

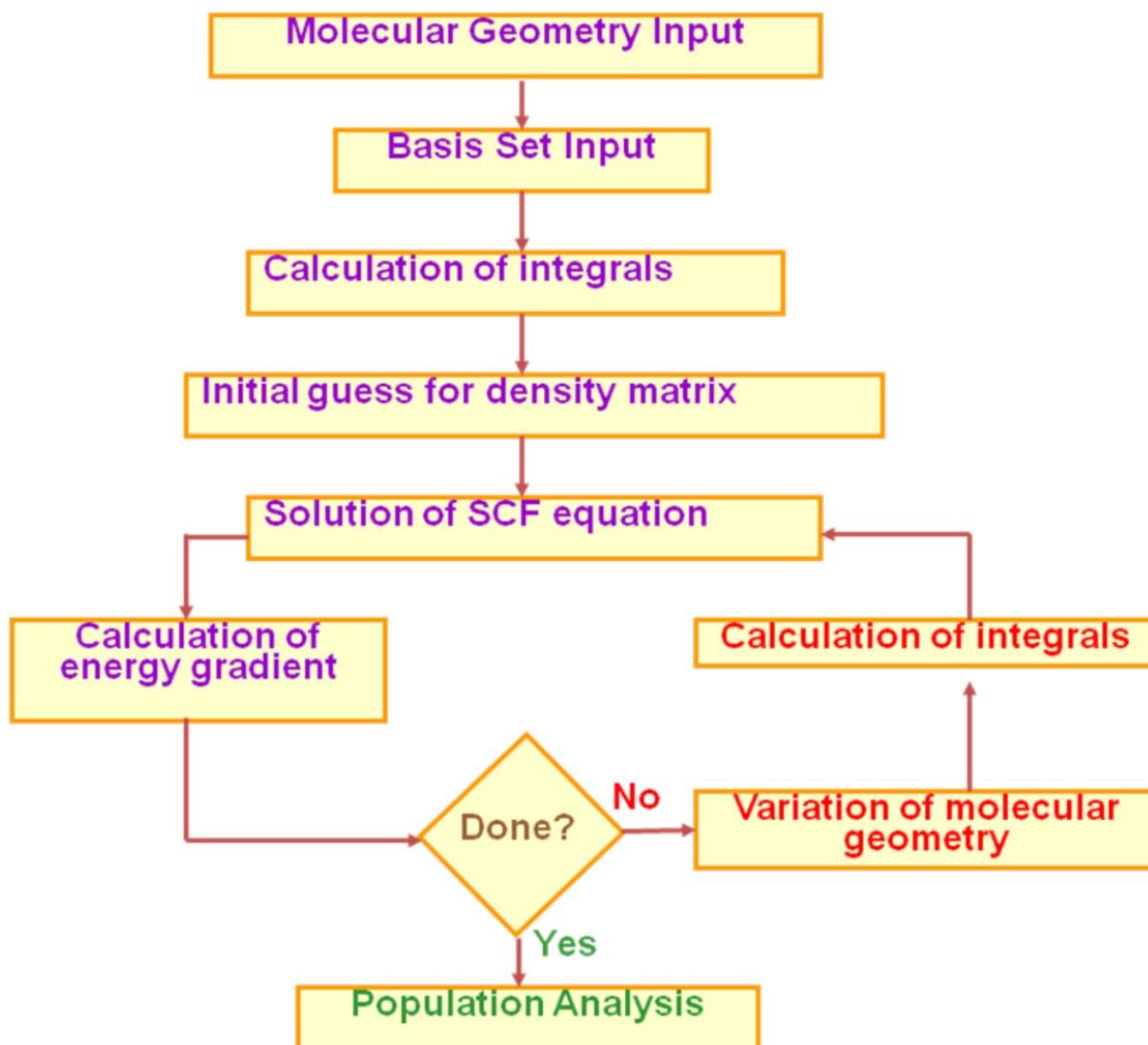
Hartree-Fock Theory and Geometry Optimization

Keywords: Ab initio, Hartree-Fock theory, geometry optimization.

In chapter 18, it is discussed on downloading 'GAMESS' and implementing it on a linux box. Making of an INPUT file for a HF calculation with appropriate atomic basis functions is also described. Examples are provided to run for energy calculation under Hartree-Fock theory applying GAMESS suit of program and the results in the OUTPUT file are discussed in detail. Now we will move to examples where energy calculations are carried out with varying geometrical parameters. This is carried out in a job for geometry optimization to find out the ground state structure of a molecule with minimum total energy. A function which has minima, its gradient or first derivative should be zero for certain values of variables of the function. A job where 'geometry optimization' is carried out, looks for the geometrical variables where calculated total energy of the system is the minimum. This essentially suggests that one has to calculate energy gradient for each steps of 'geometry optimization' job and look for the geometrical variables where the calculated gradient is zero or less than equal to a preset value. Once the preset limit of energy gradient is achieved, geometry optimization is completed and the job ends after calculating property of the molecule at those optimized geometrical parameters. Based on chemical intuition, if one supplies good geometrical parameters, this job takes less number of optimization steps to reach the minimum energy structure. As a result, the job gets completed in a shorter time compared to a job that needs more optimization steps to achieve preset cutoff energy gradient values. So, one has to be careful before supplying initial geometrical parameters of the molecule to make use of compute time efficiently. For a molecule where many conformers may exist, the final optimized geometry is the conformer that has the closest geometrical parameters with the initial geometrical parameters in the INPUT. Thus, often one has to perform several geometry optimizations considering various initial INPUT geometrical parameters to obtain geometrical parameters of all possible conformers of the molecular system.

A typical flow chart for geometry optimization in an *ab initio* calculation is as follows:

Flow Chart for Steps of Geometry Optimization



Now, we move to the description of an INPUT file for geometry optimization to run in GAMESS. We take up the same example of input file for single point energy calculation of H₂O molecule and modify it for geometry optimization. So, the following INPUT is for geometry optimization at 'Restricted Hartree Fock' level of theory with 6-31G(d,p) atomic basis functions for neutral water molecule.

```

$SYSTEM TIMLIM=600.0 MWORDS=10 MEMDDI=40 $END
$CONTRL SCFTYP=RHF ICHARG=0 MULT=1 RUNTYP=OPTIMIZE COORD=ZMT $END
$BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 $END
$DATA
Water-Geometry // RHF/6-31G(d,p)
CN 1

O
H 1 roh
H 1 roh 2 ahoh

roh=1.08
ahoh=109.5
$END

```

Note that the only change made is in the keyword 'RUNTYP' of group 'CONTRL'. The output is displayed in the following pages.

```

----- GAMESS execution script -----
This job is running on host dkml03.barc.gov.in
under operating system Linux at Fri Mar 16 13:45:47 EDT 2012
Available scratch disk space (Kbyte units) at beginning of the job is
The generated host list is
dkml03:cpus=8

```

Distributed Data Interface kickoff program.
Initiating 8 compute processes on 1 nodes to run the following command:
/home/dilip/gamess/gamess.11.adhya.socket.x water-hf-opt

```

*****
*           GAMESS VERSION =  1 OCT 2010 (R1)           *
*           FROM IOWA STATE UNIVERSITY                 *
* M.W.SCHMIDT, K.K.BALDRIDGE, J.A.BOATZ, S.T.ELBERT, *
* M.S.GORDON, J.H.JENSEN, S.KOSEKI, N.MATSUNAGA,     *
*           K.A.NGUYEN, S.J.SU, T.L.WINDUS,           *
*           TOGETHER WITH M.DUPOUIS, J.A.MONTGOMERY   *
*           J.COMPUT.CHEM.  14, 1347-1363(1993)       *
***** 64 BIT INTEL VERSION *****

