.34138	0.31584
23	C	2	S	0.20885	0.32363
24	C	2	X	0.04135	0.29454
25	C	2	Y	0.01552	0.26279
26	C	2	Z	0.23413	0.27790
27	O	3	S	1.08366	1.03188
28	O	3	S	0.91209	0.95191
29	O	3	X	0.36076	0.36940
30	O	3	Y	0.30059	0.30383
31	O	3	Z	0.25815	0.26217
32	O	3	S	1.00690	0.92034
33	O	3	X	0.79238	0.79936
34	O	3	Y	0.69249	0.70466
35	O	3	Z	0.59987	0.59755
36	O	3	S	0.94066	0.71122
37	O	3	X	0.60508	0.62304
38	O	3	Y	0.40974	0.51616
39	O	3	Z	0.58598	0.57944
40	O	4	S	1.08357	1.03134
41	O	4	S	0.91222	0.95150
42	O	4	X	0.22534	0.22863
43	O	4	Y	0.33021	0.33779
44	O	4	Z	0.36862	0.37589
45	O	4	S	0.98276	0.90644
46	O	4	X	0.58862	0.55882

47	O	4	Y	0.75508	0.75231
48	O	4	Z	0.79117	0.80872
49	O	4	S	0.96447	0.68412
50	O	4	X	0.39675	0.46445
51	O	4	Y	0.58973	0.59649
52	O	4	Z	0.74207	0.70694
53	H	5	S	0.26448	0.27472
54	H	5	S	0.46174	0.44462
55	H	5	S	0.05696	0.17548
56	H	6	S	0.26201	0.27058
57	H	6	S	0.44973	0.43603
58	H	6	S	0.05018	0.16992
59	H	7	S	0.26201	0.27058
60	H	7	S	0.44973	0.43603
61	H	7	S	0.05018	0.16992
62	H	8	S	0.26947	0.27050
63	H	8	S	0.26193	0.32309
64	H	8	S	0.04062	0.13097

----- MULLIKEN ATOMIC OVERLAP POPULATIONS -----
(OFF-DIAGONAL ELEMENTS NEED TO BE MULTIPLIED BY 2)

	1	2	3	4	5
1	5.5262012				
2	0.0341570	4.7247581			
3	-0.0833878	0.5093419	8.2805403		
4	-0.0629319	0.1993841	-0.1831868	8.5051657	
5	0.3564260	-0.0464483	0.0040128	0.0027755	0.5002332
6	0.3811758	-0.0404320	0.0014166	0.0017178	-0.0166221
7	0.3811758	-0.0404320	0.0014166	0.0017178	-0.0166221
8	0.0057518	-0.0368701	0.0181894	0.2659627	-0.0005756

	6	7	8
6	0.4468106		
7	-0.0118688	0.4468106	
8	-0.0002855	-0.0002855	0.3201341

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 C	6.538568	-0.538568	6.199229	-0.199229
2 C	5.303459	0.696541	5.653887	0.346113
3 O	8.548343	-0.548343	8.370963	-0.370963
4 O	8.730605	-0.730605	8.403459	-0.403459
5 H	0.783179	0.216821	0.894829	0.105171
6 H	0.761912	0.238088	0.876540	0.123460
7 H	0.761912	0.238088	0.876540	0.123460
8 H	0.572021	0.427979	0.724554	0.275446

BOND ORDER AND VALENCE ANALYSIS BOND ORDER THRESHOLD=0.050

ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER
1	2	1.501	0.789	1	5	1.102	0.921	1	6	1.102	0.925
1	7	1.102	0.925	2	3	1.230	1.806	2	4	1.446	0.853
4	8	0.960	0.766								

ATOM	TOTAL VALENCE	BONDED VALENCE	FREE VALENCE
1 C	3.517	3.517	0.000
2 C	3.419	3.419	0.000
3 O	1.825	1.825	0.000
4 O	1.599	1.599	0.000

5 H	0.912	0.912	0.000
6 H	0.917	0.917	0.000
7 H	0.917	0.917	0.000
8 H	0.821	0.821	0.000

ELECTROSTATIC MOMENTS

POINT	1	X	Y	Z (BOHR)	CHARGE
		0.000000	0.000000	0.000000	0.00 (A.U.)
		DX	DY	DZ	/D/ (DEBYE)
		-2.252751	1.079859	0.000000	2.498196

..... END OF PROPERTY EVALUATION

CPU	TIME:	STEP =	0.09 ,	TOTAL =	5.8 SECONDS (0.1 MIN)
WALL CLOCK TIME:	STEP =	0.09 ,	TOTAL =	5.6 SECONDS (0.1 MIN)	
CPU UTILIZATION:	STEP =	100.00%,	TOTAL =	104.84%		

.....END OF NBO ANALYSIS.....

CPU	TIME:	STEP =	0.00 ,	TOTAL =	5.8 SECONDS (0.1 MIN)
WALL CLOCK TIME:	STEP =	0.00 ,	TOTAL =	5.6 SECONDS (0.1 MIN)	
CPU UTILIZATION:	STEP =	100.00%,	TOTAL =	104.84%		

BEGINNING ONE ELECTRON GRADIENT...
..... END OF 1-ELECTRON GRADIENT

CPU	TIME:	STEP =	0.23 ,	TOTAL =	6.1 SECONDS (0.1 MIN)
WALL CLOCK TIME:	STEP =	0.24 ,	TOTAL =	5.8 SECONDS (0.1 MIN)	
CPU UTILIZATION:	STEP =	95.83%,	TOTAL =	104.47%		

GRADIENT OF THE ENERGY

SCHWARZ SCREENING SKIPPED 8716 BLOCKS, COMPUTED 48797 BLOCKS

..... END OF 2-ELECTRON GRADIENT

CPU	TIME:	STEP =	3.47 ,	TOTAL =	9.5 SECONDS (0.2 MIN)
WALL CLOCK TIME:	STEP =	3.46 ,	TOTAL =	9.3 SECONDS (0.2 MIN)	
CPU UTILIZATION:	STEP =	100.29%,	TOTAL =	102.91%		

NSERCH= 0 ENERGY= -227.7159310

GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	-0.0297657	-0.0290787	0.0000000
2	C	6.0	-0.1098196	0.0548254	0.0000000
3	O	8.0	0.0554461	0.0198191	0.0000000
4	O	8.0	0.0609473	-0.0357743	0.0000000
5	H	1.0	0.0151241	0.0170958	0.0000000
6	H	1.0	0.0000117	-0.0087930	-0.0170995
7	H	1.0	0.0000117	-0.0087930	0.0170995
8	H	1.0	0.0080444	-0.0093013	0.0000000

MAXIMUM GRADIENT = 0.1098196 RMS GRADIENT = 0.0333359
FORCE CONSTANT MATRIX NOT UPDATED --- TAKING FIRST STEP
MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
NR STEP HAS LENGTH = 0.489843
TRIM/QA LAMBDA FOR NON-TS MODES = -0.21097656

TRIM/QA STEP HAS LENGTH = 0.300000
 RADIUS OF STEP TAKEN= 0.30000 CURRENT TRUST RADIUS= 0.30000
 INSERCH= 1

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.5264637983	0.3673013438	0.0000000000
C	6.0	0.0158443437	-0.0431837662	0.0000000000
O	8.0	0.2905662507	-1.1591197744	0.0000000000
O	8.0	1.0655542665	0.8276902108	0.0000000000
H	1.0	-1.6291896673	1.4229518379	0.0000000000
H	1.0	-1.9632057545	-0.1044602893	0.9020898724
H	1.0	1.8171200452	0.1444335692	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.5264637983	0.3673013438	0.0000000000
C	6.0	0.0158443437	-0.0431837662	0.0000000000
O	8.0	0.2905662507	-1.1591197744	0.0000000000
O	8.0	1.0655542665	0.8276902108	0.0000000000
H	1.0	-1.6291896673	1.4229518379	0.0000000000
H	1.0	-1.9632057545	-0.1044602893	-0.9020898724
H	1.0	-1.9632057545	-0.1044602893	0.9020898724
H	1.0	1.8171200452	0.1444335692	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.5959989 *	2.3730907 *	2.6325872 *
2 C	1.5959989 *	0.0000000	1.1492542 *	1.3639327 *
3 O	2.3730907 *	1.1492542 *	0.0000000	2.1326088 *
4 O	2.6325872 *	1.3639327 *	2.1326088 *	0.0000000
5 H	1.0606369 *	2.2035631 *	3.2175389	2.7597067 *
6 H	1.1077313 *	2.1758125 *	2.6468020 *	3.2948533
7 H	1.1077313 *	2.1758125 *	2.6468020 *	3.2948533
8 H	3.3510033	1.8110203 *	2.0073908 *	1.0157218 *

	H	H	H	H
1 C	1.0606369 *	1.1077313 *	1.1077313 *	3.3510033
2 C	2.2035631 *	2.1758125 *	2.1758125 *	1.8110203 *
3 O	3.2175389	2.6468020 *	2.6468020 *	2.0073908 *
4 O	2.7597067 *	3.2948533	3.2948533	1.0157218 *
5 H	0.0000000	1.8050819 *	1.8050819 *	3.6758209
6 H	1.8050819 *	0.0000000	1.8041797 *	3.8944290
7 H	1.8050819 *	1.8041797 *	0.0000000	3.8944290
8 H	3.6758209	3.8944290	3.8944290	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 9.6 SECONDS (0.2 MIN)
 WALL CLOCK TIME: STEP = 0.04 , TOTAL = 9.3 SECONDS (0.2 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 102.90%
 TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 998423
 200 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.
 END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.23 , TOTAL = 11.8 SECONDS (0.2 MIN)
 WALL CLOCK TIME: STEP = 2.23 , TOTAL = 11.5 SECONDS (0.2 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 102.34%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.701102008	-227.701102008	0.085560283	0.037069295
2	1	0	-227.726599421	-0.025497412	0.029550257	0.009958182
3	2	0	-227.728325913	-0.001726492	0.007764753	0.006684944
4	3	0	-227.728850581	-0.000524669	0.003664380	0.001324582
5	4	0	-227.728880693	-0.000030112	0.000827365	0.000290773
6	5	0	-227.728883391	-0.000002698	0.000309389	0.000060047
7	6	0	-227.728883557	-0.000000166	0.000074767	0.000047616
8	7	0	-227.728883585	-0.000000027	0.000018319	0.000006910

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.8 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.2 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7288835845 AFTER 8 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 1.95 , TOTAL = 13.8 SECONDS (0.2 MIN)
WALL CLOCK TIME: STEP = 1.96 , TOTAL = 13.5 SECONDS (0.2 MIN)
CPU UTILIZATION: STEP = 99.49%, TOTAL = 101.92%
..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.24 , TOTAL = 14.0 SECONDS (0.2 MIN)
WALL CLOCK TIME: STEP = 0.23 , TOTAL = 13.7 SECONDS (0.2 MIN)
CPU UTILIZATION: STEP = 104.35%, TOTAL = 101.97%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.48 , TOTAL = 17.5 SECONDS (0.3 MIN)
WALL CLOCK TIME: STEP = 3.48 , TOTAL = 17.2 SECONDS (0.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 101.57%

NSERCH= 1 ENERGY= -227.7288836

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 C	6.0	-0.0455009	0.0215421	0.0000000
2 C	6.0	0.0723626	-0.1032863	0.0000000
3 O	8.0	-0.0226748	0.1321601	0.0000000
4 O	8.0	-0.0187828	0.0334018	0.0000000
5 H	1.0	0.0071092	-0.0101458	0.0000000
6 H	1.0	-0.0063660	-0.0109953	-0.0161751
7 H	1.0	-0.0063660	-0.0109953	0.0161751
8 H	1.0	0.0202187	-0.0516813	0.0000000

MAXIMUM GRADIENT = 0.1321601 RMS GRADIENT = 0.0418166
HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0129525622
PREDICTED ENERGY CHANGE WAS -0.0339907567 RATIO= 0.381
MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
NR STEP HAS LENGTH = 0.441121
TRIM/QA LAMBDA FOR NON-TS MODES = -0.09897543
TRIM/QA STEP HAS LENGTH = 0.300000
RADIUS OF STEP TAKEN= 0.30000 CURRENT TRUST RADIUS= 0.30000

1NSERCH= 2

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4695649336	0.3716341074	0.0000000000

C	6.0	0.0391956575	-0.0026849200	0.0000000000
O	8.0	0.2680123343	-1.2761121465	0.0000000000
O	8.0	1.0359947550	0.8276605077	0.0000000000
H	1.0	-1.6456667188	1.4184466097	0.0000000000
H	1.0	-1.9582697363	-0.0895505523	0.8771389047
H	1.0	1.7955883094	0.1913097888	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4695649336	0.3716341074	0.0000000000
C	6.0	0.0391956575	-0.0026849200	0.0000000000
O	8.0	0.2680123343	-1.2761121465	0.0000000000
O	8.0	1.0359947550	0.8276605077	0.0000000000
H	1.0	-1.6456667188	1.4184466097	0.0000000000
H	1.0	-1.9582697363	-0.0895505523	-0.8771389047
H	1.0	-1.9582697363	-0.0895505523	0.8771389047
H	1.0	1.7955883094	0.1913097888	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.5545010 *	2.3946278 *	2.5467213 *
2 C	1.5545010 *	0.0000000	1.2938215 *	1.2973365 *
3 O	2.3946278 *	1.2938215 *	0.0000000	2.2395661 *
4 O	2.5467213 *	1.2973365 *	2.2395661 *	0.0000000
5 H	1.0615217 *	2.2041724 *	3.3049681	2.7459673 *
6 H	1.1049418 *	2.1832971 *	2.6708862 *	3.2521176
7 H	1.1049418 *	2.1832971 *	2.6708862 *	3.2521176
8 H	3.2701288	1.7670736 *	2.1182104 *	0.9909211 *

	H	H	H	H
1 C	1.0615217 *	1.1049418 *	1.1049418 *	3.2701288
2 C	2.2041724 *	2.1832971 *	2.1832971 *	1.7670736 *
3 O	3.3049681	2.6708862 *	2.6708862 *	2.1182104 *
4 O	2.7459673 *	3.2521176	3.2521176	0.9909211 *
5 H	0.0000000	1.7723286 *	1.7723286 *	3.6535053
6 H	1.7723286 *	0.0000000	1.7542778 *	3.8651915
7 H	1.7723286 *	1.7542778 *	0.0000000	3.8651915
8 H	3.6535053	3.8651915	3.8651915	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU	TIME:	STEP =	0.04	,	TOTAL =	17.5 SECONDS (0.3 MIN)
WALL CLOCK TIME:	STEP =	0.04	,	TOTAL =	17.3 SECONDS (0.3 MIN)	
CPU UTILIZATION:	STEP =	100.00%		TOTAL =	101.56%		

TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 996463

200 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU	TIME:	STEP =	2.21	,	TOTAL =	19.7 SECONDS (0.3 MIN)
WALL CLOCK TIME:	STEP =	2.55	,	TOTAL =	19.8 SECONDS (0.3 MIN)	
CPU UTILIZATION:	STEP =	86.67%		TOTAL =	99.65%		

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.704390343	-227.704390343	0.040451009	0.040769034
2	1	0	-227.729144111	-0.024753768	0.029254543	0.017013815
3	2	0	-227.732450397	-0.003306286	0.009393294	0.006188703
4	3	0	-227.733058768	-0.000608371	0.004439709	0.001682648
5	4	0	-227.733160235	-0.000101467	0.002126763	0.001397481
6	5	0	-227.733190260	-0.000030025	0.000998364	0.000434130

7	6	0	-227.733194466	-0.000004207	0.000355972	0.000170246
8	7	0	-227.733195100	-0.000000634	0.000169830	0.000055385
9	8	0	-227.733195185	-0.000000084	0.000056019	0.000017131
10	9	0	-227.733195196	-0.000000011	0.000014522	0.000004015

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 2.2 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.2 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7331951961 AFTER 10 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 2.42 , TOTAL = 22.2 SECONDS (0.4 MIN)
WALL CLOCK TIME: STEP = 2.42 , TOTAL = 22.2 SECONDS (0.4 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 99.69%
..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.23 , TOTAL = 22.4 SECONDS (0.4 MIN)
WALL CLOCK TIME: STEP = 0.24 , TOTAL = 22.5 SECONDS (0.4 MIN)
CPU UTILIZATION: STEP = 95.83%, TOTAL = 99.64%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.47 , TOTAL = 25.9 SECONDS (0.4 MIN)
WALL CLOCK TIME: STEP = 3.46 , TOTAL = 25.9 SECONDS (0.4 MIN)
CPU UTILIZATION: STEP = 100.29%, TOTAL = 99.73%