```

SINCE 1993, STUDENTS AND POSTDOCS WORKING AT IOWA STATE UNIVERSITY AND ALSO IN THEIR VARIOUS JOBS AFTER LEAVING ISU HAVE MADE IMPORTANT CONTRIBUTIONS TO THE CODE:

IVANA ADAMOVIC, CHRISTINE AIKENS, YURI ALEXEEV, POOJA ARORA,
ANDREY ASADCHEV, ROB BELL, PRADIPTA BANDYOPADHYAY, JONATHAN BENTZ,
BRETT BODE, GALINA CHABAN, WEI CHEN, CHEOL HO CHOI, PAUL DAY, TIM
DUDLEY, DMITRI FEDOROV, GRAHAM FLETCHER, MARK FREITAG, KURT GLAESEMANN,
DAN KEMP, GRANT MERRILL, NORIYUKI MINEZAWA, JONATHAN MULLIN, TAKESHI

COMPUTATIONAL CHEMISTRY II

NAGATA, SEAN NEDD, HEATHER NETZLOFF, BOSILJKA NJEGIC, RYAN OLSON, MIKE PAK, JIM SHOEMAKER, LYUDMILA SLIPCHENKO, SAROM SOK, JIE SONG, TETSUYA TAKETSUGU, SIMON WEBB, SOOHAENG YOO, FEDERICO ZAHARIEV

ADDITIONAL CODE HAS BEEN PROVIDED BY COLLABORATORS IN OTHER GROUPS:
IOWA STATE UNIVERSITY: JOE IVANIC, LAIMUTIS BYTAUTAS, KLAUS RUEDENBERG
UNIVERSITY OF TOKYO: KIMIHICO HIRAO, TAKAHITO NAKAJIMA, TAKAO TSUNEDA, MUNEAKI KAMIYA, SUSUMU YANAGISAWA, KIYOSHI YAGI, MAHITO CHIBA, SEIKEN TOKURA, NAOAKI KAWAKAMI
UNIVERSITY OF AARHUS: FRANK JENSEN
UNIVERSITY OF IOWA: VISVALDAS KAIRYS, HUI LI
NATIONAL INST. OF STANDARDS AND TECHNOLOGY: WALT STEVENS, DAVID GARMER
UNIVERSITY OF PISA: BENEDETTA MENNUCCI, JACOPO TOMASI
UNIVERSITY OF MEMPHIS: HENRY KURTZ, PRAKASHAN KORAMBATH
UNIVERSITY OF ALBERTA: TOBY ZENG, MARIUSZ KLOBUKOWSKI
UNIVERSITY OF NEW ENGLAND: MARK SPACKMAN
MIE UNIVERSITY: HIROAKI UMEDA
MICHIGAN STATE UNIVERSITY: KAROL KOWALSKI, MARTA WLOCH, JEFFREY GOUR, JESSE LUTZ, PIOTR PIECUCH
UNIVERSITY OF SILESIA: MONIKA MUSIAL, STANISLAW KUCHARSKI
FACULTES UNIVERSITAIRES NOTRE-DAME DE LA PAIX: OLIVIER QUINET, BENOIT CHAMPAGNE
UNIVERSITY OF CALIFORNIA - SANTA BARBARA: BERNARD KIRTMAN
INSTITUTE FOR MOLECULAR SCIENCE: KAZUYA ISHIMURA, MICHIO KATOUDA, AND SHIGERU NAGASE
UNIVERSITY OF NOTRE DAME: DAN CHIPMAN
KYUSHU UNIVERSITY: HARUYUKI NAKANO, FENG LONG GU, JACEK KORCHOWIEC, MARCIN MAKOWSKI, AND YURIKO AOKI, HIROTOSHI MORI AND EISAKU MIYOSHI
PENNSYLVANIA STATE UNIVERSITY: TZVETELIN IORDANOV, CHET SWALINA, JONATHAN SKONE, SHARON HAMMES-SCHIFFER
WASEDA UNIVERSITY: MASATO KOBAYASHI, TOMOKO AKAMA, HIROMI NAKAI
UNIVERSITY OF NEBRASKA: PEIFENG SU, DEJUN SI, YALI WANG, HUI LI
UNIVERSITY OF ZURICH: ROBERTO PEVERATI, KIM BALDRIDGE
N. COPERNICUS UNIVERSITY AND JACKSON STATE UNIVERSITY: MARIA BARYSZ

PARALLEL VERSION RUNNING ON 8 PROCESSORS IN 1 NODES.

EXECUTION OF GAMESS BEGUN Fri Mar 16 13:45:48 2012

ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD> \$SYSTEM TIMLIM=600.0 MWORDS=10 MEMDDI=40 \$END
INPUT CARD> \$CONTRL SCFTYP=RHF ICHARG=0 MULT=1 RUNTYP=OPTIMIZE COORD=ZMT \$END
INPUT CARD> \$BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 \$END
INPUT CARD> \$DATA
INPUT CARD> Water-Energy//RHF/6-31G(d,p)
INPUT CARD> CN 1
INPUT CARD>
INPUT CARD> O
INPUT CARD> H 1 roh
INPUT CARD> H 1 roh 2 ahoh
INPUT CARD>
INPUT CARD> roh=1.08
INPUT CARD> ahoh=109.5
INPUT CARD> \$END
INPUT CARD>
INPUT CARD>

COMPUTATIONAL CHEMISTRY II

10000000 WORDS OF MEMORY AVAILABLE

BASIS OPTIONS

GBASIS=N31 IGAUSS= 6 POLAR=POP31
 NDFUNC= 1 NFFUNC= 0 DIFFSP= F
 NPFUNC= 1 DIFFS= F BASNAM=

RUN TITLE

Water-Energy//RHF/6-31G(d,p)

THE POINT GROUP OF THE MOLECULE IS CN
 THE ORDER OF THE PRINCIPAL AXIS IS 1

YOUR FULLY SUBSTITUTED Z-MATRIX IS

O
 H 1 1.0800000
 H 1 1.0800000 2 109.5000

THE MOMENTS OF INERTIA ARE (AMU-ANGSTROM**2)
 IXX= 0.695 IYY= 1.568 IZZ= 2.263

ATOM	ATOMIC CHARGE	COORDINATES (BOHR)		
		X	Y	Z
O	8.0	0.0000000000	-0.1318243316	0.0000000000
H	1.0	1.6666870710	1.0460736338	0.0000000000
H	1.0	-1.6666870710	1.0460736338	0.0000000000

INTERNUCLEAR DISTANCES (ANGS.)

	1 O	2 H	3 H
1 O	0.0000000	1.0800000 *	1.0800000 *
2 H	1.0800000 *	0.0000000	1.7639458 *
3 H	1.0800000 *	1.7639458 *	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	PRIMITIVE	EXPONENT	CONTRACTION COEFFICIENT(S)
O			
1 S	1	5484.6716600	0.001831074430
1 S	2	825.2349460	0.013950172200
1 S	3	188.0469580	0.068445078098
1 S	4	52.9645000	0.232714335992
1 S	5	16.8975704	0.470192897984
1 S	6	5.7996353	0.358520852987

COMPUTATIONAL CHEMISTRY II

2	L	7	15.5396162	-0.110777549525	0.070874268231
2	L	8	3.5999336	-0.148026262701	0.339752839147
2	L	9	1.0137618	1.130767015354	0.727158577316
3	L	10	0.2700058	1.000000000000	1.000000000000
4	D	11	0.8000000	1.000000000000	

H

5	S	12	18.7311370	0.033494604338	
5	S	13	2.8253944	0.234726953484	
5	S	14	0.6401217	0.813757326146	
6	S	15	0.1612778	1.000000000000	
7	P	16	1.1000000	1.000000000000	

H

8	S	17	18.7311370	0.033494604338	
8	S	18	2.8253944	0.234726953484	
8	S	19	0.6401217	0.813757326146	
9	S	20	0.1612778	1.000000000000	
10	P	21	1.1000000	1.000000000000	

TOTAL NUMBER OF BASIS SET SHELLS = 10
 NUMBER OF CARTESIAN GAUSSIAN BASIS FUNCTIONS = 25
 NUMBER OF ELECTRONS = 10
 CHARGE OF MOLECULE = 0
 SPIN MULTIPLICITY = 1
 NUMBER OF OCCUPIED ORBITALS (ALPHA) = 5
 NUMBER OF OCCUPIED ORBITALS (BETA) = 5
 TOTAL NUMBER OF ATOMS = 3
 THE NUCLEAR REPULSION ENERGY IS 8.1396592790

\$CONTRL OPTIONS

```

SCFTYP=RHF          RUNTYP=OPTIMIZE      EXETYP=RUN
MPLEVL=             0          CITYP =NONE      CCTYP =NONE      VBTYP =NONE
DFTTYP=NONE        TDDFT =NONE
MULT =              1          ICHARG=          0          NZVAR =          0          COORD =ZMT
PP =NONE           RELWFN=NONE          LOCAL =NONE      NUMGRD=          F
ISPHER=            -1          NOSYM =          0          MAXIT =          30         UNITS =ANGS
PLTORB=             F          MOLPLT=          F          AIMPAC=          F          FRIEND=
NPRINT=             7          IREST =          0          GEOM =INPUT
NORMF =             0          NORMP =          0          ITOL =           20         ICUT  =          9
INTTYP=BEST        GRDTYP=BEST          QMTTOL= 1.0E-06
    
```

\$SYSTEM OPTIONS

```

REPLICATED MEMORY= 10000000 WORDS (ON EVERY NODE).
DISTRIBUTED MEMDDI= 40 MILLION WORDS IN AGGREGATE,
MEMDDI DISTRIBUTED OVER 8 PROCESSORS IS 5000000 WORDS/PROCESSOR.
TOTAL MEMORY REQUESTED ON EACH PROCESSOR= 15000000 WORDS.
TIMLIM= 600.00 MINUTES, OR 0.4 DAYS.
    
```

COMPUTATIONAL CHEMISTRY II

PARALL= T BALYP= DLB KDIAG= 0 COREFL= F
 MXSEQ2= 300 MXSEQ3= 150

 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
 ORBITAL PRINTING OPTION: NPRES= 1 25 2 1

 INTEGRAL TRANSFORMATION OPTIONS

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

 INTEGRAL INPUT OPTIONS

NOPK = 1 NORDER= 0 SCHWRZ= F

--- ENCODED Z MATRIX ---

COORD	TYPE	I	J	K	L	M	N
1	1	2	1				
2	1	3	1				
3	2	3	1	2			

THE DETERMINANT OF THE G MATRIX IS 10**(-1)

 THE POINT GROUP IS CN , NAXIS= 1, ORDER= 1

DIMENSIONS OF THE SYMMETRY SUBSPACES ARE
 A = 25

..... DONE SETTING UP THE RUN
 CPU 0: STEP CPU TIME= 0.03 TOTAL CPU TIME= 0.0 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 0.1 SECONDS, CPU UTILIZATION IS 50.00%

Upto this point, GAMESS produces same output as in case of energy calculation.

 STATIONARY POINT LOCATION RUN

OBTAINING INITIAL HESSIAN, HESS=GUESS
 CARTESIAN COORDINATE OPTIMIZATION USING BADGER'S RULE FORCE CONSTANT GUESS

```

PARAMETERS CONTROLLING GEOMETRY SEARCH ARE
METHOD =QA                      UPHESS =BFGS
NNEG   =      0                  NFRZ   =      0
NSTEP  =      50                 IFOLOW =      1
HESS   =GUESS                   RESTAR =      F
IHREP  =      0                  HSSEND =      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
    
```

These are the default options for geometry optimization

One may wish to change METHOD, NSTEP & OPTTOL. NSTEP is the upper limit for number of steps & OPTTOL may be varied to calculate a rough or more accurate energy surface by putting values 1.000E-03 or 1.000E-05 respectively.

BEGINNING GEOMETRY SEARCH POINT NSERCH= 0 ...

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
O	8.0	0.0000000000	-0.0697584372	0.0000000000
H	1.0	0.8819728796	0.5535583681	0.0000000000
H	1.0	-0.8819728796	0.5535583681	0.0000000000

THE CURRENT FULLY SUBSTITUTED Z-MATRIX IS

O			
H	1	1.0800000	
H	1	1.0800000	2 109.5000000

These are the initial geometry parameters

```

*****
1 ELECTRON INTEGRALS
*****
    
```

..... END OF ONE-ELECTRON INTEGRALS

```

CPU      0: STEP CPU TIME=      0.00 TOTAL CPU TIME=      0.0 (      0.0 MIN)
TOTAL WALL CLOCK TIME=      0.2 SECONDS, CPU UTILIZATION IS 18.75%
    
```

GUESS OPTIONS

```

GUESS =HUCKEL          NORB  =      0          NORDER=      0
MIX    =      F        PRTMO =      F          PUNMO  =      F
TOLZ   = 1.0E-08      TOLE  = 1.0E-05
SYMDEN=      F        PURIFY=      F
    
```

INITIAL GUESS ORBITALS GENERATED BY HUCKEL ROUTINE.
HUCKEL GUESS REQUIRES 6979 WORDS.

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

```

5 ORBITALS ARE OCCUPIED (      1 CORE ORBITALS).
2=A      3=A      4=A      5=A      6=A      7=A      8=A
9=A      10=A     11=A     12=A     13=A     14=A     15=A
    
```

COMPUTATIONAL CHEMISTRY II

..... END OF INITIAL ORBITAL SELECTION

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.0 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 0.2 SECONDS, CPU UTILIZATION IS 13.04%

 AO INTEGRAL TECHNOLOGY

S,P,L SHELL ROTATED AXIS INTEGRALS, REPROGRAMMED BY
 KAZUYA ISHIMURA (IMS) AND JOSE SIERRA (SYNSTAR).
 S,P,D,L SHELL ROTATED AXIS INTEGRALS PROGRAMMED BY
 KAZUYA ISHIMURA (INSTITUTE FOR MOLECULAR SCIENCE).
 S,P,D,F,G SHELL TO TOTAL QUARTET ANGULAR MOMENTUM SUM 5,
 ERIC PROGRAM BY GRAHAM FLETCHER (ELORET AND NASA ADVANCED
 SUPERCOMPUTING DIVISION, AMES RESEARCH CENTER).
 S,P,D,F,G,L SHELL GENERAL RYS QUADRATURE PROGRAMMED BY
 MICHEL DUPUIS (PACIFIC NORTHWEST NATIONAL LABORATORY).

 2 ELECTRON INTEGRALS

THE -PK- OPTION IS OFF, THE INTEGRALS ARE NOT IN SUPERMATRIX FORM.
 STORING 15000 INTEGRALS/RECORD ON DISK, USING 12 BYTES/INTEGRAL.
 TWO ELECTRON INTEGRAL EVALUATION REQUIRES 90451 WORDS OF MEMORY.