NSERCH= 2 ENERGY= -227.7331952

GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	-0.0180767	0.0112652	0.0000000
2	C	6.0	0.0747412	0.1250691	0.0000000
3	O	8.0	0.0019989	-0.0893424	0.0000000
4	O	8.0	-0.0370305	0.0179538	0.0000000
5	H	1.0	0.0007733	-0.0119219	0.0000000
6	H	1.0	-0.0135879	-0.0075809	-0.0108154
7	H	1.0	-0.0135879	-0.0075809	0.0108154
8	H	1.0	0.0047696	-0.0378621	0.0000000

MAXIMUM GRADIENT = 0.1250691 RMS GRADIENT = 0.0374605
HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0043116116
PREDICTED ENERGY CHANGE WAS -0.0266697164 RATIO= 0.162
MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
NR STEP HAS LENGTH = 0.305538
TRIM/QA LAMBDA FOR NON-TS MODES = -0.00569354
TRIM/QA STEP HAS LENGTH = 0.300000
RADIUS OF STEP TAKEN= 0.30000 CURRENT TRUST RADIUS= 0.30000

1NSERCH= 3

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

	ATOM	CHARGE	X	Y	Z
C		6.0	-1.4171935478	0.3558584268	0.0000000000
C		6.0	-0.0466269087	-0.0761775221	0.0000000000
O		8.0	0.2646350972	-1.2741605289	0.0000000000
O		8.0	1.0667231136	0.7997669603	0.0000000000
H		1.0	-1.6544462114	1.4316016009	0.0000000000
H		1.0	-1.9414582791	-0.0731483744	0.8525795687
H		1.0	1.7768449466	0.2605606543	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4171935478	0.3558584268	0.0000000000
C	6.0	-0.0466269087	-0.0761775221	0.0000000000
O	8.0	0.2646350972	-1.2741605289	0.0000000000
O	8.0	1.0667231136	0.7997669603	0.0000000000
H	1.0	-1.6544462114	1.4316016009	0.0000000000
H	1.0	-1.9414582791	-0.0731483744	-0.8525795687
H	1.0	-1.9414582791	-0.0731483744	0.8525795687
H	1.0	1.7768449466	0.2605606543	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.4370484 *	2.3421164 *	2.5232710 *
2 C	1.4370484 *	0.0000000	1.2377590 *	1.4166252 *
3 O	2.3421164 *	1.2377590 *	0.0000000	2.2236278 *
4 O	2.5232710 *	1.4166252 *	2.2236278 *	0.0000000
5 H	1.1015953 *	2.2041962 *	3.3172310	2.7935600 *
6 H	1.0889409 *	2.0778082 *	2.6525780 *	3.2462330
7 H	1.0889409 *	2.0778082 *	2.6525780 *	3.2462330
8 H	3.1954598	1.8543037 *	2.1545644 *	0.8916370 *
	H	H	H	H
1 C	1.1015953 *	1.0889409 *	1.0889409 *	3.1954598
2 C	2.2041962 *	2.0778082 *	2.0778082 *	1.8543037 *
3 O	3.3172310	2.6525780 *	2.6525780 *	2.1545644 *
4 O	2.7935600 *	3.2462330	3.2462330	0.8916370 *
5 H	0.0000000	1.7531515 *	1.7531515 *	3.6256166
6 H	1.7531515 *	0.0000000	1.7051591 *	3.8293645
7 H	1.7531515 *	1.7051591 *	0.0000000	3.8293645
8 H	3.6256166	3.8293645	3.8293645	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 25.9 SECONDS (0.4 MIN)
 WALL CLOCK TIME: STEP = 0.04 , TOTAL = 26.0 SECONDS (0.4 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 99.73%
 TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1000639
 201 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.
 END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.22 , TOTAL = 28.1 SECONDS (0.5 MIN)
 WALL CLOCK TIME: STEP = 2.23 , TOTAL = 28.2 SECONDS (0.5 MIN)
 CPU UTILIZATION: STEP = 99.55%, TOTAL = 99.72%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.715832255	-227.715832255	0.044621561	0.038077304
2	1	0	-227.738734420	-0.022902165	0.027739442	0.006833156
3	2	0	-227.740289081	-0.001554661	0.006116526	0.004533066
4	3	0	-227.740446636	-0.000157554	0.001743660	0.002493713
5	4	0	-227.740493940	-0.000047305	0.000775485	0.000559634
6	5	0	-227.740499295	-0.000005355	0.000379620	0.000170237
7	6	0	-227.740500502	-0.000001207	0.000215259	0.000068742
8	7	0	-227.740500610	-0.000000107	0.000069040	0.000023170
9	8	0	-227.740500622	-0.000000013	0.000012204	0.000007050

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 2.0 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.2 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7405006223 AFTER 9 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 2.19 , TOTAL = 30.3 SECONDS (0.5 MIN)
WALL CLOCK TIME: STEP = 2.20 , TOTAL = 30.4 SECONDS (0.5 MIN)
CPU UTILIZATION: STEP = 99.55%, TOTAL = 99.70%
..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.24 , TOTAL = 30.5 SECONDS (0.5 MIN)
WALL CLOCK TIME: STEP = 0.23 , TOTAL = 30.6 SECONDS (0.5 MIN)
CPU UTILIZATION: STEP = 104.35%, TOTAL = 99.74%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.48 , TOTAL = 34.0 SECONDS (0.6 MIN)
WALL CLOCK TIME: STEP = 3.48 , TOTAL = 34.1 SECONDS (0.6 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 99.77%

NSERCH= 3 ENERGY= -227.7405006

GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	0.0529595	-0.0306905	0.0000000
2	C	6.0	-0.0834614	0.0396985	0.0000000
3	O	8.0	0.0173384	-0.0322771	0.0000000
4	O	8.0	0.1179799	-0.0287404	0.0000000
5	H	1.0	-0.0166825	0.0140168	0.0000000
6	H	1.0	-0.0080470	-0.0012412	-0.0005929
7	H	1.0	-0.0080470	-0.0012412	0.0005929
8	H	1.0	-0.0720401	0.0404752	0.0000000

MAXIMUM GRADIENT = 0.1179799 RMS GRADIENT = 0.0386287

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0073054262

PREDICTED ENERGY CHANGE WAS -0.0216688295 RATIO= 0.337

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.210415

RADIUS OF STEP TAKEN= 0.21041 CURRENT TRUST RADIUS= 0.30000

1NSERCH= 4

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4537781700	0.3646139785	0.0000000000
C	6.0	-0.0505846401	-0.1003357573	0.0000000000
O	8.0	0.2724004667	-1.2560047872	0.0000000000
O	8.0	0.9932487587	0.7986206797	0.0000000000
H	1.0	-1.6372182946	1.4308827627	0.0000000000
H	1.0	-1.9274089784	-0.0684684265	0.8480398092
H	1.0	1.8377697673	0.2503128191	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4537781700	0.3646139785	0.0000000000
C	6.0	-0.0505846401	-0.1003357573	0.0000000000
O	8.0	0.2724004667	-1.2560047872	0.0000000000
O	8.0	0.9932487587	0.7986206797	0.0000000000
H	1.0	-1.6372182946	1.4308827627	0.0000000000
H	1.0	-1.9274089784	-0.0684684265	-0.8480398092

H	1.0	-1.9274089784	-0.0684684265	0.8480398092
H	1.0	1.8377697673	0.2503128191	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.4782186 *	2.3677200 *	2.4852168 *
2 C	1.4782186 *	0.0000000	1.1999543 *	1.3775743 *
3 O	2.3677200 *	1.1999543 *	0.0000000	2.1774086 *
4 O	2.4852168 *	1.3775743 *	2.1774086 *	0.0000000
5 H	1.0819332 *	2.2050026 *	3.2963629	2.7053858 *
6 H	1.0635121 *	2.0597710 *	2.6398060 *	3.1624763
7 H	1.0635121 *	2.0597710 *	2.6398060 *	3.1624763
8 H	3.2935319	1.9206345 *	2.1724120 *	1.0069048 *

	H	H	H	H
1 C	1.0819332 *	1.0635121 *	1.0635121 *	3.2935319
2 C	2.2050026 *	2.0597710 *	2.0597710 *	1.9206345 *
3 O	3.2963629	2.6398060 *	2.6398060 *	2.1724120 *
4 O	2.7053858 *	3.1624763	3.1624763	1.0069048 *
5 H	0.0000000	1.7468360 *	1.7468360 *	3.6700528
6 H	1.7468360 *	0.0000000	1.6960796 *	3.8726430
7 H	1.7468360 *	1.6960796 *	0.0000000	3.8726430
8 H	3.6700528	3.8726430	3.8726430	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 34.1 SECONDS (0.6 MIN)
WALL CLOCK TIME: STEP = 0.04 , TOTAL = 34.1 SECONDS (0.6 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 99.77%
TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1004759
202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.
..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.24 , TOTAL = 36.3 SECONDS (0.6 MIN)
WALL CLOCK TIME: STEP = 2.25 , TOTAL = 36.4 SECONDS (0.6 MIN)
CPU UTILIZATION: STEP = 99.56%, TOTAL = 99.75%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.740149253	-227.740149253	0.033661595	0.028851885
2	1	0	-227.749603856	-0.009454602	0.012162827	0.005445103
3	2	0	-227.750390547	-0.000786691	0.004333337	0.003996063
4	3	0	-227.750620897	-0.000230350	0.001507378	0.000787403
5	4	0	-227.750629455	-0.000008559	0.000594826	0.000330404
6	5	0	-227.750631997	-0.000002541	0.000136323	0.000049242
7	6	0	-227.750632095	-0.000000099	0.000061760	0.000019130
8	7	0	-227.750632108	-0.000000013	0.000018133	0.000005960

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS=	1.8 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS=	0.1 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7506321079 AFTER 8 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 1.97 , TOTAL = 38.3 SECONDS (0.6 MIN)
WALL CLOCK TIME: STEP = 1.96 , TOTAL = 38.4 SECONDS (0.6 MIN)
CPU UTILIZATION: STEP = 100.51%, TOTAL = 99.79%

..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.24 , TOTAL = 38.5 SECONDS (0.6 MIN)
WALL CLOCK TIME: STEP = 0.24 , TOTAL = 38.6 SECONDS (0.6 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 99.79%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.53 , TOTAL = 42.0 SECONDS (0.7 MIN)
WALL CLOCK TIME: STEP = 3.56 , TOTAL = 42.2 SECONDS (0.7 MIN)
CPU UTILIZATION: STEP = 99.16%, TOTAL = 99.74%

NSERCH= 4 ENERGY= -227.7506321

GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	-0.0004963	-0.0130202	0.0000000
2	C	6.0	-0.0336745	-0.0184678	0.0000000
3	O	8.0	0.0091411	0.0284015	0.0000000
4	O	8.0	-0.0142975	0.0254021	0.0000000
5	H	1.0	-0.0104329	0.0038003	0.0000000
6	H	1.0	0.0058249	0.0032539	0.0114604
7	H	1.0	0.0058249	0.0032539	-0.0114604
8	H	1.0	0.0381103	-0.0326237	0.0000000

MAXIMUM GRADIENT = 0.0381103 RMS GRADIENT = 0.0162998

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0101314856

PREDICTED ENERGY CHANGE WAS -0.0163142656 RATIO= 0.621

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.162218

RADIUS OF STEP TAKEN= 0.16222 CURRENT TRUST RADIUS= 0.21041

1NSERCH= 5

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

	ATOM	CHARGE	X	Y	Z
	C	6.0	-1.4629906171	0.3860282434	0.0000000000
	C	6.0	-0.0003392760	-0.1001466162	0.0000000000
	O	8.0	0.2575177675	-1.2743027472	0.0000000000
	O	8.0	0.9887378272	0.7709329166	0.0000000000
	H	1.0	-1.6204347118	1.4246522863	0.0000000000
	H	1.0	-1.9310286404	-0.0711989263	0.8607316819
	H	1.0	1.8065862224	0.2863866121	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

	ATOM	CHARGE	X	Y	Z
	C	6.0	-1.4629906171	0.3860282434	0.0000000000
	C	6.0	-0.0003392760	-0.1001466162	0.0000000000
	O	8.0	0.2575177675	-1.2743027472	0.0000000000
	O	8.0	0.9887378272	0.7709329166	0.0000000000
	H	1.0	-1.6204347118	1.4246522863	0.0000000000
	H	1.0	-1.9310286404	-0.0711989263	-0.8607316819
	H	1.0	-1.9310286404	-0.0711989263	0.8607316819
	H	1.0	1.8065862224	0.2863866121	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

		C	C	O	O
1	C	0.0000000	1.5413354 *	2.3909931 *	2.4817582 *
2	C	1.5413354 *	0.0000000	1.2021368 *	1.3179731 *

3	O	2.3909931 *	1.2021368 *	0.0000000	2.1720202 *
4	O	2.4817582 *	1.3179731 *	2.1720202 *	0.0000000
5	H	1.0504897 *	2.2247968 *	3.2880182	2.6898198 *
6	H	1.0811916 *	2.1140621 *	2.6416005 *	3.1583352
7	H	1.0811916 *	2.1140621 *	2.6416005 *	3.1583352
8	H	3.2710948	1.8478062 *	2.1989462 *	0.9506109 *

	H		H		H		H
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1	C	1.0504897 *	1.0811916 *	1.0811916 *	3.2710948
2	C	2.2247968 *	2.1140621 *	2.1140621 *	1.8478062 *
3	O	3.2880182	2.6416005 *	2.6416005 *	2.1989462 *
4	O	2.6898198 *	3.1583352	3.1583352	0.9506109 *
5	H	0.0000000	1.7535388 *	1.7535388 *	3.6111108
6	H	1.7535388 *	0.0000000	1.7214634 *	3.8520762
7	H	1.7535388 *	1.7214634 *	0.0000000	3.8520762
8	H	3.6111108	3.8520762	3.8520762	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.05 , TOTAL = 42.1 SECONDS (0.7 MIN)
 WALL CLOCK TIME: STEP = 0.04 , TOTAL = 42.2 SECONDS (0.7 MIN)
 CPU UTILIZATION: STEP = 125.00%, TOTAL = 99.76%
 TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1004019

201 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.37 , TOTAL = 44.5 SECONDS (0.7 MIN)
 WALL CLOCK TIME: STEP = 2.53 , TOTAL = 44.7 SECONDS (0.7 MIN)
 CPU UTILIZATION: STEP = 93.68%, TOTAL = 99.42%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.746605969	-227.746605969	0.029089602	0.016168128
2	1	0	-227.752686334	-0.006080365	0.014789587	0.005739380
3	2	0	-227.753294285	-0.000607951	0.003489855	0.002698001
4	3	0	-227.753421728	-0.000127443	0.000774479	0.000634928
5	4	0	-227.753426812	-0.000005084	0.000563801	0.000321019
6	5	0	-227.753428423	-0.000001611	0.000120728	0.000089287
7	6	0	-227.753428556	-0.000000133	0.000072290	0.000024658
8	7	0	-227.753428576	-0.000000020	0.000027887	0.000008796
9	8	0	-227.753428578	-0.000000003	0.000007812	0.000002429

 DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 2.1 SECONDS (0.2 SEC/ITER)
 TIME TO SOLVE SCF EQUATIONS= 0.2 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7534285783 AFTER 9 ITERATIONS
 END OF RHF CALCULATION

CPU TIME: STEP = 2.35 , TOTAL = 46.8 SECONDS (0.8 MIN)
 WALL CLOCK TIME: STEP = 2.43 , TOTAL = 47.2 SECONDS (0.8 MIN)
 CPU UTILIZATION: STEP = 96.71%, TOTAL = 99.28%
 END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.26 , TOTAL = 47.1 SECONDS (0.8 MIN)
 WALL CLOCK TIME: STEP = 0.37 , TOTAL = 47.5 SECONDS (0.8 MIN)
 CPU UTILIZATION: STEP = 70.27%, TOTAL = 99.05%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.57 , TOTAL = 50.6 SECONDS (0.8 MIN)

WALL CLOCK TIME: STEP = 6.34 , TOTAL = 53.9 SECONDS (0.9 MIN)
 CPU UTILIZATION: STEP = 56.31%, TOTAL = 94.02%

NSERCH= 5 ENERGY= -227.7534286

 GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	-0.0257986	0.0311222	0.0000000
2	C	6.0	0.0477094	-0.0020935	0.0000000
3	O	8.0	-0.0011081	0.0240590	0.0000000
4	O	8.0	-0.0086812	-0.0193616	0.0000000
5	H	1.0	-0.0042494	-0.0190517	0.0000000
6	H	1.0	-0.0002138	-0.0034707	0.0012385
7	H	1.0	-0.0002138	-0.0034707	-0.0012385
8	H	1.0	-0.0074444	-0.0077330	0.0000000