II,JST,KST,LST = 1 1 1 1 NREC = 1 INTLOC = 1
 II,JST,KST,LST = 2 1 1 1 NREC = 1 INTLOC = 1
 II,JST,KST,LST = 3 1 1 1 NREC = 1 INTLOC = 2
 II,JST,KST,LST = 4 1 1 1 NREC = 1 INTLOC = 55
 II,JST,KST,LST = 5 1 1 1 NREC = 1 INTLOC = 55
 II,JST,KST,LST = 6 1 1 1 NREC = 1 INTLOC = 220
 II,JST,KST,LST = 7 1 1 1 NREC = 1 INTLOC = 220
 II,JST,KST,LST = 8 1 1 1 NREC = 1 INTLOC = 1031
 II,JST,KST,LST = 9 1 1 1 NREC = 1 INTLOC = 1304
 II,JST,KST,LST = 10 1 1 1 NREC = 1 INTLOC = 1588

TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 25620

8 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU 0: STEP CPU TIME= 0.02 TOTAL CPU TIME= 0.0 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 0.3 SECONDS, CPU UTILIZATION IS 18.52%

 RHF SCF CALCULATION

NUCLEAR ENERGY = 8.1396592790
 MAXIT = 30 NPUNCH= 2
 EXTRAP=T DAMP=F SHIFT=F RSTRCT=F DIIS=F DEM=F SOSCF=T
 DENSITY MATRIX CONV= 1.00E-05
 SOSCF WILL OPTIMIZE 100 ORBITAL ROTATIONS, SOGTOL= 0.250
 MEMORY REQUIRED FOR RHF ITERS= 35125 WORDS.

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
1	0	0	-75.7578553061	-75.7578553061	0.209790063	0.000000000
-----START SECOND ORDER SCF-----						
2	1	0	-75.9776712959	-0.2198159897	0.060105249	0.055579571
3	2	0	-75.9898226716	-0.0121513757	0.036044572	0.012329435
4	3	0	-75.9911251216	-0.0013024500	0.008480690	0.006920777
5	4	0	-75.9912714182	-0.0001462966	0.001806672	0.002252616

COMPUTATIONAL CHEMISTRY II

6	5	0	-75.9912902644	-0.0000188462	0.001544622	0.000526249
7	6	0	-75.9912928398	-0.0000025753	0.000095376	0.000061739
8	7	0	-75.9912928561	-0.0000000163	0.000027725	0.000016646
9	8	0	-75.9912928568	-0.0000000007	0.000007368	0.000003064
10	9	0	-75.9912928569	0.0000000000	0.000001111	0.000000614

 DENSITY CONVERGED

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

FINAL RHF ENERGY IS -75.9912928569 AFTER 10 ITERATIONS

 EIGENVECTORS

				1	2	3	4	5
				-20.5781	-1.2830	-0.6497	-0.5374	-0.4882
				A	A	A	A	A
1	O	1	S	0.994767	-0.213706	0.000000	0.065290	0.000000
2	O	1	S	0.020762	0.486905	0.000000	-0.146234	0.000000
3	O	1	X	0.000000	0.000000	0.483992	0.000000	0.000000
4	O	1	Y	0.001262	0.057821	0.000000	0.546864	0.000000
5	O	1	Z	0.000000	0.000000	0.000000	0.000000	0.642629
6	O	1	S	0.003837	0.463759	0.000000	-0.302230	0.000000
7	O	1	X	0.000000	0.000000	0.295897	0.000000	0.000000
8	O	1	Y	-0.000437	0.034045	0.000000	0.400541	0.000000
9	O	1	Z	0.000000	0.000000	0.000000	0.000000	0.500932
10	O	1	XX	-0.003999	0.010757	0.000000	0.004221	0.000000
11	O	1	YY	-0.003897	0.008641	0.000000	0.034207	0.000000
12	O	1	ZZ	-0.003712	0.001011	0.000000	-0.008318	0.000000
13	O	1	XY	0.000000	0.000000	0.033087	0.000000	0.000000
14	O	1	XZ	0.000000	0.000000	0.000000	0.000000	0.000000
15	O	1	YZ	0.000000	0.000000	0.000000	0.000000	0.023861
16	H	2	S	0.000317	0.112181	0.225091	0.144810	0.000000
17	H	2	S	-0.000210	0.017898	0.156445	0.123400	0.000000
18	H	2	X	0.000051	-0.016944	-0.013432	-0.014117	0.000000
19	H	2	Y	0.000060	-0.010819	-0.016001	0.004091	0.000000
20	H	2	Z	0.000000	0.000000	0.000000	0.000000	0.017204
21	H	3	S	0.000317	0.112181	-0.225091	0.144810	0.000000
22	H	3	S	-0.000210	0.017898	-0.156445	0.123400	0.000000
23	H	3	X	-0.000051	0.016944	-0.013432	0.014117	0.000000
24	H	3	Y	0.000060	-0.010819	0.016001	0.004091	0.000000
25	H	3	Z	0.000000	0.000000	0.000000	0.000000	0.017204

				6	7	8	9	10
				0.1812	0.2705	0.9752	0.9775	1.1356
				A	A	A	A	A
1	O	1	S	-0.096688	0.000000	0.000000	0.031408	-0.024856
2	O	1	S	0.078577	0.000000	0.000000	-0.337578	-0.898240
3	O	1	X	0.000000	-0.361760	0.261342	0.000000	0.000000
4	O	1	Y	0.255523	0.000000	0.000000	-0.338322	0.709469
5	O	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
6	O	1	S	1.161540	0.000000	0.000000	0.680835	1.741220

COMPUTATIONAL CHEMISTRY II

7	O	1	X	0.000000	-0.793690	0.020189	0.000000	0.000000
8	O	1	Y	0.496642	0.000000	0.000000	0.154161	-0.745241
9	O	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
10	O	1	XX	-0.049288	0.000000	0.000000	0.165562	-0.327593
11	O	1	YY	-0.035555	0.000000	0.000000	-0.048815	-0.349301
12	O	1	ZZ	-0.057267	0.000000	0.000000	-0.193437	-0.318957
13	O	1	XY	0.000000	-0.020832	-0.251328	0.000000	0.000000
14	O	1	XZ	0.000000	0.000000	0.000000	0.000000	0.000000
15	O	1	YZ	0.000000	0.000000	0.000000	0.000000	0.000000
16	H	2	S	-0.088086	0.072985	-0.796539	0.769567	0.117540
17	H	2	S	-0.931551	1.163937	0.822048	-0.717852	-0.230268
18	H	2	X	-0.001354	-0.006412	-0.042271	0.125061	-0.039305
19	H	2	Y	0.001961	0.000763	-0.091287	0.027756	-0.054821
20	H	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
21	H	3	S	-0.088086	-0.072985	0.796539	0.769567	0.117540
22	H	3	S	-0.931551	-1.163937	-0.822048	-0.717852	-0.230268
23	H	3	X	0.001354	-0.006412	-0.042271	-0.125061	0.039305
24	H	3	Y	0.001961	-0.000763	0.091287	0.027756	-0.054821
25	H	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000

				11	12	13	14	15
				1.1692	1.3064	1.3755	1.7915	1.8570
				A	A	A	A	A
1	O	1	S	0.000000	0.000000	-0.073945	0.000000	0.022866
2	O	1	S	0.000000	0.000000	-1.289182	0.000000	0.288077
3	O	1	X	0.000000	-0.905167	0.000000	0.000000	0.000000
4	O	1	Y	0.000000	0.000000	-0.523164	0.000000	0.136323
5	O	1	Z	-0.959491	0.000000	0.000000	0.000000	0.000000
6	O	1	S	0.000000	0.000000	3.054571	0.000000	-0.718126
7	O	1	X	0.000000	1.640905	0.000000	0.000000	0.000000
8	O	1	Y	0.000000	0.000000	1.013831	0.000000	-0.475892
9	O	1	Z	1.022637	0.000000	0.000000	0.000000	0.000000
10	O	1	XX	0.000000	0.000000	-0.591897	0.000000	-0.278944
11	O	1	YY	0.000000	0.000000	-0.319649	0.000000	0.820779
12	O	1	ZZ	0.000000	0.000000	-0.298692	0.000000	-0.271989
13	O	1	XY	0.000000	-0.006624	0.000000	0.000000	0.000000
14	O	1	XZ	0.000000	0.000000	0.000000	0.680899	0.000000
15	O	1	YZ	0.017485	0.000000	0.000000	0.000000	0.000000
16	H	2	S	0.000000	-0.160301	-0.290390	0.000000	0.216613
17	H	2	S	0.000000	-0.681711	-0.621226	0.000000	0.100849
18	H	2	X	0.000000	0.170004	-0.003860	0.000000	-0.170938
19	H	2	Y	0.000000	0.054002	0.129285	0.000000	0.270140
20	H	2	Z	0.026283	0.000000	0.000000	0.378513	0.000000
21	H	3	S	0.000000	0.160301	-0.290390	0.000000	0.216613
22	H	3	S	0.000000	0.681711	-0.621226	0.000000	0.100849
23	H	3	X	0.000000	0.170004	0.003860	0.000000	0.170938
24	H	3	Y	0.000000	-0.054002	0.129285	0.000000	0.270140
25	H	3	Z	0.026283	0.000000	0.000000	-0.378513	0.000000