MAXIMUM GRADIENT = 0.0477094 RMS GRADIENT = 0.0150949

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0027964704

PREDICTED ENERGY CHANGE WAS -0.0058384914 RATIO= 0.479

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.110630

RADIUS OF STEP TAKEN= 0.11063 CURRENT TRUST RADIUS= 0.16222

1NSERCH= 6

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4369530703	0.3662422509	0.0000000000
C	6.0	-0.0152468278	-0.1134861787	0.0000000000
O	8.0	0.2446489760	-1.3015499079	0.0000000000
O	8.0	0.9822580376	0.7893598692	0.0000000000
H	1.0	-1.6128610613	1.4392116485	0.0000000000
H	1.0	-1.9310631396	-0.0669059708	0.8627193306
H	1.0	1.8073001561	0.3051871022	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4369530703	0.3662422509	0.0000000000
C	6.0	-0.0152468278	-0.1134861787	0.0000000000
O	8.0	0.2446489760	-1.3015499079	0.0000000000
O	8.0	0.9822580376	0.7893598692	0.0000000000
H	1.0	-1.6128610613	1.4392116485	0.0000000000
H	1.0	-1.9310631396	-0.0669059708	-0.8627193306
H	1.0	-1.9310631396	-0.0669059708	0.8627193306
H	1.0	1.8073001561	0.3051871022	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.5004626 *	2.3683995 *	2.4559338 *
2 C	1.5004626 *	0.0000000	1.2161584 *	1.3454170 *
3 O	2.3683995 *	1.2161584 *	0.0000000	2.2171989 *
4 O	2.4559338 *	1.3454170 *	2.2171989 *	0.0000000
5 H	1.0872934 *	2.2278334 *	3.3109089	2.6752477 *
6 H	1.0844569 *	2.1016200 *	2.6461960 *	3.1567255
7 H	1.0844569 *	2.1016200 *	2.6461960 *	3.1567255
8 H	3.2448277	1.8700173 *	2.2413127 *	0.9566179 *
	H	H	H	H

1	C	1.0872934 *	1.0844569 *	1.0844569 *	3.2448277
2	C	2.2278334 *	2.1016200 *	2.1016200 *	1.8700173 *
3	O	3.3109089	2.6461960 *	2.6461960 *	2.2413127 *
4	O	2.6752477 *	3.1567255	3.1567255	0.9566179 *
5	H	0.0000000	1.7646324 *	1.7646324 *	3.6032644
6	H	1.7646324 *	0.0000000	1.7254387 *	3.8546203
7	H	1.7646324 *	1.7254387 *	0.0000000	3.8546203
8	H	3.6032644	3.8546203	3.8546203	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 50.7 SECONDS (0.8 MIN)
WALL CLOCK TIME: STEP = 0.10 , TOTAL = 54.0 SECONDS (0.9 MIN)
CPU UTILIZATION: STEP = 40.00%, TOTAL = 93.92%

TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1003781

201 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.21 , TOTAL = 52.9 SECONDS (0.9 MIN)
WALL CLOCK TIME: STEP = 4.45 , TOTAL = 58.4 SECONDS (1.0 MIN)
CPU UTILIZATION: STEP = 49.66%, TOTAL = 90.55%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.755044948	-227.755044948	0.012976425	0.011408440
2	1	0	-227.756544211	-0.001499263	0.005273260	0.001949306
3	2	0	-227.756665884	-0.000121673	0.001342459	0.000997932
4	3	0	-227.756680953	-0.000015069	0.000476256	0.000231118
5	4	0	-227.756681991	-0.000001038	0.000284911	0.000067568
6	5	0	-227.756682135	-0.000000144	0.000037115	0.000036246
7	6	0	-227.756682147	-0.000000012	0.000024128	0.000014463
8	7	0	-227.756682150	-0.000000003	0.000007024	0.000003009

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.8 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.1 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7566821502 AFTER 8 ITERATIONS

..... END OF RHF CALCULATION

CPU TIME: STEP = 1.97 , TOTAL = 54.9 SECONDS (0.9 MIN)
WALL CLOCK TIME: STEP = 3.87 , TOTAL = 62.3 SECONDS (1.0 MIN)
CPU UTILIZATION: STEP = 50.90%, TOTAL = 88.09%

..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.24 , TOTAL = 55.1 SECONDS (0.9 MIN)
WALL CLOCK TIME: STEP = 0.49 , TOTAL = 62.8 SECONDS (1.0 MIN)
CPU UTILIZATION: STEP = 48.98%, TOTAL = 87.78%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.51 , TOTAL = 58.6 SECONDS (1.0 MIN)
WALL CLOCK TIME: STEP = 7.04 , TOTAL = 69.8 SECONDS (1.2 MIN)
CPU UTILIZATION: STEP = 49.86%, TOTAL = 83.96%

NSERCH= 6 ENERGY= -227.7566822

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ

1	C	6.0	0.0044292	-0.0034677	0.0000000
2	C	6.0	0.0126258	0.0092503	0.0000000
3	O	8.0	-0.0013895	-0.0047981	0.0000000
4	O	8.0	0.0021820	0.0069284	0.0000000
5	H	1.0	-0.0109952	0.0070868	0.0000000
6	H	1.0	-0.0025402	-0.0021080	-0.0006719
7	H	1.0	-0.0025402	-0.0021080	0.0006719
8	H	1.0	-0.0017720	-0.0107838	0.0000000

MAXIMUM GRADIENT = 0.0126258 RMS GRADIENT = 0.0052741

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0032535719

PREDICTED ENERGY CHANGE WAS -0.0032197087 RATIO= 1.011

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.099243

RADIUS OF STEP TAKEN= 0.09924 CURRENT TRUST RADIUS= 0.22126

1NSERCH= 7

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4352045508	0.3677938680	0.0000000000
C	6.0	-0.0357781487	-0.1312216332	0.0000000000
O	8.0	0.2406323735	-1.3126558729	0.0000000000
O	8.0	0.9660968702	0.7823175608	0.0000000000
H	1.0	-1.5907542121	1.4318645391	0.0000000000
H	1.0	-1.9254198268	-0.0605687622	0.8608159079
H	1.0	1.8128672528	0.3341919050	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4352045508	0.3677938680	0.0000000000
C	6.0	-0.0357781487	-0.1312216332	0.0000000000
O	8.0	0.2406323735	-1.3126558729	0.0000000000
O	8.0	0.9660968702	0.7823175608	0.0000000000
H	1.0	-1.5907542121	1.4318645391	0.0000000000
H	1.0	-1.9254198268	-0.0605687622	-0.8608159079
H	1.0	-1.9254198268	-0.0605687622	0.8608159079
H	1.0	1.8128672528	0.3341919050	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.4857358 *	2.3732553 *	2.4368173 *
2 C	1.4857358 *	0.0000000	1.2133382 *	1.3558420 *
3 O	2.3732553 *	1.2133382 *	0.0000000	2.2170278 *
4 O	2.4368173 *	1.3558420 *	2.2170278 *	0.0000000
5 H	1.0753800 *	2.2048104 *	3.2994498	2.6380672 *
6 H	1.0792634 *	2.0776770 *	2.6458474 *	3.1324639
7 H	1.0792634 *	2.0776770 *	2.6458474 *	3.1324639
8 H	3.2482456	1.9063314 *	2.2768465 *	0.9580379 *

	H	H	H	H
1 C	1.0753800 *	1.0792634 *	1.0792634 *	3.2482456
2 C	2.2048104 *	2.0776770 *	2.0776770 *	1.9063314 *
3 O	3.2994498	2.6458474 *	2.6458474 *	2.2768465 *
4 O	2.6380672 *	3.1324639	3.1324639	0.9580379 *
5 H	0.0000000	1.7550961 *	1.7550961 *	3.5762444
6 H	1.7550961 *	0.0000000	1.7216318 *	3.8563753
7 H	1.7550961 *	1.7216318 *	0.0000000	3.8563753
8 H	3.5762444	3.8563753	3.8563753	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 58.7 SECONDS (1.0 MIN)
WALL CLOCK TIME: STEP = 0.04 , TOTAL = 69.9 SECONDS (1.2 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 83.97%
TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1005005
202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.
..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.22 , TOTAL = 60.9 SECONDS (1.0 MIN)
WALL CLOCK TIME: STEP = 4.44 , TOTAL = 74.3 SECONDS (1.2 MIN)
CPU UTILIZATION: STEP = 50.00%, TOTAL = 81.94%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.757505256	-227.757505256	0.006983211	0.005854873
2	1	0	-227.758009293	-0.000504037	0.003484463	0.001187350
3	2	0	-227.758054319	-0.000045026	0.000984792	0.000512300
4	3	0	-227.758059410	-0.000005090	0.000253988	0.000192744
5	4	0	-227.758059815	-0.000000405	0.000089824	0.000062883
6	5	0	-227.758059893	-0.000000078	0.000033798	0.000020680
7	6	0	-227.758059900	-0.000000008	0.000021178	0.000007873
8	7	0	-227.758059902	-0.000000002	0.000006006	0.000003191

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.8 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.2 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7580599020 AFTER 8 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 2.04 , TOTAL = 62.9 SECONDS (1.0 MIN)
WALL CLOCK TIME: STEP = 2.34 , TOTAL = 76.6 SECONDS (1.3 MIN)
CPU UTILIZATION: STEP = 87.18%, TOTAL = 82.10%
..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.21 , TOTAL = 63.1 SECONDS (1.1 MIN)
WALL CLOCK TIME: STEP = 0.24 , TOTAL = 76.9 SECONDS (1.3 MIN)
CPU UTILIZATION: STEP = 87.50%, TOTAL = 82.11%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.53 , TOTAL = 66.7 SECONDS (1.1 MIN)
WALL CLOCK TIME: STEP = 3.61 , TOTAL = 80.5 SECONDS (1.3 MIN)
CPU UTILIZATION: STEP = 97.78%, TOTAL = 82.82%

NSERCH= 7 ENERGY= -227.7580599

GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	0.0062202	0.0034649	0.0000000
2	C	6.0	-0.0103028	0.0021348	0.0000000
3	O	8.0	0.0026138	-0.0011069	0.0000000
4	O	8.0	0.0050202	0.0058230	0.0000000
5	H	1.0	-0.0096729	-0.0003798	0.0000000
6	H	1.0	0.0010125	-0.0011542	0.0017470
7	H	1.0	0.0010125	-0.0011542	-0.0017470
8	H	1.0	0.0040964	-0.0076275	0.0000000

MAXIMUM GRADIENT = 0.0103028 RMS GRADIENT = 0.0041234

HESSIAN UPDATED USING THE BFGS FORMULA
 ACTUAL ENERGY CHANGE WAS -0.0013777519
 PREDICTED ENERGY CHANGE WAS -0.0010599781 RATIO= 1.300
 MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
 NR STEP HAS LENGTH = 0.174925
 TRIM/QA LAMBDA FOR NON-TS MODES = -0.01568856
 TRIM/QA STEP HAS LENGTH = 0.140350
 RADIUS OF STEP TAKEN= 0.14035 CURRENT TRUST RADIUS= 0.14035

1NSERCH= 8

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4377053440	0.3539975817	0.0000000000
C	6.0	-0.0419109845	-0.1524464938	0.0000000000
O	8.0	0.2302473923	-1.3291403855	0.0000000000
O	8.0	0.9410629097	0.7700185679	0.0000000000
H	1.0	-1.5519946754	1.4333975379	0.0000000000
H	1.0	-1.9221468964	-0.0516680092	0.8630644394
H	1.0	1.8116144257	0.3786620527	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4377053440	0.3539975817	0.0000000000
C	6.0	-0.0419109845	-0.1524464938	0.0000000000
O	8.0	0.2302473923	-1.3291403855	0.0000000000
O	8.0	0.9410629097	0.7700185679	0.0000000000
H	1.0	-1.5519946754	1.4333975379	0.0000000000
H	1.0	-1.9221468964	-0.0516680092	-0.8630644394
H	1.0	-1.9221468964	-0.0516680092	0.8630644394
H	1.0	1.8116144257	0.3786620527	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.4848325 *	2.3696033 *	2.4148731 *
2 C	1.4848325 *	0.0000000	1.2077577 *	1.3480280 *
3 O	2.3696033 *	1.2077577 *	0.0000000	2.2162416 *
4 O	2.4148731 *	1.3480280 *	2.2162416 *	0.0000000
5 H	1.0854337 *	2.1898069 *	3.2875527	2.5798077 *
6 H	1.0696394 *	2.0713096 *	2.6475681 *	3.1012932
7 H	1.0696394 *	2.0713096 *	2.6475681 *	3.1012932
8 H	3.2494134	1.9281164 *	2.3275117 *	0.9544736 *

	H	H	H	H
1 C	1.0854337 *	1.0696394 *	1.0696394 *	3.2494134
2 C	2.1898069 *	2.0713096 *	2.0713096 *	1.9281164 *
3 O	3.2875527	2.6475681 *	2.6475681 *	2.3275117 *
4 O	2.5798077 *	3.1012932	3.1012932	0.9544736 *
5 H	0.0000000	1.7570750 *	1.7570750 *	3.5251004
6 H	1.7570750 *	0.0000000	1.7261289 *	3.8562985
7 H	1.7570750 *	1.7261289 *	0.0000000	3.8562985
8 H	3.5251004	3.8562985	3.8562985	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 66.7 SECONDS (1.1 MIN)
 WALL CLOCK TIME: STEP = 0.04 , TOTAL = 80.5 SECONDS (1.3 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 82.83%
 TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1006657
 202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.28 , TOTAL = 69.0 SECONDS (1.1 MIN)
WALL CLOCK TIME: STEP = 2.67 , TOTAL = 83.2 SECONDS (1.4 MIN)
CPU UTILIZATION: STEP = 85.39% , TOTAL = 82.91%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.758467340	-227.758467340	0.007617791	0.007715837
2	1	0	-227.759153546	-0.000686206	0.003417411	0.001346250
3	2	0	-227.759212461	-0.000058914	0.000680118	0.000319995
4	3	0	-227.759214868	-0.000002407	0.000230315	0.000158497
5	4	0	-227.759215329	-0.000000461	0.000083128	0.000053799
6	5	0	-227.759215370	-0.000000041	0.000037039	0.000019754
7	6	0	-227.759215376	-0.000000006	0.000008906	0.000007958
8	7	0	-227.759215377	-0.000000001	0.000003862	0.000001767

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.8 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.2 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7592153765 AFTER 8 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 1.98 , TOTAL = 71.0 SECONDS (1.2 MIN)
WALL CLOCK TIME: STEP = 2.01 , TOTAL = 85.2 SECONDS (1.4 MIN)
CPU UTILIZATION: STEP = 98.51% , TOTAL = 83.28%
..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.24 , TOTAL = 71.2 SECONDS (1.2 MIN)
WALL CLOCK TIME: STEP = 0.24 , TOTAL = 85.4 SECONDS (1.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 83.32%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.56 , TOTAL = 74.8 SECONDS (1.2 MIN)
WALL CLOCK TIME: STEP = 3.60 , TOTAL = 89.0 SECONDS (1.5 MIN)
CPU UTILIZATION: STEP = 98.89% , TOTAL = 83.95%

NSERCH= 8 ENERGY= -227.7592154

GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	-0.0020388	-0.0115199	0.0000000
2	C	6.0	-0.0060908	-0.0011329	0.0000000
3	O	8.0	-0.0008803	0.0072967	0.0000000
4	O	8.0	0.0015382	-0.0032219	0.0000000
5	H	1.0	-0.0076000	0.0069008	0.0000000
6	H	1.0	0.0054159	0.0019917	0.0056959
7	H	1.0	0.0054159	0.0019917	-0.0056959
8	H	1.0	0.0042399	-0.0023062	0.0000000

MAXIMUM GRADIENT = 0.0115199 RMS GRADIENT = 0.0045742

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0011554745

PREDICTED ENERGY CHANGE WAS -0.0010930292 RATIO= 1.057

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.224896

RADIUS OF STEP TAKEN= 0.22490 CURRENT TRUST RADIUS= 0.28070

1NSERCH= 9

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4301495765	0.3542634302	0.0000000000
C	6.0	-0.0494816281	-0.1871632492	0.0000000000
O	8.0	0.2168022830	-1.3667365976	0.0000000000
O	8.0	0.9047628868	0.7660976032	0.0000000000
H	1.0	-1.4837273911	1.4248742469	0.0000000000
H	1.0	-1.9279349465	-0.0429040442	0.8777347870
H	1.0	1.8046832502	0.4456254973	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4301495765	0.3542634302	0.0000000000
C	6.0	-0.0494816281	-0.1871632492	0.0000000000
O	8.0	0.2168022830	-1.3667365976	0.0000000000
O	8.0	0.9047628868	0.7660976032	0.0000000000
H	1.0	-1.4837273911	1.4248742469	0.0000000000
H	1.0	-1.9279349465	-0.0429040442	-0.8777347870
H	1.0	-1.9279349465	-0.0429040442	0.8777347870
H	1.0	1.8046832502	0.4456254973	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.4830330 *	2.3820771 *	2.3709542 *
2 C	1.4830330 *	0.0000000	1.2092561 *	1.3488102 *
3 O	2.3820771 *	1.2092561 *	0.0000000	2.2410425 *
4 O	2.3709542 *	1.3488102 *	2.2410425 *	0.0000000
5 H	1.0719506 *	2.1577131 *	3.2687753	2.4776748 *
6 H	1.0844126 *	2.0784167 *	2.6688666 *	3.0739354
7 H	1.0844126 *	2.0784167 *	2.6688666 *	3.0739354
8 H	3.2361227	1.9591705 *	2.4095689 *	0.9552796 *
	H	H	H	H
1 C	1.0719506 *	1.0844126 *	1.0844126 *	3.2361227
2 C	2.1577131 *	2.0784167 *	2.0784167 *	1.9591705 *
3 O	3.2687753	2.6688666 *	2.6688666 *	2.4095689 *
4 O	2.4776748 *	3.0739354	3.0739354	0.9552796 *
5 H	0.0000000	1.7669499 *	1.7669499 *	3.4311183
6 H	1.7669499 *	0.0000000	1.7554696 *	3.8654260
7 H	1.7669499 *	1.7554696 *	0.0000000	3.8654260
8 H	3.4311183	3.8654260	3.8654260	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 74.8 SECONDS (1.2 MIN)
WALL CLOCK TIME: STEP = 0.04 , TOTAL = 89.1 SECONDS (1.5 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 83.96%

TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1007695

202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.26 , TOTAL = 77.1 SECONDS (1.3 MIN)
WALL CLOCK TIME: STEP = 2.31 , TOTAL = 91.4 SECONDS (1.5 MIN)
CPU UTILIZATION: STEP = 97.84%, TOTAL = 84.31%

ITER EX DEM TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD

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

1	0	0	-227.758523923	-227.758523923	0.009650078	0.009797160
2	1	0	-227.759985724	-0.001461800	0.005351541	0.002136814

3	2	0	-227.760118358	-0.000132634	0.001287591	0.000832671
4	3	0	-227.760126436	-0.000008078	0.000468647	0.000485118
5	4	0	-227.760129064	-0.000002628	0.000194392	0.000055277
6	5	0	-227.760129123	-0.000000059	0.000039291	0.000014625
7	6	0	-227.760129131	-0.000000008	0.000009556	0.000004326
8	7	0	-227.760129132	-0.000000001	0.000003779	0.000001894

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.8 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.1 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7601291319 AFTER 8 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 1.99 , TOTAL = 79.0 SECONDS (1.3 MIN)
WALL CLOCK TIME: STEP = 2.04 , TOTAL = 93.4 SECONDS (1.6 MIN)
CPU UTILIZATION: STEP = 97.55%, TOTAL = 84.60%
..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.22 , TOTAL = 79.3 SECONDS (1.3 MIN)
WALL CLOCK TIME: STEP = 0.24 , TOTAL = 93.7 SECONDS (1.6 MIN)
CPU UTILIZATION: STEP = 91.67%, TOTAL = 84.62%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.56 , TOTAL = 82.8 SECONDS (1.4 MIN)
WALL CLOCK TIME: STEP = 3.60 , TOTAL = 97.3 SECONDS (1.6 MIN)
CPU UTILIZATION: STEP = 98.89%, TOTAL = 85.15%

NSERCH= 9 ENERGY= -227.7601291

GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	0.0057551	0.0084019	0.0000000
2	C	6.0	-0.0049358	-0.0022190	0.0000000
3	O	8.0	-0.0031875	-0.0003687	0.0000000
4	O	8.0	-0.0054826	-0.0004705	0.0000000
5	H	1.0	-0.0037061	-0.0013524	0.0000000
6	H	1.0	0.0021133	-0.0024824	-0.0034898
7	H	1.0	0.0021133	-0.0024824	0.0034898
8	H	1.0	0.0073303	0.0009735	0.0000000

MAXIMUM GRADIENT = 0.0084019 RMS GRADIENT = 0.0034727

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0009137554

PREDICTED ENERGY CHANGE WAS -0.0011292026 RATIO= 0.809

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.039136

RADIUS OF STEP TAKEN= 0.03914 CURRENT TRUST RADIUS= 0.31805

1NSERCH= 10

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

	ATOM	CHARGE	X	Y	Z
	C	6.0	-1.4379463932	0.3483709541	0.0000000000
	C	6.0	-0.0455500831	-0.1854852421	0.0000000000
	O	8.0	0.2229114983	-1.3660396796	0.0000000000
	O	8.0	0.9106358528	0.7712372435	0.0000000000
	H	1.0	-1.4747981082	1.4223515816	0.0000000000
	H	1.0	-1.9327506066	-0.0407567764	0.8757104941
	H	1.0	1.7972683779	0.4422315377	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4379463932	0.3483709541	0.0000000000
C	6.0	-0.0455500831	-0.1854852421	0.0000000000
O	8.0	0.2229114983	-1.3660396796	0.0000000000
O	8.0	0.9106358528	0.7712372435	0.0000000000
H	1.0	-1.4747981082	1.4223515816	0.0000000000
H	1.0	-1.9327506066	-0.0407567764	-0.8757104941
H	1.0	-1.9327506066	-0.0407567764	0.8757104941
H	1.0	1.7972683779	0.4422315377	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.4912310 *	2.3869757 *	2.3863475 *
2 C	1.4912310 *	0.0000000	1.2106942 *	1.3526306 *
3 O	2.3869757 *	1.2106942 *	0.0000000	2.2451988 *
4 O	2.3863475 *	1.3526306 *	2.2451988 *	0.0000000
5 H	1.0746127 *	2.1512529 *	3.2645587	2.4727000 *
6 H	1.0784806 *	2.0855074 *	2.6777085 *	3.0839990
7 H	1.0784806 *	2.0855074 *	2.6777085 *	3.0839990
8 H	3.2365760	1.9467943 *	2.3975914 *	0.9457071 *

	H	H	H	H
1 C	1.0746127 *	1.0784806 *	1.0784806 *	3.2365760
2 C	2.1512529 *	2.0855074 *	2.0855074 *	1.9467943 *
3 O	3.2645587	2.6777085 *	2.6777085 *	2.3975914 *
4 O	2.4727000 *	3.0839990	3.0839990	0.9457071 *
5 H	0.0000000	1.7655808 *	1.7655808 *	3.4157070
6 H	1.7655808 *	0.0000000	1.7514210 *	3.8617597
7 H	1.7655808 *	1.7514210 *	0.0000000	3.8617597
8 H	3.4157070	3.8617597	3.8617597	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 82.9 SECONDS (1.4 MIN)
 WALL CLOCK TIME: STEP = 0.04 , TOTAL = 97.3 SECONDS (1.6 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 85.15%
 TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1006723
 202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.
 END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.25 , TOTAL = 85.1 SECONDS (1.4 MIN)
 WALL CLOCK TIME: STEP = 2.29 , TOTAL = 99.6 SECONDS (1.7 MIN)
 CPU UTILIZATION: STEP = 98.25%, TOTAL = 85.45%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.760281290	-227.760281290	0.003689761	0.002250811
2	1	0	-227.760403037	-0.000121747	0.001254312	0.000532671
3	2	0	-227.760412870	-0.000009832	0.000530886	0.000256604
4	3	0	-227.760414276	-0.000001407	0.000174883	0.000051457
5	4	0	-227.760414349	-0.000000073	0.000040727	0.000033615
6	5	0	-227.760414363	-0.000000014	0.000014406	0.000011232
7	6	0	-227.760414364	-0.000000002	0.000007258	0.000003532
8	7	0	-227.760414365	0.000000000	0.000003077	0.000001607

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.8 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.1 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7604143646 AFTER 8 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 1.97 , TOTAL = 87.1 SECONDS (1.5 MIN)
WALL CLOCK TIME: STEP = 2.20 , TOTAL = 101.8 SECONDS (1.7 MIN)
CPU UTILIZATION: STEP = 89.55%, TOTAL = 85.54%
..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.23 , TOTAL = 87.3 SECONDS (1.5 MIN)
WALL CLOCK TIME: STEP = 0.24 , TOTAL = 102.0 SECONDS (1.7 MIN)
CPU UTILIZATION: STEP = 95.83%, TOTAL = 85.57%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.59 , TOTAL = 90.9 SECONDS (1.5 MIN)
WALL CLOCK TIME: STEP = 3.60 , TOTAL = 105.6 SECONDS (1.8 MIN)
CPU UTILIZATION: STEP = 99.72%, TOTAL = 86.05%

NSERCH= 10 ENERGY= -227.7604144

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 C	6.0	-0.0049642	0.0019775	0.0000000
2 C	6.0	-0.0007456	-0.0007661	0.0000000
3 O	8.0	-0.0035716	-0.0033337	0.0000000
4 O	8.0	0.0076262	-0.0000386	0.0000000
5 H	1.0	-0.0017900	0.0002534	0.0000000
6 H	1.0	0.0034439	-0.0007175	-0.0004400
7 H	1.0	0.0034439	-0.0007175	0.0004400
8 H	1.0	-0.0034425	0.0033426	0.0000000

MAXIMUM GRADIENT = 0.0076262 RMS GRADIENT = 0.0026073

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0002852327

PREDICTED ENERGY CHANGE WAS -0.0002875582 RATIO= 0.992

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.043332

RADIUS OF STEP TAKEN= 0.04333 CURRENT TRUST RADIUS= 0.07827

1NSERCH= 11

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4353344847	0.3418295933	0.0000000000
C	6.0	-0.0429408952	-0.1824381337	0.0000000000
O	8.0	0.2332675336	-1.3598784383	0.0000000000
O	8.0	0.9072281253	0.7712066525	0.0000000000
H	1.0	-1.4657344518	1.4197697882	0.0000000000
H	1.0	-1.9416416722	-0.0382660377	0.8738844741
H	1.0	1.7938174484	0.4371954559	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4353344847	0.3418295933	0.0000000000
C	6.0	-0.0429408952	-0.1824381337	0.0000000000
O	8.0	0.2332675336	-1.3598784383	0.0000000000
O	8.0	0.9072281253	0.7712066525	0.0000000000
H	1.0	-1.4657344518	1.4197697882	0.0000000000
H	1.0	-1.9416416722	-0.0382660377	-0.8738844741
H	1.0	-1.9416416722	-0.0382660377	0.8738844741

H 1.0 1.7938174484 0.4371954559 0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.4878228 *	2.3832841 *	2.3815886 *
2 C	1.4878228 *	0.0000000	1.2094035 *	1.3462019 *
3 O	2.3832841 *	1.2094035 *	0.0000000	2.2351167 *
4 O	2.3815886 *	1.3462019 *	2.2351167 *	0.0000000
5 H	1.0783688 *	2.1427580 *	3.2577679	2.4599971 *
6 H	1.0791171 *	2.0951192 *	2.6908295 *	3.0878762
7 H	1.0791171 *	2.0951192 *	2.6908295 *	3.0878762
8 H	3.2305598	1.9384600 *	2.3800821 *	0.9474197 *

	H	H	H	H
1 C	1.0783688 *	1.0791171 *	1.0791171 *	3.2305598
2 C	2.1427580 *	2.0951192 *	2.0951192 *	1.9384600 *
3 O	3.2577679	2.6908295 *	2.6908295 *	2.3800821 *
4 O	2.4599971 *	3.0878762	3.0878762	0.9474197 *
5 H	0.0000000	1.7652281 *	1.7652281 *	3.4044281
6 H	1.7652281 *	0.0000000	1.7477689 *	3.8656684
7 H	1.7652281 *	1.7477689 *	0.0000000	3.8656684
8 H	3.4044281	3.8656684	3.8656684	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 91.0 SECONDS (1.5 MIN)
WALL CLOCK TIME: STEP = 0.04 , TOTAL = 105.7 SECONDS (1.8 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 86.05%

TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1007678

202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.21 , TOTAL = 93.2 SECONDS (1.6 MIN)
WALL CLOCK TIME: STEP = 2.29 , TOTAL = 108.0 SECONDS (1.8 MIN)
CPU UTILIZATION: STEP = 96.51%, TOTAL = 86.28%

ITER EX DEM TOTAL ENERGY E CHANGE DENSITY CHANGE ORB. GRAD
-----START SECOND ORDER SCF-----

1	0	0	-227.760567942	-227.760567942	0.003849784	0.001472322
2	1	0	-227.760649525	-0.000081583	0.001171156	0.000498040
3	2	0	-227.760656385	-0.000006860	0.000401026	0.000292309
4	3	0	-227.760657469	-0.000001084	0.000134085	0.000092184
5	4	0	-227.760657575	-0.000000106	0.000046912	0.000019863
6	5	0	-227.760657581	-0.000000006	0.000011154	0.000003912
7	6	0	-227.760657581	0.000000000	0.000001756	0.000001510
8	7	0	-227.760657581	0.000000000	0.000000515	0.000000252

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.8 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.1 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7606575815 AFTER 8 ITERATIONS

..... END OF RHF CALCULATION

CPU TIME: STEP = 1.98 , TOTAL = 95.1 SECONDS (1.6 MIN)
WALL CLOCK TIME: STEP = 2.41 , TOTAL = 110.4 SECONDS (1.8 MIN)
CPU UTILIZATION: STEP = 82.16%, TOTAL = 86.19%

..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.23 , TOTAL = 95.4 SECONDS (1.6 MIN)
WALL CLOCK TIME: STEP = 0.23 , TOTAL = 110.6 SECONDS (1.8 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 86.21%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.57 , TOTAL = 98.9 SECONDS (1.6 MIN)
WALL CLOCK TIME: STEP = 3.61 , TOTAL = 114.2 SECONDS (1.9 MIN)
CPU UTILIZATION: STEP = 98.89%, TOTAL = 86.61%

NSERCH= 11 ENERGY= -227.7606576

GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	-0.0014066	-0.0041339	0.0000000
2	C	6.0	0.0022428	0.0026506	0.0000000
3	O	8.0	-0.0036555	0.0006463	0.0000000
4	O	8.0	0.0025992	-0.0033449	0.0000000
5	H	1.0	-0.0010349	0.0025075	0.0000000
6	H	1.0	0.0015888	-0.0001860	-0.0003054
7	H	1.0	0.0015888	-0.0001860	0.0003054
8	H	1.0	-0.0019224	0.0020466	0.0000000

MAXIMUM GRADIENT = 0.0041339 RMS GRADIENT = 0.0018641

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0002432168

PREDICTED ENERGY CHANGE WAS -0.0001908147 RATIO= 1.275

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.055015

RADIUS OF STEP TAKEN= 0.05502 CURRENT TRUST RADIUS= 0.06128

1NSERCH= 12

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

	ATOM	CHARGE	X	Y	Z
	C	6.0	-1.4345834721	0.3388107412	0.0000000000
	C	6.0	-0.0431683451	-0.1871401021	0.0000000000
	O	8.0	0.2470061003	-1.3608785431	0.0000000000
	O	8.0	0.9006543492	0.7748140013	0.0000000000
	H	1.0	-1.4490895506	1.4148595536	0.0000000000
	H	1.0	-1.9514198897	-0.0337264635	0.8713918797
	H	1.0	1.7890406291	0.4381401184	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

	ATOM	CHARGE	X	Y	Z
	C	6.0	-1.4345834721	0.3388107412	0.0000000000
	C	6.0	-0.0431683451	-0.1871401021	0.0000000000
	O	8.0	0.2470061003	-1.3608785431	0.0000000000
	O	8.0	0.9006543492	0.7748140013	0.0000000000
	H	1.0	-1.4490895506	1.4148595536	0.0000000000
	H	1.0	-1.9514198897	-0.0337264635	-0.8713918797
	H	1.0	-1.9514198897	-0.0337264635	0.8713918797
	H	1.0	1.7890406291	0.4381401184	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

		C	C	O	O
1	C	0.0000000	1.4875014 *	2.3909595 *	2.3755914 *
2	C	1.4875014 *	0.0000000	1.2090753 *	1.3476487 *
3	O	2.3909595 *	1.2090753 *	0.0000000	2.2334813 *