				16	17	18	19	20
				1.9437	2.3970	2.4173	2.5782	2.8126
				A	A	A	A	A
1	O	1	S	0.000000	0.018454	0.000000	0.000000	0.000000
2	O	1	S	0.000000	0.420560	0.000000	0.000000	0.000000
3	O	1	X	0.000000	0.000000	-0.261376	-0.287042	0.000000
4	O	1	Y	0.000000	0.241769	0.000000	0.000000	0.000000
5	O	1	Z	0.036973	0.000000	0.000000	0.000000	0.065287
6	O	1	S	0.000000	-0.791706	0.000000	0.000000	0.000000

COMPUTATIONAL CHEMISTRY II

7	O	1	X	0.000000	0.000000	0.610299	0.084468	0.000000
8	O	1	Y	0.000000	-0.425040	0.000000	0.000000	0.000000
9	O	1	Z	-0.217240	0.000000	0.000000	0.000000	-0.371699
10	O	1	XX	0.000000	-0.461412	0.000000	0.000000	0.000000
11	O	1	YY	0.000000	-0.098121	0.000000	0.000000	0.000000
12	O	1	ZZ	0.000000	0.950826	0.000000	0.000000	0.000000
13	O	1	XY	0.000000	0.000000	0.208049	0.660073	0.000000
14	O	1	XZ	0.000000	0.000000	0.000000	0.000000	0.000000
15	O	1	YZ	0.797333	0.000000	0.000000	0.000000	-0.658691
16	H	2	S	0.000000	0.455610	-0.324372	-0.337921	0.000000
17	H	2	S	0.000000	-0.027873	0.010651	0.247208	0.000000
18	H	2	X	0.000000	0.169455	-0.514771	-0.113937	0.000000
19	H	2	Y	0.000000	0.212805	0.435518	-0.485331	0.000000
20	H	2	Z	0.321675	0.000000	0.000000	0.000000	0.702322
21	H	3	S	0.000000	0.455610	0.324372	0.337921	0.000000
22	H	3	S	0.000000	-0.027873	-0.010651	-0.247208	0.000000
23	H	3	X	0.000000	-0.169455	-0.514771	-0.113937	0.000000
24	H	3	Y	0.000000	0.212805	-0.435518	0.485331	0.000000
25	H	3	Z	0.321675	0.000000	0.000000	0.000000	0.702322

				21	22	23	24	25
				2.8619	3.1264	3.4944	3.7855	4.0613
				A	A	A	A	A
1	O	1	S	0.000000	-0.002816	-0.226360	0.000000	-0.397384
2	O	1	S	0.000000	-0.107621	-0.084650	0.000000	0.473347
3	O	1	X	0.000000	0.000000	0.000000	0.358489	0.000000
4	O	1	Y	0.000000	-0.044069	0.233774	0.000000	-0.239501
5	O	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
6	O	1	S	0.000000	0.271718	2.515976	0.000000	2.488579
7	O	1	X	0.000000	0.000000	0.000000	1.227071	0.000000
8	O	1	Y	0.000000	0.424723	0.723642	0.000000	-0.048712
9	O	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
10	O	1	XX	0.000000	-0.618418	0.228951	0.000000	-1.801089
11	O	1	YY	0.000000	0.763764	-0.455836	0.000000	-1.442617
12	O	1	ZZ	0.000000	-0.093404	-1.158677	0.000000	-1.172881
13	O	1	XY	0.000000	0.000000	0.000000	1.327850	0.000000
14	O	1	XZ	0.818884	0.000000	0.000000	0.000000	0.000000
15	O	1	YZ	0.000000	0.000000	0.000000	0.000000	0.000000
16	H	2	S	0.000000	-0.076696	-0.594532	-0.853472	0.385591
17	H	2	S	0.000000	-0.095731	-0.497905	-0.448478	-0.238219
18	H	2	X	0.000000	0.483891	0.700275	0.777261	-0.380824
19	H	2	Y	0.000000	-0.545041	0.488399	0.573125	-0.317490
20	H	2	Z	-0.651986	0.000000	0.000000	0.000000	0.000000
21	H	3	S	0.000000	-0.076696	-0.594532	0.853472	0.385591
22	H	3	S	0.000000	-0.095731	-0.497905	0.448478	-0.238219
23	H	3	X	0.000000	-0.483891	-0.700275	0.777261	0.380824
24	H	3	Y	0.000000	-0.545041	0.488399	-0.573125	-0.317490
25	H	3	Z	0.651986	0.000000	0.000000	0.000000	0.000000

..... END OF RHF CALCULATION

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.0 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 0.7 SECONDS, CPU UTILIZATION IS 7.58%

 PROPERTY VALUES FOR THE RHF SELF-CONSISTENT FIELD WAVEFUNCTION

 ENERGY COMPONENTS

```

-----
WAVEFUNCTION NORMALIZATION =      1.0000000000
      ONE ELECTRON ENERGY =     -121.1891250574
      TWO ELECTRON ENERGY =      37.0581729215
      NUCLEAR REPULSION ENERGY =      8.1396592790
-----
      TOTAL ENERGY =     -75.9912928569
ELECTRON-ELECTRON POTENTIAL ENERGY =      37.0581729215
NUCLEUS-ELECTRON POTENTIAL ENERGY =    -196.6003884075
NUCLEUS-NUCLEUS POTENTIAL ENERGY =      8.1396592790
-----
      TOTAL POTENTIAL ENERGY =    -151.4025562070
      TOTAL KINETIC ENERGY =      75.4112633501
      VIRIAL RATIO (V/T) =      2.0076915501

```

..... PI ENERGY ANALYSIS

```

ENERGY ANALYSIS:
      FOCK ENERGY=     -47.0727736009
      BARE H ENERGY=   -121.1891250574
      ELECTRONIC ENERGY =   -84.1309493291
      KINETIC ENERGY=     75.4112633501
      N-N REPULSION=      8.1396592790
      TOTAL ENERGY=    -75.9912900502
      SIGMA PART(1+2)=   -76.6253226641
      (K,V1,2)=         70.8366325450   -177.9908078866
30.5288526775
      PI PART(1+2)=     -7.5056266650
      (K,V1,2)=         4.5746308052   -18.6095805209
6.5293230507
      SIGMA SKELETON, ERROR=  -68.4856633852   0.0000000000
      MIXED PART= 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
..... END OF PI ENERGY ANALYSIS .....
```

MULLIKEN AND LOWDIN POPULATION ANALYSES

ATOMIC MULLIKEN POPULATION IN EACH MOLECULAR ORBITAL

	1	2	3	4	5
	2.000000	2.000000	2.000000	2.000000	2.000000
1	2.000035	1.757253	1.267358	1.691368	1.986773
2	-0.000017	0.121374	0.366321	0.154316	0.006613
3	-0.000017	0.121374	0.366321	0.154316	0.006613