4	O	2.3755914 *	1.3476487 *	2.2334813 *	0.0000000
5	H	1.0761466 *	2.1314355 *	3.2529160	2.4353551 *
6	H	1.0794571 *	2.1033981 *	2.7117768 *	3.0898849
7	H	1.0794571 *	2.1033981 *	2.7117768 *	3.0898849
8	H	3.2251541	1.9359662 *	2.3694596 *	0.9500418 *

		H	H	H	H
1	C	1.0761466 *	1.0794571 *	1.0794571 *	3.2251541
2	C	2.1314355 *	2.1033981 *	2.1033981 *	1.9359662 *
3	O	3.2529160	2.7117768 *	2.7117768 *	2.3694596 *
4	O	2.4353551 *	3.0898849	3.0898849	0.9500418 *
5	H	0.0000000	1.7635365 *	1.7635365 *	3.3822282
6	H	1.7635365 *	0.0000000	1.7427838 *	3.8694996
7	H	1.7635365 *	1.7427838 *	0.0000000	3.8694996
8	H	3.3822282	3.8694996	3.8694996	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 99.0 SECONDS (1.6 MIN)
WALL CLOCK TIME: STEP = 0.04 , TOTAL = 114.3 SECONDS (1.9 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 86.62%
TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1007838
202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.
..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.25 , TOTAL = 101.2 SECONDS (1.7 MIN)
WALL CLOCK TIME: STEP = 2.38 , TOTAL = 116.6 SECONDS (1.9 MIN)
CPU UTILIZATION: STEP = 94.54%, TOTAL = 86.78%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.760688529	-227.760688529	0.003025657	0.002210078
2	1	0	-227.760815000	-0.000126471	0.001289944	0.000608569
3	2	0	-227.760826070	-0.000011070	0.000453940	0.000395999
4	3	0	-227.760827881	-0.000001811	0.000113245	0.000115088
5	4	0	-227.760828008	-0.000000126	0.000064723	0.000025750
6	5	0	-227.760828021	-0.000000013	0.000018677	0.000008552
7	6	0	-227.760828024	-0.000000003	0.000006609	0.000004524
8	7	0	-227.760828024	0.000000000	0.000002015	0.000001340

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.8 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.2 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7608280240 AFTER 8 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 1.96 , TOTAL = 103.2 SECONDS (1.7 MIN)
WALL CLOCK TIME: STEP = 2.52 , TOTAL = 119.2 SECONDS (2.0 MIN)
CPU UTILIZATION: STEP = 77.78%, TOTAL = 86.59%
..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.24 , TOTAL = 103.4 SECONDS (1.7 MIN)
WALL CLOCK TIME: STEP = 0.24 , TOTAL = 119.4 SECONDS (2.0 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 86.62%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.56 , TOTAL = 107.0 SECONDS (1.8 MIN)
WALL CLOCK TIME: STEP = 3.61 , TOTAL = 123.0 SECONDS (2.1 MIN)
CPU UTILIZATION: STEP = 98.61%, TOTAL = 86.97%

NSERCH= 12 ENERGY= -227.7608280

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 C	6.0	-0.0001942	-0.0026800	0.0000000
2 C	6.0	0.0017132	0.0016844	0.0000000
3 O	8.0	-0.0022161	0.0010040	0.0000000
4 O	8.0	-0.0002610	-0.0010771	0.0000000
5 H	1.0	-0.0000080	0.0008950	0.0000000
6 H	1.0	0.0003426	-0.0000605	0.0001309
7 H	1.0	0.0003426	-0.0000605	-0.0001309
8 H	1.0	0.0002809	0.0002946	0.0000000

MAXIMUM GRADIENT = 0.0026800 RMS GRADIENT = 0.0009439

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0001704425

PREDICTED ENERGY CHANGE WAS -0.0001268714 RATIO= 1.343

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.032057

RADIUS OF STEP TAKEN= 0.03206 CURRENT TRUST RADIUS= 0.05502

1NSERCH= 13

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4345082483	0.3385029443	0.0000000000
C	6.0	-0.0440518050	-0.1916757557	0.0000000000
O	8.0	0.2559432822	-1.3631548012	0.0000000000
O	8.0	0.8966719467	0.7763651083	0.0000000000
H	1.0	-1.4401112761	1.4130092954	0.0000000000
H	1.0	-1.9562268208	-0.0309200945	0.8705511332
H	1.0	1.7855296733	0.4399462404	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4345082483	0.3385029443	0.0000000000
C	6.0	-0.0440518050	-0.1916757557	0.0000000000
O	8.0	0.2559432822	-1.3631548012	0.0000000000
O	8.0	0.8966719467	0.7763651083	0.0000000000
H	1.0	-1.4401112761	1.4130092954	0.0000000000
H	1.0	-1.9562268208	-0.0309200945	-0.8705511332
H	1.0	-1.9562268208	-0.0309200945	0.8705511332
H	1.0	1.7855296733	0.4399462404	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.4881057 *	2.3985966 *	2.3719453 *
2 C	1.4881057 *	0.0000000	1.2092809 *	1.3498386 *
3 O	2.3985966 *	1.2092809 *	0.0000000	2.2334007 *
4 O	2.3719453 *	1.3498386 *	2.2334007 *	0.0000000
5 H	1.0745210 *	2.1269688 *	3.2532581	2.4219562 *
6 H	1.0800569 *	2.1071580 *	2.7251431 *	3.0900809
7 H	1.0800569 *	2.1071580 *	2.7251431 *	3.0900809
8 H	3.2216354	1.9355399 *	2.3644889 *	0.9503924 *
	H	H	H	H
1 C	1.0745210 *	1.0800569 *	1.0800569 *	3.2216354
2 C	2.1269688 *	2.1071580 *	2.1071580 *	1.9355399 *

3	O	3.2532581	2.7251431 *	2.7251431 *	2.3644889 *
4	O	2.4219562 *	3.0900809	3.0900809	0.9503924 *
5	H	0.0000000	1.7632829 *	1.7632829 *	3.3692152
6	H	1.7632829 *	0.0000000	1.7411023 *	3.8704413
7	H	1.7632829 *	1.7411023 *	0.0000000	3.8704413
8	H	3.3692152	3.8704413	3.8704413	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 107.0 SECONDS (1.8 MIN)
 WALL CLOCK TIME: STEP = 0.04 , TOTAL = 123.1 SECONDS (2.1 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 86.97%
 TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1007694
 202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.
 END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.24 , TOTAL = 109.3 SECONDS (1.8 MIN)
 WALL CLOCK TIME: STEP = 2.38 , TOTAL = 125.4 SECONDS (2.1 MIN)
 CPU UTILIZATION: STEP = 94.12%, TOTAL = 87.11%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.760803580	-227.760803580	0.002076444	0.001612494
2	1	0	-227.760860217	-0.000056637	0.000939470	0.000434464
3	2	0	-227.760865129	-0.000004911	0.000316827	0.000303247
4	3	0	-227.760866137	-0.000001008	0.000080790	0.000069634
5	4	0	-227.760866191	-0.000000054	0.000036294	0.000015882
6	5	0	-227.760866195	-0.000000005	0.000015719	0.000005757
7	6	0	-227.760866196	-0.000000001	0.000003771	0.000001796
8	7	0	-227.760866196	0.000000000	0.000001417	0.000000803

 DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.8 SECONDS (0.2 SEC/ITER)
 TIME TO SOLVE SCF EQUATIONS= 0.1 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7608661963 AFTER 8 ITERATIONS
 END OF RHF CALCULATION

CPU TIME: STEP = 1.96 , TOTAL = 111.2 SECONDS (1.9 MIN)
 WALL CLOCK TIME: STEP = 1.99 , TOTAL = 127.4 SECONDS (2.1 MIN)
 CPU UTILIZATION: STEP = 98.49%, TOTAL = 87.29%
 END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.24 , TOTAL = 111.5 SECONDS (1.9 MIN)
 WALL CLOCK TIME: STEP = 0.24 , TOTAL = 127.7 SECONDS (2.1 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 87.31%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.50 , TOTAL = 115.0 SECONDS (1.9 MIN)
 WALL CLOCK TIME: STEP = 3.60 , TOTAL = 131.3 SECONDS (2.2 MIN)
 CPU UTILIZATION: STEP = 97.22%, TOTAL = 87.58%

NSERCH= 13 ENERGY= -227.7608662

 GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	0.0003150	-0.0002092	0.0000000
2	C	6.0	0.0001574	0.0002503	0.0000000

3	O	8.0	-0.0006255	0.0003206	0.0000000
4	O	8.0	-0.0001365	0.0003627	0.0000000
5	H	1.0	0.0003249	-0.0001660	0.0000000
6	H	1.0	-0.0002204	-0.0002052	0.0000881
7	H	1.0	-0.0002204	-0.0002052	-0.0000881
8	H	1.0	0.0004056	-0.0001479	0.0000000

MAXIMUM GRADIENT = 0.0006255 RMS GRADIENT = 0.0002408

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0000381723

PREDICTED ENERGY CHANGE WAS -0.0000346397 RATIO= 1.102

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.004620

RADIUS OF STEP TAKEN= 0.00462 CURRENT TRUST RADIUS= 0.05000

1NSERCH= 14

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4347174291	0.3386918868	0.0000000000
C	6.0	-0.0442084440	-0.1926526550	0.0000000000
O	8.0	0.2574780162	-1.3638696222	0.0000000000
O	8.0	0.8959380904	0.7760129962	0.0000000000
H	1.0	-1.4399002370	1.4132490778	0.0000000000
H	1.0	-1.9562476141	-0.0303213260	0.8706719544
H	1.0	1.7849251632	0.4403638109	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4347174291	0.3386918868	0.0000000000
C	6.0	-0.0442084440	-0.1926526550	0.0000000000
O	8.0	0.2574780162	-1.3638696222	0.0000000000
O	8.0	0.8959380904	0.7760129962	0.0000000000
H	1.0	-1.4399002370	1.4132490778	0.0000000000
H	1.0	-1.9562476141	-0.0303213260	-0.8706719544
H	1.0	-1.9562476141	-0.0303213260	0.8706719544
H	1.0	1.7849251632	0.4403638109	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.4885705 *	2.4004669 *	2.3713298 *
2 C	1.4885705 *	0.0000000	1.2094478 *	1.3498847 *
3 O	2.4004669 *	1.2094478 *	0.0000000	2.2330985 *
4 O	2.3713298 *	1.3498847 *	2.2330985 *	0.0000000
5 H	1.0745697 *	2.1276456 *	3.2547628	2.4212002 *
6 H	1.0799232 *	2.1072055 *	2.7270867 *	3.0892083
7 H	1.0799232 *	2.1072055 *	2.7270867 *	3.0892083
8 H	3.2212475	1.9355722 *	2.3639698 *	0.9502412 *

	H	H	H	H
1 C	1.0745697 *	1.0799232 *	1.0799232 *	3.2212475
2 C	2.1276456 *	2.1072055 *	2.1072055 *	1.9355722 *
3 O	3.2547628	2.7270867 *	2.7270867 *	2.3639698 *
4 O	2.4212002 *	3.0892083	3.0892083	0.9502412 *
5 H	0.0000000	1.7631165 *	1.7631165 *	3.3683831
6 H	1.7631165 *	0.0000000	1.7413439 *	3.8698822
7 H	1.7631165 *	1.7413439 *	0.0000000	3.8698822
8 H	3.3683831	3.8698822	3.8698822	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 115.0 SECONDS (1.9 MIN)
WALL CLOCK TIME: STEP = 0.04 , TOTAL = 131.3 SECONDS (2.2 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 87.59%
TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1007658
202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.
..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.23 , TOTAL = 117.2 SECONDS (2.0 MIN)
WALL CLOCK TIME: STEP = 2.60 , TOTAL = 133.9 SECONDS (2.2 MIN)
CPU UTILIZATION: STEP = 85.77%, TOTAL = 87.55%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.760867409	-227.760867409	0.000399939	0.000303036
2	1	0	-227.760868803	-0.000001393	0.000164610	0.000086731
3	2	0	-227.760868925	-0.000000122	0.000050619	0.000035739
4	3	0	-227.760868938	-0.000000013	0.000017212	0.000013172
5	4	0	-227.760868940	-0.000000002	0.000005839	0.000001918
6	5	0	-227.760868940	0.000000000	0.000003214	0.000000684

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.3 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.1 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7608689403 AFTER 6 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 1.50 , TOTAL = 118.7 SECONDS (2.0 MIN)
WALL CLOCK TIME: STEP = 1.51 , TOTAL = 135.4 SECONDS (2.3 MIN)
CPU UTILIZATION: STEP = 99.34%, TOTAL = 87.68%
..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.24 , TOTAL = 119.0 SECONDS (2.0 MIN)
WALL CLOCK TIME: STEP = 0.24 , TOTAL = 135.7 SECONDS (2.3 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 87.70%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.60 , TOTAL = 122.6 SECONDS (2.0 MIN)
WALL CLOCK TIME: STEP = 3.97 , TOTAL = 139.6 SECONDS (2.3 MIN)
CPU UTILIZATION: STEP = 90.68%, TOTAL = 87.79%

NSERCH= 14 ENERGY= -227.7608689

GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	C	6.0	0.0000368	0.0001223	0.0000000
2	C	6.0	-0.0000497	0.0000705	0.0000000
3	O	8.0	-0.0001856	0.0000462	0.0000000
4	O	8.0	-0.0000600	0.0002411	0.0000000
5	H	1.0	0.0002144	-0.0001018	0.0000000
6	H	1.0	-0.0001067	-0.0001512	0.0001233
7	H	1.0	-0.0001067	-0.0001512	-0.0001233
8	H	1.0	0.0002574	-0.0000760	0.0000000

MAXIMUM GRADIENT = 0.0002574 RMS GRADIENT = 0.0001206
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0000027441
PREDICTED ENERGY CHANGE WAS -0.0000020101 RATIO= 1.365
MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.003022
 RADIUS OF STEP TAKEN= 0.00302 CURRENT TRUST RADIUS= 0.05000
 INSERCH= 15

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4347160226	0.3387176422	0.0000000000
C	6.0	-0.0441795203	-0.1931317737	0.0000000000
O	8.0	0.2582397223	-1.3642045868	0.0000000000
O	8.0	0.8956321033	0.7756351530	0.0000000000
H	1.0	-1.4405293848	1.4134476442	0.0000000000
H	1.0	-1.9559653408	-0.0298704099	0.8709990498
H	1.0	1.7845037148	0.4404295834	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4347160226	0.3387176422	0.0000000000
C	6.0	-0.0441795203	-0.1931317737	0.0000000000
O	8.0	0.2582397223	-1.3642045868	0.0000000000
O	8.0	0.8956321033	0.7756351530	0.0000000000
H	1.0	-1.4405293848	1.4134476442	0.0000000000
H	1.0	-1.9559653408	-0.0298704099	-0.8709990498
H	1.0	-1.9559653408	-0.0298704099	0.8709990498
H	1.0	1.7845037148	0.4404295834	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O
1 C	0.0000000	1.4887765 *	2.4012587 *	2.3709532 *
2 C	1.4887765 *	0.0000000	1.2094912 *	1.3497241 *
3 O	2.4012587 *	1.2094912 *	0.0000000	2.2327524 *
4 O	2.3709532 *	1.3497241 *	2.2327524 *	0.0000000
5 H	1.0747457 *	2.1285888 *	3.2559435	2.4216637 *
6 H	1.0799062 *	2.1071826 *	2.7279646 *	3.0885412
7 H	1.0799062 *	2.1071826 *	2.7279646 *	3.0885412
8 H	3.2208261	1.9353249 *	2.3635114 *	0.9499766 *

	H	H	H	H
1 C	1.0747457 *	1.0799062 *	1.0799062 *	3.2208261
2 C	2.1285888 *	2.1071826 *	2.1071826 *	1.9353249 *
3 O	3.2559435	2.7279646 *	2.7279646 *	2.3635114 *
4 O	2.4216637 *	3.0885412	3.0885412	0.9499766 *
5 H	0.0000000	1.7628047 *	1.7628047 *	3.3686203
6 H	1.7628047 *	0.0000000	1.7419981 *	3.8692286
7 H	1.7628047 *	1.7419981 *	0.0000000	3.8692286
8 H	3.3686203	3.8692286	3.8692286	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 122.6 SECONDS (2.0 MIN)
 WALL CLOCK TIME: STEP = 0.04 , TOTAL = 139.7 SECONDS (2.3 MIN)
 CPU UTILIZATION: STEP = 100.00%, TOTAL = 87.79%

TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1007662

202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.25 , TOTAL = 124.9 SECONDS (2.1 MIN)
 WALL CLOCK TIME: STEP = 2.35 , TOTAL = 142.0 SECONDS (2.4 MIN)
 CPU UTILIZATION: STEP = 95.74%, TOTAL = 87.92%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-227.760869488	-227.760869488	0.000202062	0.000138983
2	1	0	-227.760869793	-0.000000305	0.000083919	0.000044324
3	2	0	-227.760869820	-0.000000027	0.000022083	0.000011279
4	3	0	-227.760869823	-0.000000003	0.000011486	0.000002979
5	4	0	-227.760869823	0.000000000	0.000003278	0.000001399
6	5	0	-227.760869823	0.000000000	0.000000957	0.000000490

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 1.3 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.1 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7608698233 AFTER 6 ITERATIONS
..... END OF RHF CALCULATION

CPU TIME: STEP = 1.50 , TOTAL = 126.4 SECONDS (2.1 MIN)
WALL CLOCK TIME: STEP = 1.51 , TOTAL = 143.5 SECONDS (2.4 MIN)
CPU UTILIZATION: STEP = 99.34% , TOTAL = 88.04%
..... END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.23 , TOTAL = 126.6 SECONDS (2.1 MIN)
WALL CLOCK TIME: STEP = 0.23 , TOTAL = 143.8 SECONDS (2.4 MIN)
CPU UTILIZATION: STEP = 100.00% , TOTAL = 88.06%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.54 , TOTAL = 130.1 SECONDS (2.2 MIN)
WALL CLOCK TIME: STEP = 4.01 , TOTAL = 147.8 SECONDS (2.5 MIN)
CPU UTILIZATION: STEP = 88.28% , TOTAL = 88.07%

NSERCH= 15 ENERGY= -227.7608698

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 C	6.0	0.00000004	0.0001469	0.00000000
2 C	6.0	-0.0000592	-0.0000556	0.00000000
3 O	8.0	0.0000197	0.0000039	0.00000000
4 O	8.0	0.0000715	0.0000018	0.00000000
5 H	1.0	0.0000481	0.0000269	0.00000000
6 H	1.0	-0.0000332	-0.0000761	0.0000636
7 H	1.0	-0.0000332	-0.0000761	-0.0000636
8 H	1.0	-0.0000141	0.0000283	0.00000000

MAXIMUM GRADIENT = 0.0001469 RMS GRADIENT = 0.0000498

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0000008829

PREDICTED ENERGY CHANGE WAS -0.0000007628 RATIO= 1.157

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.000936

RADIUS OF STEP TAKEN= 0.00094 CURRENT TRUST RADIUS= 0.05000

1NSERCH= 16

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4347258493	0.3386007117	0.0000000000
C	6.0	-0.0441481017	-0.1931578094	0.0000000000
O	8.0	0.2583043419	-1.3642534964	0.0000000000
O	8.0	0.8955696427	0.7755843945	0.0000000000
H	1.0	-1.4407632218	1.4133759933	0.0000000000

H	1.0	-1.9558343223	-0.0296990276	0.8711730756
H	1.0	1.7844517641	0.4404011039	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z

C	6.0	-1.4347258493	0.3386007117	0.0000000000
C	6.0	-0.0441481017	-0.1931578094	0.0000000000
O	8.0	0.2583043419	-1.3642534964	0.0000000000
O	8.0	0.8955696427	0.7755843945	0.0000000000
H	1.0	-1.4407632218	1.4133759933	0.0000000000
H	1.0	-1.9558343223	-0.0296990276	-0.8711730756
H	1.0	-1.9558343223	-0.0296990276	0.8711730756
H	1.0	1.7844517641	0.4404011039	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	C	C	O	O

1 C	0.0000000	1.4887826 *	2.4012629 *	2.3709137 *
2 C	1.4887826 *	0.0000000	1.2095216 *	1.3496410 *
3 O	2.4012629 *	1.2095216 *	0.0000000	2.2327143 *
4 O	2.3709137 *	1.3496410 *	2.2327143 *	0.0000000
5 H	1.0747922 *	2.1287284 *	3.2560799	2.4218236 *
6 H	1.0798802 *	2.1071795 *	2.7280741 *	3.0883537
7 H	1.0798802 *	2.1071795 *	2.7280741 *	3.0883537
8 H	3.2207868	1.9352453 *	2.3634518 *	0.9499786 *

	H	H	H	H

1 C	1.0747922 *	1.0798802 *	1.0798802 *	3.2207868
2 C	2.1287284 *	2.1071795 *	2.1071795 *	1.9352453 *
3 O	3.2560799	2.7280741 *	2.7280741 *	2.3634518 *
4 O	2.4218236 *	3.0883537	3.0883537	0.9499786 *
5 H	0.0000000	1.7625851 *	1.7625851 *	3.3687820
6 H	1.7625851 *	0.0000000	1.7423462 *	3.8690666
7 H	1.7625851 *	1.7423462 *	0.0000000	3.8690666
8 H	3.3687820	3.8690666	3.8690666	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU TIME: STEP = 0.04 , TOTAL = 130.2 SECONDS (2.2 MIN)
WALL CLOCK TIME: STEP = 0.04 , TOTAL = 147.8 SECONDS (2.5 MIN)
CPU UTILIZATION: STEP = 100.00%, TOTAL = 88.07%
TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 1007653
202 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.
..... END OF TWO-ELECTRON INTEGRALS

CPU TIME: STEP = 2.25 , TOTAL = 132.4 SECONDS (2.2 MIN)
WALL CLOCK TIME: STEP = 3.28 , TOTAL = 151.1 SECONDS (2.5 MIN)
CPU UTILIZATION: STEP = 68.60%, TOTAL = 87.65%

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD

-----START SECOND ORDER SCF-----						
1	0	0	-227.760869919	-227.760869919	0.000078325	0.000037732
2	1	0	-227.760869936	-0.000000017	0.000024190	0.000008167
3	2	0	-227.760869937	-0.000000001	0.000006964	0.000005783
4	3	0	-227.760869938	0.000000000	0.000002690	0.000001062

DENSITY CONVERGED

TIME TO FORM FOCK OPERATORS= 0.9 SECONDS (0.2 SEC/ITER)
TIME TO SOLVE SCF EQUATIONS= 0.1 SECONDS (0.0 SEC/ITER)

FINAL ENERGY IS -227.7608699377 AFTER 4 ITERATIONS
 END OF RHF CALCULATION

CPU TIME: STEP = 1.04 , TOTAL = 133.5 SECONDS (2.2 MIN)
 WALL CLOCK TIME: STEP = 1.06 , TOTAL = 152.1 SECONDS (2.5 MIN)
 CPU UTILIZATION: STEP = 98.11%, TOTAL = 87.72%
 END OF 1-ELECTRON GRADIENT

CPU TIME: STEP = 0.23 , TOTAL = 133.7 SECONDS (2.2 MIN)
 WALL CLOCK TIME: STEP = 0.24 , TOTAL = 152.4 SECONDS (2.5 MIN)
 CPU UTILIZATION: STEP = 95.83%, TOTAL = 87.74%

..... END OF 2-ELECTRON GRADIENT

CPU TIME: STEP = 3.56 , TOTAL = 137.3 SECONDS (2.3 MIN)
 WALL CLOCK TIME: STEP = 3.61 , TOTAL = 156.0 SECONDS (2.6 MIN)
 CPU UTILIZATION: STEP = 98.61%, TOTAL = 87.99%

NSERCH= 16 ENERGY= -227.7608699

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 C	6.0	-0.0000171	0.0000413	0.0000000
2 C	6.0	-0.0000208	0.0000047	0.0000000
3 O	8.0	0.0000301	-0.0000338	0.0000000
4 O	8.0	0.0000235	-0.0000319	0.0000000
5 H	1.0	0.0000062	0.0000476	0.0000000
6 H	1.0	-0.0000032	-0.0000257	0.0000396
7 H	1.0	-0.0000032	-0.0000257	-0.0000396
8 H	1.0	-0.0000155	0.0000236	0.0000000

MAXIMUM GRADIENT = 0.0000476 RMS GRADIENT = 0.0000238
 1 ***** EQUILIBRIUM GEOMETRY LOCATED *****

HAc(Z) generated by Kimball.exe
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4347258493	0.3386007117	0.0000000000
C	6.0	-0.0441481017	-0.1931578094	0.0000000000
O	8.0	0.2583043419	-1.3642534964	0.0000000000
O	8.0	0.8955696427	0.7755843945	0.0000000000
H	1.0	-1.4407632218	1.4133759933	0.0000000000
H	1.0	-1.9558343223	-0.0296990276	0.8711730756
H	1.0	1.7844517641	0.4404011039	0.0000000000

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.4347258493	0.3386007117	0.0000000000
C	6.0	-0.0441481017	-0.1931578094	0.0000000000
O	8.0	0.2583043419	-1.3642534964	0.0000000000
O	8.0	0.8955696427	0.7755843945	0.0000000000
H	1.0	-1.4407632218	1.4133759933	0.0000000000
H	1.0	-1.9558343223	-0.0296990276	-0.8711730756
H	1.0	-1.9558343223	-0.0296990276	0.8711730756
H	1.0	1.7844517641	0.4404011039	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

C C O O

1	C	0.0000000	1.4887826 *	2.4012629 *	2.3709137 *
2	C	1.4887826 *	0.0000000	1.2095216 *	1.3496410 *
3	O	2.4012629 *	1.2095216 *	0.0000000	2.2327143 *
4	O	2.3709137 *	1.3496410 *	2.2327143 *	0.0000000
5	H	1.0747922 *	2.1287284 *	3.2560799	2.4218236 *
6	H	1.0798802 *	2.1071795 *	2.7280741 *	3.0883537
7	H	1.0798802 *	2.1071795 *	2.7280741 *	3.0883537
8	H	3.2207868	1.9352453 *	2.3634518 *	0.9499786 *

H	H	H	H
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1	C	1.0747922 *	1.0798802 *	1.0798802 *	3.2207868
2	C	2.1287284 *	2.1071795 *	2.1071795 *	1.9352453 *
3	O	3.2560799	2.7280741 *	2.7280741 *	2.3634518 *
4	O	2.4218236 *	3.0883537	3.0883537	0.9499786 *
5	H	0.0000000	1.7625851 *	1.7625851 *	3.3687820
6	H	1.7625851 *	0.0000000	1.7423462 *	3.8690666
7	H	1.7625851 *	1.7423462 *	0.0000000	3.8690666
8	H	3.3687820	3.8690666	3.8690666	0.0000000

* ... LESS THAN 3.000

NUCLEAR ENERGY	=	121.5183649393
ELECTRONIC ENERGY	=	-349.2792348770
TOTAL ENERGY	=	-227.7608699377

MOLECULAR ORBITALS

			1	2	3	4	5
			-20.6136	-20.5600	-11.4159	-11.2516	-1.4906
			A'	A'	A'	A'	A'
1	C	1 S	0.000000	0.000000	0.001157	0.563243	-0.008661
2	C	1 S	0.000003	0.000006	0.000907	0.466504	-0.014489
3	C	1 X	-0.000001	-0.000008	0.000118	0.000373	0.009275
4	C	1 Y	-0.000002	-0.000016	-0.000057	-0.000260	-0.002987
5	C	1 Z	0.000000	0.000000	0.000000	0.000000	0.000000
6	C	1 S	-0.000020	-0.000036	0.000199	0.004855	0.037587
7	C	1 X	-0.000025	0.000014	0.000209	-0.000129	0.017101
8	C	1 Y	0.000006	0.000053	-0.000046	0.000109	-0.006123
9	C	1 Z	0.000000	0.000000	0.000000	0.000000	0.000000
10	C	1 S	-0.000055	0.000492	0.001112	-0.001691	0.015428
11	C	1 X	-0.000016	0.000196	0.000507	-0.000023	0.002956
12	C	1 Y	-0.000188	0.000059	-0.000166	-0.000007	0.009155
13	C	1 Z	0.000000	0.000000	0.000000	0.000000	0.000000
14	C	2 S	-0.000004	0.000007	0.563424	-0.001269	-0.063655
15	C	2 S	-0.000027	-0.000080	0.466638	-0.001113	-0.104851
16	C	2 X	0.000048	0.000036	0.001307	-0.000191	0.042049
17	C	2 Y	0.000083	-0.000144	-0.000057	0.000077	-0.021494
18	C	2 Z	0.000000	0.000000	0.000000	0.000000	0.000000
19	C	2 S	0.000110	0.000347	0.004009	0.000303	0.282760
20	C	2 X	0.000103	0.000070	-0.000669	-0.000147	0.058631
21	C	2 Y	-0.000011	-0.000214	-0.000103	0.000049	-0.020817
22	C	2 Z	0.000000	0.000000	0.000000	0.000000	0.000000
23	C	2 S	0.000180	0.000002	-0.001412	0.000365	-0.022292
24	C	2 X	0.000147	0.000360	0.001054	-0.000205	-0.040115
25	C	2 Y	0.000419	-0.000589	-0.000264	0.000049	-0.006734
26	C	2 Z	0.000000	0.000000	0.000000	0.000000	0.000000
27	O	3 S	-0.000195	0.551468	-0.000194	0.000004	-0.061295
28	O	3 S	-0.000160	0.471683	-0.000311	0.000008	-0.102513
29	O	3 X	-0.000007	-0.000553	-0.000088	0.000006	-0.005673
30	O	3 Y	0.000000	0.002506	0.000242	-0.000002	0.044028
31	O	3 Z	0.000000	0.000000	0.000000	0.000000	0.000000
32	O	3 S	-0.000040	0.005523	0.000732	-0.000021	0.290686

33	O	3	X	0.000008	0.000191	-0.000135	0.000032	-0.014640
34	O	3	Y	-0.000033	-0.000861	0.000774	-0.000025	0.080129
35	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
36	O	3	S	0.000123	-0.000877	-0.000064	-0.000038	0.213746
37	O	3	X	-0.000104	-0.000043	-0.000121	0.000039	0.003611
38	O	3	Y	-0.000046	0.000053	-0.000222	-0.000003	0.033396
39	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
40	O	4	S	0.551436	0.000198	-0.000091	0.000005	-0.081687
41	O	4	S	0.471652	0.000172	-0.000161	0.000010	-0.136699
42	O	4	X	0.000438	-0.000006	-0.000111	-0.000001	-0.004221
43	O	4	Y	-0.002259	0.000004	-0.000114	0.000000	-0.037061
44	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
45	O	4	S	0.005669	0.000001	0.000412	-0.000033	0.385126
46	O	4	X	-0.000218	0.000038	-0.000326	0.000049	-0.002675
47	O	4	Y	0.000815	0.000007	-0.000393	0.000017	-0.073874
48	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
49	O	4	S	-0.000591	-0.000019	0.000097	-0.000039	0.336367
50	O	4	X	0.000263	-0.000197	0.000018	-0.000044	-0.009252
51	O	4	Y	-0.000239	0.000146	0.000095	-0.000005	-0.054015
52	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
53	H	5	S	-0.000007	-0.000002	-0.000008	0.000356	0.004280
54	H	5	S	0.000023	-0.000075	-0.000087	0.000133	-0.002557
55	H	5	S	0.000137	-0.000028	0.000015	0.000300	-0.004462
56	H	6	S	0.000002	0.000011	0.000001	0.000348	0.003253
57	H	6	S	-0.000021	-0.000041	-0.000062	0.000152	0.001176
58	H	6	S	-0.000021	0.000017	0.000098	0.000267	0.000157
59	H	7	S	0.000002	0.000011	0.000001	0.000348	0.003253
60	H	7	S	-0.000021	-0.000041	-0.000062	0.000152	0.001176
61	H	7	S	-0.000021	0.000017	0.000098	0.000267	0.000157
62	H	8	S	0.000211	0.000010	-0.000024	-0.000005	0.063177
63	H	8	S	-0.000147	0.000095	-0.000071	0.000059	0.017281
64	H	8	S	0.000111	-0.000004	-0.000092	0.000011	0.005492