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

				MULLIKEN	LOWDIN
1	O	1	S	1.99551	1.97782
2	O	1	S	0.91149	0.71635
3	O	1	X	0.73653	0.66318
4	O	1	Y	0.89909	0.84812
5	O	1	Z	1.15271	1.12651

COMPUTATIONAL CHEMISTRY II

6	O	1	S	0.93303	0.50069
7	O	1	X	0.51832	0.58802
8	O	1	Y	0.68628	0.72667
9	O	1	Z	0.83265	0.83601
10	O	1	XX	0.01421	0.18780
11	O	1	YY	0.00541	0.17487
12	O	1	ZZ	0.00364	0.17539
13	O	1	XY	0.01251	0.01650
14	O	1	XZ	0.00000	0.00000
15	O	1	YZ	0.00142	0.00086
16	H	2	S	0.42027	0.39468
17	H	2	S	0.19835	0.26629
18	H	2	X	0.01427	0.03047
19	H	2	Y	0.00911	0.02086
20	H	2	Z	0.00661	0.01831
21	H	3	S	0.42027	0.39468
22	H	3	S	0.19835	0.26629
23	H	3	X	0.01427	0.03047
24	H	3	Y	0.00911	0.02086
25	H	3	Z	0.00661	0.01831

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

	1	2	3
1	8.1635208		
2	0.2696328	0.3962585	
3	0.2696328	-0.0172845	0.3962585

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL. POP.	CHARGE	LOW. POP.	CHARGE
1 O	8.702786	-0.702786	8.538781	-0.538781
2 H	0.648607	0.351393	0.730609	0.269391
3 H	0.648607	0.351393	0.730609	0.269391

BOND ORDER AND VALENCE ANALYSIS BOND ORDER THRESHOLD=0.050

BOND				BOND				
BOND ORDER	ATOM	PAIR	DIST	ORDER	ATOM	PAIR	DIST	
1	1	2	1.080	0.864	1	3	1.080	0.864

ATOM	TOTAL VALENCE	BONDED VALENCE	FREE VALENCE
1 O	1.727	1.727	0.000
2 H	0.868	0.868	0.000
3 H	0.868	0.868	0.000

ELECTROSTATIC MOMENTS

POINT	1	X	Y	Z (BOHR)	CHARGE
		0.000000	0.000000	0.000000	0.00 (A.U.)

COMPUTATIONAL CHEMISTRY II

DX DY DZ /D/ (DEBYE)
 0.000000 2.173861 0.000000 2.173861
 END OF PROPERTY EVALUATION
 CPU 0: STEP CPU TIME= 0.01 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 0.7 SECONDS, CPU UTILIZATION IS 8.11%

BEGINNING ONE ELECTRON GRADIENT...
 END OF 1-ELECTRON GRADIENT
 CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 0.8 SECONDS, CPU UTILIZATION IS 7.41%

 GRADIENT OF THE ENERGY

THE MINIMUM MEMORY REQUIRED FOR THIS RUN IS 71766 WORDS.
 USING 1047286 WORDS FOR 2E- DERIVATIVE INTEGRAL CONTRIBUTIONS.
 THE COARSE/FINE SCHWARZ SCREENINGS SKIPPED 0/ 0
 BLOCKS.

THE NUMBER OF GRADIENT INTEGRAL BLOCKS COMPUTED WAS 1443
 END OF 2-ELECTRON GRADIENT
 CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 0.9 SECONDS, CPU UTILIZATION IS 6.98%

NSERCH= 0 ENERGY= -75.9912929

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 O	8.0	0.0000000	-0.1024982	0.0000000
2 H	1.0	0.0919966	0.0512491	0.0000000
3 H	1.0	-0.0919966	0.0512491	0.0000000

MAXIMUM GRADIENT = 0.1024982 RMS GRADIENT = 0.0602638
 FORCE CONSTANT MATRIX NOT UPDATED --- TAKING FIRST STEP
 MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
 NR STEP HAS LENGTH = 0.393418
 TRIM/QA LAMBDA FOR NON-TS MODES = -0.10231703
 TRIM/QA STEP HAS LENGTH = 0.300000
 RADIUS OF STEP TAKEN= 0.30000 CURRENT TRUST RADIUS= 0.30000

BEGINNING GEOMETRY SEARCH POINT NSERCH= 1 ...

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
O	8.0	0.0000000000	0.0079117195	0.0000000000
H	1.0	0.7921018869	0.5147232897	0.0000000000
H	1.0	-0.7921018869	0.5147232897	0.0000000000

THE CURRENT FULLY SUBSTITUTED Z-MATRIX IS

O				
H	1	0.9403634		
H	1	0.9403634	2	114.7752302

INTERNUCLEAR DISTANCES (ANGS.)

COMPUTATIONAL CHEMISTRY II

```

-----
                1 O          2 H          3 H
1 O          0.0000000    0.9403634 *  0.9403634 *
2 H          0.9403634 *  0.0000000    1.5842038 *
3 H          0.9403634 *  1.5842038 *  0.0000000

```

* ... LESS THAN 3.000

```

..... END OF ONE-ELECTRON INTEGRALS .....
CPU      0: STEP CPU TIME=      0.00 TOTAL CPU TIME=      0.1 (  0.0 MIN)
TOTAL WALL CLOCK TIME=      0.9 SECONDS, CPU UTILIZATION IS  6.67%
TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS =      25620
      8 INTEGRAL RECORDS WERE STORED ON DISK FILE  8.
..... END OF TWO-ELECTRON INTEGRALS .....
CPU      0: STEP CPU TIME=      0.00 TOTAL CPU TIME=      0.1 (  0.0 MIN)
TOTAL WALL CLOCK TIME=      1.0 SECONDS, CPU UTILIZATION IS  6.19%

```

RHF SCF CALCULATION

DENSITY MATRIX CONV= 2.00E-04

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-76.0093152823	-76.0093152823	0.056153824	0.042531890
2	1	0	-76.0203748666	-0.0110595844	0.028893134	0.021343871
3	2	0	-76.0214648394	-0.0010899728	0.006199477	0.006327896
4	3	0	-76.0216364370	-0.0001715976	0.001762537	0.000855592
5	4	0	-76.0216428406	-0.0000064035	0.000783492	0.000282955
6	5	0	-76.0216433681	-0.0000005276	0.000116765	0.000046512
7	6	0	-76.0216433828	-0.0000000147	0.000019540	0.000010102
8	7	0	-76.0216433835	-0.0000000007	0.000003152	0.000001932

DENSITY CONVERGED

```

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

```

```

FINAL RHF ENERGY IS      -76.0216433835 AFTER  8 ITERATIONS
..... END OF RHF CALCULATION .....
CPU      0: STEP CPU TIME=      0.01 TOTAL CPU TIME=      0.1 (  0.0 MIN)
TOTAL WALL CLOCK TIME=      1.3 SECONDS, CPU UTILIZATION IS  5.47%
..... END OF 1-ELECTRON GRADIENT .....
CPU      0: STEP CPU TIME=      0.01 TOTAL CPU TIME=      0.1 (  0.0 MIN)
TOTAL WALL CLOCK TIME=      1.3 SECONDS, CPU UTILIZATION IS  6.02%
..... END OF 2-ELECTRON GRADIENT .....
CPU      0: STEP CPU TIME=      0.00 TOTAL CPU TIME=      0.1 (  0.0 MIN)
TOTAL WALL CLOCK TIME=      1.4 SECONDS, CPU UTILIZATION IS  5.84%

```

NSERCH= 1 ENERGY= -76.0216434

GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
------	------	-------	-------	-------

COMPUTATIONAL CHEMISTRY II

```

-----
 1 O          8.0    0.0000000    0.0224439    0.0000000
 2 H          1.0    0.0085673   -0.0112219    0.0000000
 3 H          1.0   -0.0085673   -0.0112219    0.0000000

MAXIMUM GRADIENT = 0.0224439    RMS GRADIENT = 0.0100133
HESSIAN UPDATED USING THE BFGS FORMULA
ACTUAL ENERGY CHANGE WAS -0.0303505266
PREDICTED ENERGY CHANGE WAS -0.0315113346 RATIO= 0.963
MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
NR STEP HAS LENGTH           = 0.656701
TRIM/QA LAMBDA FOR NON-TS MODES = -0.01249316
TRIM/QA STEP HAS LENGTH           = 0.500000
RADIUS OF STEP TAKEN= 0.50000 CURRENT TRUST RADIUS= 0.50000

```

BEGINNING GEOMETRY SEARCH POINT NSERCH= 2 ...