				6	7	8	9	10
				-1.3811	-1.0448	-0.8465	-0.7036	-0.6881
				A'	A'	A'	A'	A'
1	C	1	S	-0.002499	-0.093407	-0.038765	-0.009619	-0.016570
2	C	1	S	-0.004296	-0.157470	-0.065818	-0.016062	-0.028979
3	C	1	X	-0.000008	0.020580	-0.053206	-0.036816	-0.092366
4	C	1	Y	-0.006287	-0.006448	-0.000833	0.069917	0.043634
5	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
6	C	1	S	0.011434	0.406934	0.166508	0.035995	0.064304
7	C	1	X	0.004677	0.036644	-0.091516	-0.071668	-0.131700
8	C	1	Y	-0.007065	-0.013468	0.000304	0.121050	0.062864
9	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
10	C	1	S	0.004945	0.316638	0.207363	0.108970	0.273870
11	C	1	X	-0.008328	0.008584	-0.006518	0.010501	-0.023366
12	C	1	Y	-0.021204	-0.000196	-0.013572	0.048852	0.026080
13	C	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
14	C	2	S	-0.024043	-0.041112	0.052417	0.047118	0.001887
15	C	2	S	-0.038972	-0.070235	0.090764	0.081814	0.002146
16	C	2	X	-0.010884	-0.071497	-0.047736	0.041387	0.135785
17	C	2	Y	-0.103551	0.048661	-0.065185	0.088109	-0.013571
18	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
19	C	2	S	0.108140	0.206778	-0.271819	-0.259668	0.011137
20	C	2	X	-0.014220	-0.114050	-0.088369	0.073598	0.253173
21	C	2	Y	-0.139139	0.082893	-0.121201	0.173168	-0.038758
22	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
23	C	2	S	0.026037	0.057047	-0.162784	-0.159931	-0.130439
24	C	2	X	0.022981	-0.017503	0.027703	0.082394	0.189659
25	C	2	Y	0.056559	0.010741	-0.029766	-0.006390	-0.069418
26	C	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
27	O	3	S	-0.085155	0.023083	-0.020225	-0.049456	0.013563
28	O	3	S	-0.142655	0.038889	-0.034076	-0.083526	0.022783
29	O	3	X	-0.017185	-0.017479	-0.013918	0.080618	0.102456
30	O	3	Y	0.045948	-0.000081	-0.034981	-0.148733	0.077601

31	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
32	O	3	S	0.404735	-0.112613	0.098783	0.244805	-0.062871
33	O	3	X	-0.028496	-0.027086	-0.019533	0.123025	0.164060
34	O	3	Y	0.089884	-0.001516	-0.054043	-0.213863	0.108743
35	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
36	O	3	S	0.322920	-0.099215	0.108583	0.346036	-0.144156
37	O	3	X	-0.016796	-0.012309	-0.015203	0.073470	0.115354
38	O	3	Y	0.031289	0.004537	-0.036589	-0.139618	0.070000
39	O	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000
40	O	4	S	0.075510	0.013896	-0.013975	-0.015021	0.024779
41	O	4	S	0.126542	0.023535	-0.023693	-0.025562	0.041911
42	O	4	X	-0.006118	-0.050196	0.172979	-0.092315	0.009723
43	O	4	Y	0.017503	0.002476	0.048890	0.048955	-0.152115
44	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
45	O	4	S	-0.356514	-0.068480	0.069740	0.080209	-0.126014
46	O	4	X	-0.015083	-0.086428	0.291178	-0.148661	0.017748
47	O	4	Y	0.043955	0.006730	0.076567	0.074669	-0.234688
48	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
49	O	4	S	-0.341310	-0.068343	0.076821	0.074684	-0.164031
50	O	4	X	0.002464	-0.033984	0.167265	-0.112625	0.007416
51	O	4	Y	0.035078	0.002999	0.048802	0.085879	-0.187939
52	O	4	Z	0.000000	0.000000	0.000000	0.000000	0.000000
53	H	5	S	-0.001584	0.070355	0.037380	0.068552	0.053014
54	H	5	S	0.002196	0.055407	0.033117	0.091523	0.048524
55	H	5	S	0.000075	-0.012397	0.006698	0.024545	-0.001879
56	H	6	S	0.002313	0.069442	0.055647	0.007581	0.043713
57	H	6	S	-0.000227	0.057468	0.057679	0.002632	0.042807
58	H	6	S	-0.000753	-0.010627	0.009146	0.011231	0.007465
59	H	7	S	0.002313	0.069442	0.055647	0.007581	0.043713
60	H	7	S	-0.000227	0.057468	0.057679	0.002632	0.042807
61	H	7	S	-0.000753	-0.010627	0.009146	0.011231	0.007465
62	H	8	S	-0.064545	-0.046314	0.133369	-0.068834	0.021279
63	H	8	S	-0.018147	-0.042316	0.135826	-0.075884	0.028835
64	H	8	S	-0.002553	-0.004417	0.022717	-0.009250	-0.018336

				11	12	13	14	15
				-0.6603	-0.5819	-0.5733	-0.5699	-0.4782
				A''	A'	A'	A''	A''
1	C	1	S	0.000000	-0.000912	0.004003	0.000000	0.000000
2	C	1	S	0.000000	-0.001655	0.007018	0.000000	0.000000
3	C	1	X	0.000000	0.055111	-0.108954	0.000000	0.000000
4	C	1	Y	0.000000	0.164613	-0.025215	0.000000	0.000000
5	C	1	Z	0.103083	0.000000	0.000000	0.155194	-0.042188
6	C	1	S	0.000000	0.006138	-0.020786	0.000000	0.000000
7	C	1	X	0.000000	0.097841	-0.201534	0.000000	0.000000
8	C	1	Y	0.000000	0.287423	-0.039373	0.000000	0.000000
9	C	1	Z	0.181031	0.000000	0.000000	0.270021	-0.069642
10	C	1	S	0.000000	-0.023684	-0.101654	0.000000	0.000000
11	C	1	X	0.000000	0.040586	-0.132009	0.000000	0.000000
12	C	1	Y	0.000000	0.166656	-0.057042	0.000000	0.000000
13	C	1	Z	0.082879	0.000000	0.000000	0.189346	-0.102643
14	C	2	S	0.000000	-0.006909	0.011406	0.000000	0.000000
15	C	2	S	0.000000	-0.011772	0.019712	0.000000	0.000000
16	C	2	X	0.000000	-0.004776	0.068866	0.000000	0.000000
17	C	2	Y	0.000000	-0.066646	-0.103151	0.000000	0.000000
18	C	2	Z	0.117780	0.000000	0.000000	-0.035311	0.076150
19	C	2	S	0.000000	0.042744	-0.052286	0.000000	0.000000
20	C	2	X	0.000000	-0.006323	0.130232	0.000000	0.000000
21	C	2	Y	0.000000	-0.099904	-0.166612	0.000000	0.000000
22	C	2	Z	0.211797	0.000000	0.000000	-0.061983	0.138968
23	C	2	S	0.000000	0.008172	-0.032852	0.000000	0.000000
24	C	2	X	0.000000	-0.022657	0.003600	0.000000	0.000000
25	C	2	Y	0.000000	0.035984	0.078427	0.000000	0.000000
26	C	2	Z	0.123574	0.000000	0.000000	-0.061023	0.121221
27	O	3	S	0.000000	0.010675	0.012617	0.000000	0.000000
28	O	3	S	0.000000	0.017854	0.021171	0.000000	0.000000

29	O	3	X	0.000000	-0.019422	-0.020842	0.000000	0.000000
30	O	3	Y	0.000000	0.092505	0.122108	0.000000	0.000000
31	O	3	Z	0.102122	0.000000	0.000000	-0.038206	0.210701
32	O	3	S	0.000000	-0.054617	-0.065852	0.000000	0.000000
33	O	3	X	0.000000	-0.029785	-0.031118	0.000000	0.000000
34	O	3	Y	0.000000	0.148693	0.191324	0.000000	0.000000
35	O	3	Z	0.163787	0.000000	0.000000	-0.061822	0.330950
36	O	3	S	0.000000	-0.051010	-0.054348	0.000000	0.000000
37	O	3	X	0.000000	-0.022116	-0.034023	0.000000	0.000000
38	O	3	Y	0.000000	0.114671	0.143801	0.000000	0.000000
39	O	3	Z	0.127328	0.000000	0.000000	-0.049010	0.338739
40	O	4	S	0.000000	0.000480	-0.029080	0.000000	0.000000
41	O	4	S	0.000000	0.000941	-0.049545	0.000000	0.000000
42	O	4	X	0.000000	0.032907	-0.085449	0.000000	0.000000
43	O	4	Y	0.000000	0.062637	0.158340	0.000000	0.000000
44	O	4	Z	0.155273	0.000000	0.000000	-0.162914	-0.169257
45	O	4	S	0.000000	-0.000664	0.155277	0.000000	0.000000
46	O	4	X	0.000000	0.058098	-0.144061	0.000000	0.000000
47	O	4	Y	0.000000	0.103851	0.242466	0.000000	0.000000
48	O	4	Z	0.244999	0.000000	0.000000	-0.251390	-0.254761
49	O	4	S	0.000000	-0.028383	0.176141	0.000000	0.000000
50	O	4	X	0.000000	0.039686	-0.087791	0.000000	0.000000
51	O	4	Y	0.000000	0.093913	0.241478	0.000000	0.000000
52	O	4	Z	0.217930	0.000000	0.000000	-0.260585	-0.313518
53	H	5	S	0.000000	0.153933	-0.020925	0.000000	0.000000
54	H	5	S	0.000000	0.231361	-0.015920	0.000000	0.000000
55	H	5	S	0.000000	0.074741	0.026330	0.000000	0.000000
56	H	6	S	-0.070731	-0.076056	0.053298	-0.119601	0.036232
57	H	6	S	-0.103576	-0.113008	0.085774	-0.177904	0.045295
58	H	6	S	-0.030492	-0.039608	0.025299	-0.053834	-0.000939
59	H	7	S	0.070731	-0.076056	0.053298	0.119601	-0.036232
60	H	7	S	0.103576	-0.113008	0.085774	0.177904	-0.045295
61	H	7	S	0.030492	-0.039608	0.025299	0.053834	0.000939
62	H	8	S	0.000000	0.011313	-0.092149	0.000000	0.000000
63	H	8	S	0.000000	0.027737	-0.125521	0.000000	0.000000
64	H	8	S	0.000000	0.008213	-0.026376	0.000000	0.000000

				16	17	18	19	20
				-0.4573	0.1457	0.1564	0.1754	0.2200
				A'	A'	A''	A'	A'
1	C	1	S	-0.010023	-0.035642	0.000000	-0.027218	0.004345
2	C	1	S	-0.018049	-0.058405	0.000000	-0.044106	0.006879
3	C	1	X	0.066918	-0.018925	0.000000	-0.059987	-0.030150
4	C	1	Y	-0.048521	-0.000737	0.000000	0.003926	-0.124712
5	C	1	Z	0.000000	0.000000	0.037379	0.000000	0.000000
6	C	1	S	0.049961	0.064672	0.000000	0.045677	-0.005216
7	C	1	X	0.145101	0.010637	0.000000	-0.078844	-0.019877
8	C	1	Y	-0.099624	-0.008087	0.000000	0.012498	-0.131515
9	C	1	Z	0.000000	0.000000	0.043032	0.000000	0.000000
10	C	1	S	0.155830	1.664835	0.000000	1.054582	-0.191272
11	C	1	X	0.093604	-0.160014	0.000000	-0.508771	-0.327623
12	C	1	Y	-0.064561	-0.141826	0.000000	0.117677	-1.178591
13	C	1	Z	0.000000	0.000000	0.526586	0.000000	0.000000
14	C	2	S	-0.009123	0.007054	0.000000	-0.002059	0.001534
15	C	2	S	-0.015973	0.012377	0.000000	-0.003035	0.002213
16	C	2	X	-0.056237	-0.007100	0.000000	0.011825	-0.013500
17	C	2	Y	0.006615	-0.018897	0.000000	0.010393	-0.013238
18	C	2	Z	0.000000	0.000000	0.196771	0.000000	0.000000
19	C	2	S	0.049558	-0.019239	0.000000	0.006836	0.004767
20	C	2	X	-0.077479	-0.018605	0.000000	0.062144	-0.036576
21	C	2	Y	0.033781	-0.039355	0.000000	0.018842	-0.034154
22	C	2	Z	0.000000	0.000000	0.362405	0.000000	0.000000
23	C	2	S	0.085830	-0.161751	0.000000	-0.068466	-0.138300
24	C	2	X	0.097433	0.298636	0.000000	-0.492626	0.022282
25	C	2	Y	0.081615	0.028691	0.000000	0.042134	-0.005851
26	C	2	Z	0.000000	0.000000	0.549418	0.000000	0.000000

27	O	3	S	0.001233	-0.009064	0.000000	-0.000998	0.002126
28	O	3	S	0.002231	-0.015409	0.000000	-0.001393	0.003873
29	O	3	X	0.249250	0.014144	0.000000	-0.036513	0.015160
30	O	3	Y	0.058328	0.006682	0.000000	-0.001335	-0.011070
31	O	3	Z	0.000000	0.000000	-0.142722	0.000000	0.000000
32	O	3	S	-0.010615	0.044252	0.000000	-0.004204	-0.013672
33	O	3	X	0.389240	0.025055	0.000000	-0.060313	0.021752
34	O	3	Y	0.094894	0.006927	0.000000	-0.000554	-0.022734
35	O	3	Z	0.000000	0.000000	-0.196747	0.000000	0.000000
36	O	3	S	0.016767	0.126337	0.000000	0.127432	-0.006646
37	O	3	X	0.380066	-0.010117	0.000000	-0.039141	0.042786
38	O	3	Y	0.098852	0.033807	0.000000	0.042241	-0.026864
39	O	3	Z	0.000000	0.000000	-0.421210	0.000000	0.000000
40	O	4	S	0.004952	-0.025879	0.000000	0.015472	-0.000713
41	O	4	S	0.008147	-0.043736	0.000000	0.026232	-0.001258
42	O	4	X	0.036548	0.046735	0.000000	-0.073651	-0.009256
43	O	4	Y	0.102203	-0.018113	0.000000	0.018333	-0.028707
44	O	4	Z	0.000000	0.000000	-0.092303	0.000000	0.000000
45	O	4	S	-0.007961	0.113616	0.000000	-0.068728	0.000221
46	O	4	X	0.066190	0.060623	0.000000	-0.092296	-0.021649
47	O	4	Y	0.174947	-0.050233	0.000000	0.046528	-0.042870
48	O	4	Z	0.000000	0.000000	-0.128628	0.000000	0.000000
49	O	4	S	-0.184628	0.477489	0.000000	-0.274789	0.037383
50	O	4	X	0.086219	0.168320	0.000000	-0.312879	-0.008366
51	O	4	Y	0.198675	0.009152	0.000000	-0.044582	-0.104463
52	O	4	Z	0.000000	0.000000	-0.258522	0.000000	0.000000
53	H	5	S	-0.039742	-0.001067	0.000000	-0.012581	0.028966
54	H	5	S	-0.083462	0.046614	0.000000	0.005329	-0.040238
55	H	5	S	-0.036785	-0.486906	0.000000	-0.578276	2.325029
56	H	6	S	-0.007059	-0.009169	0.051404	-0.005089	-0.011213
57	H	6	S	-0.013439	-0.025788	0.163438	0.051633	-0.000993
58	H	6	S	-0.027442	-0.750264	0.824411	-0.815936	-0.957069
59	H	7	S	-0.007059	-0.009169	-0.051404	-0.005089	-0.011213
60	H	7	S	-0.013439	-0.025788	-0.163438	0.051633	-0.000993
61	H	7	S	-0.027442	-0.750264	-0.824411	-0.815936	-0.957069
62	H	8	S	0.009666	-0.043430	0.000000	0.031044	-0.002220
63	H	8	S	0.026918	0.064291	0.000000	-0.056563	-0.044870
64	H	8	S	0.028949	-1.090733	0.000000	1.213575	0.001284

				21	22	23	24	25
				0.2321	0.3453	0.4094	0.4222	0.4651
				A' '	A'	A'	A'	A' '
1	C	1	S	0.000000	0.015801	0.005803	0.000688	0.000000
2	C	1	S	0.000000	0.022060	0.012708	-0.000660	0.000000
3	C	1	X	0.000000	-0.074767	-0.065874	0.000838	0.000000
4	C	1	Y	0.000000	0.024419	0.019083	-0.005049	0.000000
5	C	1	Z	0.126506	0.000000	0.000000	0.000000	0.031992
6	C	1	S	0.000000	0.090684	-0.069018	0.025646	0.000000
7	C	1	X	0.000000	-0.010310	-0.212347	0.097283	0.000000
8	C	1	Y	0.000000	0.003464	0.033000	-0.062076	0.000000
9	C	1	Z	0.125763	0.000000	0.000000	0.000000	-0.012801
10	C	1	S	0.000000	-2.190795	0.520628	0.094591	0.000000
11	C	1	X	0.000000	-2.420650	0.131343	-0.616539	0.000000
12	C	1	Y	0.000000	0.951423	0.307433	-0.499120	0.000000
13	C	1	Z	1.056642	0.000000	0.000000	0.000000	1.987859
14	C	2	S	0.000000	-0.051145	-0.017461	0.006093	0.000000
15	C	2	S	0.000000	-0.092154	-0.025355	0.007855	0.000000
16	C	2	X	0.000000	-0.082455	0.025881	-0.093260	0.000000
17	C	2	Y	0.000000	0.057848	-0.015922	-0.050601	0.000000
18	C	2	Z	-0.089956	0.000000	0.000000	0.000000	-0.081578
19	C	2	S	0.000000	0.241608	-0.141106	0.083635	0.000000
20	C	2	X	0.000000	-0.196677	0.082030	-0.267776	0.000000
21	C	2	Y	0.000000	0.145916	-0.108582	-0.071981	0.000000
22	C	2	Z	-0.149196	0.000000	0.000000	0.000000	-0.193333
23	C	2	S	0.000000	3.069812	2.812850	-0.885741	0.000000
24	C	2	X	0.000000	-1.636766	1.020201	-0.656196	0.000000