COORDINATES OF ALL ATOMS ARE (ANGS)

```

ATOM  CHARGE      X              Y              Z
-----
O          8.0    0.0000000000   -0.1283630141   0.0000000000
H          1.0    0.6469279643    0.5828606565   0.0000000000
H          1.0   -0.6469279643    0.5828606565   0.0000000000

```

THE CURRENT FULLY SUBSTITUTED Z-MATRIX IS

```

O
H      1    0.9614338
H      1    0.9614338  2    84.5792146

```

INTERNUCLEAR DISTANCES (ANGS.)

```

-----
          1 O          2 H          3 H
1 O      0.0000000    0.9614338 *  0.9614338 *
2 H      0.9614338 *  0.0000000    1.2938559 *
3 H      0.9614338 *  1.2938559 *  0.0000000

```

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

```

CPU      0: STEP CPU TIME=      0.00 TOTAL CPU TIME=      0.1 (    0.0 MIN)
TOTAL WALL CLOCK TIME=      1.4 SECONDS, CPU UTILIZATION IS  5.67%
TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS =      25620
      8 INTEGRAL RECORDS WERE STORED ON DISK FILE  8.

```

..... END OF TWO-ELECTRON INTEGRALS

```

CPU      0: STEP CPU TIME=      0.00 TOTAL CPU TIME=      0.1 (    0.0 MIN)
TOTAL WALL CLOCK TIME=      1.5 SECONDS, CPU UTILIZATION IS  5.52%

```

RHF SCF CALCULATION

DENSITY MATRIX CONV= 5.00E-05

```

ITER EX DEM      TOTAL ENERGY      E CHANGE  DENSITY CHANGE      ORB. GRAD
-----START SECOND ORDER SCF-----
 1  0  0      -75.9981658453    -75.9981658453    0.066330264    0.044729119
 2  1  0      -76.0091131189    -0.0109472736    0.016683503    0.015438389

```

COMPUTATIONAL CHEMISTRY II

3	2	0	-76.0100494027	-0.0009362838	0.007130494	0.004360309
4	3	0	-76.0101286072	-0.0000792045	0.001158220	0.001204443
5	4	0	-76.0101342122	-0.0000056050	0.000411355	0.000208631
6	5	0	-76.0101345689	-0.0000003567	0.000163757	0.000056450
7	6	0	-76.0101345973	-0.0000000284	0.000029919	0.000019541
8	7	0	-76.0101345993	-0.0000000020	0.000011613	0.000006288

 DENSITY CONVERGED

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

FINAL RHF ENERGY IS -76.0101345993 AFTER 8 ITERATIONS

..... END OF RHF CALCULATION

CPU 0: STEP CPU TIME= 0.01 TOTAL CPU TIME= 0.1 (0.0 MIN)

TOTAL WALL CLOCK TIME= 1.8 SECONDS, CPU UTILIZATION IS 4.97%

..... END OF 1-ELECTRON GRADIENT

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)

TOTAL WALL CLOCK TIME= 1.9 SECONDS, CPU UTILIZATION IS 4.76%

..... END OF 2-ELECTRON GRADIENT

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)

TOTAL WALL CLOCK TIME= 1.9 SECONDS, CPU UTILIZATION IS 4.69%

NSERCH= 2 ENERGY= -76.0101346

 GRADIENT (HARTREE/BOHR)

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	O	8.0	0.0000000	-0.0638307	0.0000000
2	H	1.0	-0.0255335	0.0319154	0.0000000
3	H	1.0	0.0255335	0.0319154	0.0000000

MAXIMUM GRADIENT = 0.0638307 RMS GRADIENT = 0.0287043

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS 0.0115087842

PREDICTED ENERGY CHANGE WAS -0.0082468177 RATIO= -1.396

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.371862

TRIM/QA LAMBDA FOR NON-TS MODES = -0.09547439

TRIM/QA STEP HAS LENGTH = 0.250000

RADIUS OF STEP TAKEN= 0.25000 CURRENT TRUST RADIUS= 0.25000

BEGINNING GEOMETRY SEARCH POINT NSERCH= 3 ...

COORDINATES OF ALL ATOMS ARE (ANGS)

	ATOM	CHARGE	X	Y	Z
O		8.0	0.0000000000	-0.0552551403	0.0000000000
H		1.0	0.7157924806	0.5463067196	0.0000000000
H		1.0	-0.7157924806	0.5463067196	0.0000000000

THE CURRENT FULLY SUBSTITUTED Z-MATRIX IS

O				
H	1	0.9350056		
H	1	0.9350056	2	99.9116875

INTERNUCLEAR DISTANCES (ANGS.)

	1 O	2 H	3 H
1 O	0.0000000	0.9350056 *	0.9350056 *
2 H	0.9350056 *	0.0000000	1.4315850 *
3 H	0.9350056 *	1.4315850 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 2.0 SECONDS, CPU UTILIZATION IS 4.62%
 TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 25620

8 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 2.0 SECONDS, CPU UTILIZATION IS 4.52%

RHF SCF CALCULATION

DENSITY MATRIX CONV= 2.00E-04

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
-----START SECOND ORDER SCF-----						
1	0	0	-76.0184073774	-76.0184073774	0.042167726	0.026463983
2	1	0	-76.0220422103	-0.0036348329	0.012182976	0.007203973
3	2	0	-76.0222879131	-0.0002457028	0.003175486	0.003186514
4	3	0	-76.0223289385	-0.0000410255	0.000647256	0.000430853
5	4	0	-76.0223306287	-0.0000016901	0.000410014	0.000170334
6	5	0	-76.0223308598	-0.0000002312	0.000039711	0.000023531
7	6	0	-76.0223308634	-0.0000000035	0.000012303	0.000006708

DENSITY CONVERGED

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

FINAL RHF ENERGY IS -76.0223308634 AFTER 7 ITERATIONS

..... END OF RHF CALCULATION

CPU 0: STEP CPU TIME= 0.02 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 2.3 SECONDS, CPU UTILIZATION IS 4.87%

..... END OF 1-ELECTRON GRADIENT

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 2.3 SECONDS, CPU UTILIZATION IS 4.72%

..... END OF 2-ELECTRON GRADIENT

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 2.4 SECONDS, CPU UTILIZATION IS 4.64%

NSERCH= 3 ENERGY= -76.0223309

GRADIENT (HARTREE/BOHR)

COMPUTATIONAL CHEMISTRY II

	ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1	O	8.0	0.0000000	-0.0008732	0.0000000
2	H	1.0	-0.0178187	0.0004366	0.0000000
3	H	1.0	0.0178187	0.0004366	0.0000000

MAXIMUM GRADIENT = 0.0178187 RMS GRADIENT = 0.0084074

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0121962640

PREDICTED ENERGY CHANGE WAS -0.0129202204 RATIO= 0.944

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.133857

RADIUS OF STEP TAKEN= 0.13386 CURRENT TRUST RADIUS= 0.50000

BEGINNING GEOMETRY SEARCH POINT NSERCH= 4 ...