25	C	2	Y	0.000000	0.968396	-1.533139	-0.882512	0.000000
26	C	2	Z	-0.467038	0.000000	0.000000	0.000000	-0.725023
27	O	3	S	0.000000	-0.002245	0.044404	0.010142	0.000000
28	O	3	S	0.000000	-0.003017	0.072725	0.018010	0.000000
29	O	3	X	0.000000	0.020852	-0.001653	0.071613	0.000000
30	O	3	Y	0.000000	-0.025985	-0.067539	0.015468	0.000000
31	O	3	Z	0.088790	0.000000	0.000000	0.000000	0.046298
32	O	3	S	0.000000	-0.008366	-0.113977	-0.065641	0.000000
33	O	3	X	0.000000	0.008203	0.008544	0.096495	0.000000
34	O	3	Y	0.000000	-0.045020	-0.090679	0.024020	0.000000
35	O	3	Z	0.120925	0.000000	0.000000	0.000000	0.064953
36	O	3	S	0.000000	0.246311	-2.221009	-0.191465	0.000000
37	O	3	X	0.000000	0.222259	0.061061	0.280579	0.000000
38	O	3	Y	0.000000	0.015665	-0.876010	0.068240	0.000000
39	O	3	Z	0.283711	0.000000	0.000000	0.000000	0.206409
40	O	4	S	0.000000	0.007808	0.007611	-0.029561	0.000000
41	O	4	S	0.000000	0.013180	0.012612	-0.049644	0.000000
42	O	4	X	0.000000	0.043606	0.048085	-0.077644	0.000000
43	O	4	Y	0.000000	0.020090	0.066064	-0.030929	0.000000
44	O	4	Z	0.044258	0.000000	0.000000	0.000000	0.010698
45	O	4	S	0.000000	-0.029924	-0.022300	0.109895	0.000000
46	O	4	X	0.000000	0.042445	0.084303	-0.069836	0.000000
47	O	4	Y	0.000000	0.051266	0.075718	-0.038957	0.000000
48	O	4	Z	0.061344	0.000000	0.000000	0.000000	-0.017148
49	O	4	S	0.000000	-0.260353	-0.301927	0.974796	0.000000
50	O	4	X	0.000000	0.366826	0.233660	-0.666722	0.000000
51	O	4	Y	0.000000	-0.007390	0.478384	-0.343512	0.000000
52	O	4	Z	0.143216	0.000000	0.000000	0.000000	0.175919
53	H	5	S	0.000000	-0.029916	0.027916	0.058738	0.000000
54	H	5	S	0.000000	-0.351880	0.073228	0.857370	0.000000
55	H	5	S	0.000000	-0.048727	-0.230243	-0.444520	0.000000
56	H	6	S	-0.005852	-0.017341	-0.019581	-0.036047	0.046084
57	H	6	S	-0.185201	-0.113172	-0.000712	-0.601767	1.183550
58	H	6	S	1.731832	-0.234069	-0.166626	0.216130	-0.011773
59	H	7	S	0.005852	-0.017341	-0.019581	-0.036047	-0.046084
60	H	7	S	0.185201	-0.113172	-0.000712	-0.601767	-1.183550
61	H	7	S	-1.731832	-0.234069	-0.166626	0.216130	0.011773
62	H	8	S	0.000000	0.008357	-0.038821	-0.023451	0.000000
63	H	8	S	0.000000	-0.028732	-0.270877	0.025156	0.000000
64	H	8	S	0.000000	-0.024097	-0.339000	0.435469	0.000000

26
0.5268
A'

1	C	1	S	0.001441
2	C	1	S	0.003934
3	C	1	X	-0.018237
4	C	1	Y	-0.008465
5	C	1	Z	0.000000
6	C	1	S	-0.052896
7	C	1	X	-0.019334
8	C	1	Y	0.113480
9	C	1	Z	0.000000
10	C	1	S	0.420213
11	C	1	X	-0.618859
12	C	1	Y	-2.646689
13	C	1	Z	0.000000
14	C	2	S	-0.022671
15	C	2	S	-0.040060
16	C	2	X	0.087028
17	C	2	Y	0.077447
18	C	2	Z	0.000000
19	C	2	S	0.081536
20	C	2	X	0.199727
21	C	2	Y	0.202980
22	C	2	Z	0.000000

23	C	2	S	0.241484
24	C	2	X	1.636502
25	C	2	Y	2.698585
26	C	2	Z	0.000000
27	O	3	S	-0.006389
28	O	3	S	-0.006780
29	O	3	X	-0.025002
30	O	3	Y	-0.035168
31	O	3	Z	0.000000
32	O	3	S	-0.078674
33	O	3	X	0.014855
34	O	3	Y	-0.058257
35	O	3	Z	0.000000
36	O	3	S	1.347571
37	O	3	X	-0.534782
38	O	3	Y	0.178862
39	O	3	Z	0.000000
40	O	4	S	0.036322
41	O	4	S	0.061363
42	O	4	X	0.060155
43	O	4	Y	0.055176
44	O	4	Z	0.000000
45	O	4	S	-0.130841
46	O	4	X	0.081147
47	O	4	Y	0.060515
48	O	4	Z	0.000000
49	O	4	S	-1.765772
50	O	4	X	0.559415
51	O	4	Y	0.597406
52	O	4	Z	0.000000
53	H	5	S	0.005707
54	H	5	S	1.113639
55	H	5	S	0.458292
56	H	6	S	0.001799
57	H	6	S	-0.584999
58	H	6	S	-0.188516
59	H	7	S	0.001799
60	H	7	S	-0.584999
61	H	7	S	-0.188516
62	H	8	S	0.016285
63	H	8	S	0.214300
64	H	8	S	-0.560853

ENERGY COMPONENTS

WAVEFUNCTION NORMALIZATION =	1.0000000000
ONE ELECTRON ENERGY =	-551.9249602296
TWO ELECTRON ENERGY =	202.6457253526
NUCLEAR REPULSION ENERGY =	121.5183649393
TOTAL ENERGY =	-227.7608699377
ELECTRON-ELECTRON POTENTIAL ENERGY =	202.6457253526
NUCLEUS-ELECTRON POTENTIAL ENERGY =	-779.8280660418
NUCLEUS-NUCLEUS POTENTIAL ENERGY =	121.5183649393
TOTAL POTENTIAL ENERGY =	-455.6639757499
TOTAL KINETIC ENERGY =	227.9031058122
VIRIAL RATIO (V/T) =	1.9993758932

MULLIKEN AND LOWDIN POPULATION ANALYSES

MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL

	1	2	3	4	5
	2.000000	2.000000	2.000000	2.000000	2.000000
1	-0.000003	0.000010	0.000293	1.999615	0.018976
2	0.000096	0.000176	1.999674	0.000125	0.318151
3	-0.000001	1.999815	0.000016	-0.000001	0.583589
4	1.999906	-0.000001	0.000013	0.000001	1.026624
5	0.000003	0.000000	0.000000	0.000089	-0.001599
6	0.000000	0.000000	0.000005	0.000085	0.000250
7	0.000000	0.000000	0.000005	0.000085	0.000250
8	-0.000001	0.000000	-0.000008	0.000000	0.053759

	6	7	8	9	10
	2.000000	2.000000	2.000000	2.000000	2.000000
1	0.010513	1.169894	0.282028	0.209283	0.306691
2	0.214832	0.402255	0.375662	0.361533	0.519057
3	0.973041	0.062802	0.087402	0.966304	0.423841
4	0.754788	0.095226	0.862652	0.295830	0.642083
5	-0.000060	0.077626	0.025317	0.103432	0.039914
6	-0.000062	0.080334	0.061730	0.001695	0.031115
7	-0.000062	0.080334	0.061730	0.001695	0.031115
8	0.047011	0.031529	0.243480	0.060228	0.006184

	11	12	13	14	15
	2.000000	2.000000	2.000000	2.000000	2.000000
1	0.347757	0.888719	0.364084	0.731787	0.055313
2	0.514282	0.064454	0.251975	0.030740	0.156634
3	0.292516	0.205916	0.326549	0.037669	1.127035
4	0.621934	0.109229	0.812207	0.628316	0.623584
5	0.000000	0.489877	0.007314	0.000000	0.000000
6	0.111755	0.118936	0.062518	0.285744	0.018718
7	0.111755	0.118936	0.062518	0.285744	0.018718
8	0.000000	0.003933	0.112836	0.000000	0.000000

	16
	2.000000
1	0.203518
2	0.099159
3	1.414730
4	0.218592
5	0.040213
6	0.004962
7	0.004962
8	0.013864

----- POPULATIONS IN EACH AO -----

			MULLIKEN	LOWDIN
1	C	1 S	1.10317	1.04656
2	C	1 S	0.89078	0.92843
3	C	1 X	0.18893	0.19405
4	C	1 Y	0.20950	0.21433
5	C	1 Z	0.20689	0.21091
6	C	1 S	0.74588	0.57652
7	C	1 X	0.54586	0.53707
8	C	1 Y	0.58869	0.54747
9	C	1 Z	0.58466	0.54304

10	C	1	S	0.71784	0.36640
11	C	1	X	0.16533	0.32317
12	C	1	Y	0.29764	0.35881
13	C	1	Z	0.34331	0.38235
14	C	2	S	1.10390	1.04726
15	C	2	S	0.89008	0.92684
16	C	2	X	0.21009	0.21696
17	C	2	Y	0.22819	0.23585
18	C	2	Z	0.11795	0.11993
19	C	2	S	0.84304	0.58238
20	C	2	X	0.57200	0.55051
21	C	2	Y	0.52666	0.52077
22	C	2	Z	0.35530	0.32756
23	C	2	S	0.12673	0.29934
24	C	2	X	0.11823	0.27956
25	C	2	Y	-0.01176	0.28519
26	C	2	Z	0.22840	0.27544
27	O	3	S	1.08366	1.03187
28	O	3	S	0.91208	0.95183
29	O	3	X	0.36776	0.37760
30	O	3	Y	0.28754	0.28892
31	O	3	Z	0.26372	0.26831
32	O	3	S	1.00921	0.91376
33	O	3	X	0.80937	0.81114
34	O	3	Y	0.66874	0.67892
35	O	3	Z	0.61459	0.60818
36	O	3	S	0.92099	0.69989
37	O	3	X	0.60954	0.63517
38	O	3	Y	0.37512	0.50220
39	O	3	Z	0.57891	0.58118
40	O	4	S	1.08351	1.03129
41	O	4	S	0.91222	0.95143
42	O	4	X	0.25037	0.25577
43	O	4	Y	0.32245	0.32957
44	O	4	Z	0.36060	0.36837
45	O	4	S	0.98499	0.89648
46	O	4	X	0.64971	0.60676
47	O	4	Y	0.74606	0.74633
48	O	4	Z	0.78564	0.79883
49	O	4	S	0.92816	0.64661
50	O	4	X	0.35480	0.42901
51	O	4	Y	0.58487	0.60558
52	O	4	Z	0.72760	0.68975
53	H	5	S	0.27453	0.28384
54	H	5	S	0.45160	0.44419
55	H	5	S	0.05599	0.17273
56	H	6	S	0.27153	0.28018
57	H	6	S	0.44892	0.43984
58	H	6	S	0.05734	0.16995
59	H	7	S	0.27153	0.28018
60	H	7	S	0.44892	0.43984
61	H	7	S	0.05734	0.16995
62	H	8	S	0.27505	0.27447
63	H	8	S	0.26319	0.32464
64	H	8	S	0.03458	0.11874

----- MULLIKEN ATOMIC OVERLAP POPULATIONS -----
(OFF-DIAGONAL ELEMENTS NEED TO BE MULTIPLIED BY 2)

	1	2	3	4	5
1	5.5605606				
2	0.1307942	4.5941509			
3	-0.0987037	0.5481214	8.1557223		
4	-0.1178773	0.1694721	-0.1191436	8.4851503	
5	0.3570326	-0.0352651	0.0038882	0.0094573	0.4860898

6	0.3737189	-0.0368583	0.0031864	0.0033554	-0.0192373
7	0.3737189	-0.0368583	0.0031864	0.0033554	-0.0192373
8	0.0092346	-0.0247508	0.0049660	0.2572119	-0.0006014

	6		7		8
6	0.4706867				
7	-0.0166428	0.4706867			
8	-0.0004249	-0.0004249	0.3276051		

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 C	6.588479	-0.588479	6.229117	-0.229117
2 C	5.308806	0.691194	5.667585	0.332415
3 O	8.501223	-0.501223	8.348981	-0.348981
4 O	8.690981	-0.690981	8.355768	-0.355768
5 H	0.782127	0.217873	0.900755	0.099245
6 H	0.777784	0.222216	0.889969	0.110031
7 H	0.777784	0.222216	0.889969	0.110031
8 H	0.572816	0.427184	0.717854	0.282146

BOND ORDER AND VALENCE ANALYSIS

BOND ORDER THRESHOLD=0.050

ATOM PAIR DIST	BOND ORDER	ATOM PAIR DIST	BOND ORDER	ATOM PAIR DIST	BOND ORDER
1 2 1.489	0.826	1 5 1.075	0.929	1 6 1.080	0.934
1 7 1.080	0.934	2 3 1.210	1.873	2 4 1.350	0.894
4 8 0.950	0.770				

ATOM	TOTAL VALENCE	BONDED VALENCE	FREE VALENCE
1 C	3.574	3.574	0.000
2 C	3.560	3.560	0.000
3 O	1.896	1.896	0.000
4 O	1.646	1.646	0.000
5 H	0.918	0.918	0.000
6 H	0.918	0.918	0.000
7 H	0.918	0.918	0.000
8 H	0.809	0.809	0.000

ELECTROSTATIC MOMENTS

POINT	1	X	Y	Z (BOHR)	CHARGE
		-0.090873	-0.184560	0.000000	0.00 (A.U.)
		DX	DY	DZ	/D/ (DEBYE)
		-0.574824	1.804849	0.000000	1.894176

..... END OF PROPERTY EVALUATION

CPU	TIME:	STEP =	0.14 ,	TOTAL =	137.4 SECONDS (2.3 MIN)
WALL CLOCK TIME:	STEP =	0.14 ,	TOTAL =	156.1 SECONDS (2.6 MIN)	
CPU UTILIZATION:	STEP =	100.00%,	TOTAL =	88.00%		

.....END OF NBO ANALYSIS.....

CPU	TIME:	STEP =	0.00 ,	TOTAL =	137.4 SECONDS (2.3 MIN)
WALL CLOCK TIME:	STEP =	0.00 ,	TOTAL =	156.1 SECONDS (2.6 MIN)	
CPU UTILIZATION:	STEP =	100.00%,	TOTAL =	88.00%		

\$VIB

IVIB=	0	IATOM=	0	ICOORD=	0	E=	-227.7608699377
-1.708715793E-05	4.125613396E-05	0.0000000000E+00	-2.081452500E-05	4.658639815E-06			

0.000000000E+00 3.007717889E-05-3.382485258E-05 0.000000000E+00 2.345257770E-05
-3.185653102E-05 0.000000000E+00 6.249756707E-06 4.758929338E-05 0.000000000E+00
-3.191904729E-06-2.570307294E-05 3.959330710E-05-3.191904729E-06-2.570307294E-05
-3.959330710E-05-1.549401671E-05 2.358346195E-05 0.000000000E+00
-5.748243418E-01 1.804849229E+00-2.257541709E-15
.....END OF GEOMETRY SEARCH.....

CPU	TIME:	STEP =	0.00 ,	TOTAL =	137.4 SECONDS (2.3 MIN)
WALL CLOCK TIME:	STEP =	0.01 ,	TOTAL =	156.1 SECONDS (2.6 MIN)	
CPU UTILIZATION:	STEP =	0.00%,	TOTAL =	87.99%		

AN INPUT FILE FOR -PLTORB- HAS BEEN PUNCHED.

100000 WORDS OF DYNAMIC MEMORY USED
EXECUTION OF GAMESS TERMINATED NORMALLY 10:01:55 LT 3-JUL-1999