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
O	8.0	0.0000000000	-0.0359688707	0.0000000000
H	1.0	0.7630129853	0.5366635848	0.0000000000
H	1.0	-0.7630129853	0.5366635848	0.0000000000

THE CURRENT FULLY SUBSTITUTED Z-MATRIX IS

O				
H	1	0.9539899		
H	1	0.9539899	2	106.2243887

INTERNUCLEAR DISTANCES (ANGS.)

	1 O	2 H	3 H
1 O	0.0000000	0.9539899 *	0.9539899 *
2 H	0.9539899 *	0.0000000	1.5260260 *
3 H	0.9539899 *	1.5260260 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)

TOTAL WALL CLOCK TIME= 2.4 SECONDS, CPU UTILIZATION IS 4.58%

TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 25620

8 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)

TOTAL WALL CLOCK TIME= 2.5 SECONDS, CPU UTILIZATION IS 4.49%

RHF SCF CALCULATION

DENSITY MATRIX CONV= 5.00E-05

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
			-----START	SECOND	ORDER	SCF-----
1	0	0	-76.0227430973	-76.0227430973	0.013986000	0.010200218
2	1	0	-76.0233154868	-0.0005723896	0.002807722	0.002468997
3	2	0	-76.0233428544	-0.0000273675	0.000924465	0.000851092

COMPUTATIONAL CHEMISTRY II

4	3	0	-76.0233456363	-0.0000027819	0.000127909	0.000118885
5	4	0	-76.0233457128	-0.0000000765	0.000018932	0.000018922
6	5	0	-76.0233457147	-0.0000000018	0.000006116	0.000003777
7	6	0	-76.0233457147	-0.0000000001	0.000001801	0.000000899

 DENSITY CONVERGED

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

FINAL RHF ENERGY IS -76.0233457147 AFTER 7 ITERATIONS

..... END OF RHF CALCULATION

CPU 0: STEP CPU TIME= 0.01 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 2.7 SECONDS, CPU UTILIZATION IS 4.41%

..... END OF 1-ELECTRON GRADIENT

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 2.8 SECONDS, CPU UTILIZATION IS 4.35%

..... END OF 2-ELECTRON GRADIENT

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 2.8 SECONDS, CPU UTILIZATION IS 4.29%

NSERCH= 4 ENERGY= -76.0233457

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 O	8.0	0.0000000	-0.0133855	0.0000000
2 H	1.0	0.0107971	0.0066927	0.0000000
3 H	1.0	-0.0107971	0.0066927	0.0000000

MAXIMUM GRADIENT = 0.0133855 RMS GRADIENT = 0.0074678

HESSIAN UPDATED USING THE BFGS FORMULA

ACTUAL ENERGY CHANGE WAS -0.0010148514

PREDICTED ENERGY CHANGE WAS -0.0016139019 RATIO= 0.629

MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP

NR STEP HAS LENGTH = 0.027732

RADIUS OF STEP TAKEN= 0.02773 CURRENT TRUST RADIUS= 0.13386

BEGINNING GEOMETRY SEARCH POINT NSERCH= 5 ...

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
O	8.0	0.0000000000	-0.0327525001	0.0000000000
H	1.0	0.7530169678	0.5350553995	0.0000000000
H	1.0	-0.7530169678	0.5350553995	0.0000000000

THE CURRENT FULLY SUBSTITUTED Z-MATRIX IS

O				
H	1	0.9431015		
H	1	0.9431015	2	105.9642013

INTERNUCLEAR DISTANCES (ANGS.)

COMPUTATIONAL CHEMISTRY II

	1 O	2 H	3 H
1 O	0.0000000	0.9431015 *	0.9431015 *
2 H	0.9431015 *	0.0000000	1.5060339 *
3 H	0.9431015 *	1.5060339 *	0.0000000

* ... LESS THAN 3.000

..... END OF ONE-ELECTRON INTEGRALS

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 2.8 SECONDS, CPU UTILIZATION IS 4.24%
 TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS = 25620
 8 INTEGRAL RECORDS WERE STORED ON DISK FILE 8.

..... END OF TWO-ELECTRON INTEGRALS

CPU 0: STEP CPU TIME= 0.01 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 2.9 SECONDS, CPU UTILIZATION IS 4.53%

 RHF SCF CALCULATION

DENSITY MATRIX CONV= 5.00E-05

ITER	EX	DEM	TOTAL ENERGY	E CHANGE	DENSITY CHANGE	ORB. GRAD
			-----START	SECOND ORDER SCF	-----	
1	0	0	-76.0235377068	-76.0235377068	0.003717747	0.003032072
2	1	0	-76.0236076862	-0.0000699793	0.002040698	0.001520218
3	2	0	-76.0236142696	-0.0000065834	0.000410631	0.000356478
4	3	0	-76.0236149661	-0.0000006965	0.000139577	0.000078357
5	4	0	-76.0236150119	-0.0000000459	0.000036556	0.000019255
6	5	0	-76.0236150146	-0.0000000026	0.000009705	0.000004505

 DENSITY CONVERGED

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

FINAL RHF ENERGY IS -76.0236150146 AFTER 6 ITERATIONS

..... END OF RHF CALCULATION

CPU 0: STEP CPU TIME= 0.01 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 3.1 SECONDS, CPU UTILIZATION IS 4.52%

..... END OF 1-ELECTRON GRADIENT

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 3.2 SECONDS, CPU UTILIZATION IS 4.40%

..... END OF 2-ELECTRON GRADIENT

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.1 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 3.2 SECONDS, CPU UTILIZATION IS 4.35%

NSERCH= 5 ENERGY= -76.0236150

 GRADIENT (HARTREE/BOHR)

ATOM	ZNUC	DE/DX	DE/DY	DE/DZ
1 O	8.0	0.0000000	-0.0000689	0.0000000
2 H	1.0	0.0000378	0.0000345	0.0000000
3 H	1.0	-0.0000378	0.0000345	0.0000000

MAXIMUM GRADIENT = 0.0000689 RMS GRADIENT = 0.0000333

***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
O	8.0	0.0000000000	-0.0327525001	0.0000000000
H	1.0	0.7530169678	0.5350553995	0.0000000000
H	1.0	-0.7530169678	0.5350553995	0.0000000000

THE CURRENT FULLY SUBSTITUTED Z-MATRIX IS

O				
H	1	0.9431015		
H	1	0.9431015	2	105.9642013

These are the final geometrical parameters

Geometry optimization is over after 5 steps as the calculated gradient is less than the preset limit. Property calculation starts with this geometry as in case of the previous job for energy calculation.

Compare the initial and final geometrical parameters.

O				
H	1	1.0800000		
H	1	1.0800000	2	109.5000

These were the initial geometrical parameters

INTERNUCLEAR DISTANCES (ANGS.)

	1 O	2 H	3 H
1 O	0.0000000	0.9431015 *	0.9431015 *
2 H	0.9431015 *	0.0000000	1.5060339 *
3 H	0.9431015 *	1.5060339 *	0.0000000

* ... LESS THAN 3.000

NUCLEAR ENERGY = 9.3290226296
 ELECTRONIC ENERGY = -85.3526376442
 TOTAL ENERGY = -76.0236150146

MOLECULAR ORBITALS

You can see these MO by using a suitable visualization program

For MO, see at the end of this calculation.

1 2 3 4 5

COMPUTATIONAL CHEMISTRY II

			-20.5573	-1.3464	-0.7139	-0.5683	-0.4976	
			A	A	A	A	A	
1	O	1	S	-0.994665	0.210625	0.000000	0.072601	0.000000
2	O	1	S	-0.021212	-0.471371	0.000000	-0.161976	0.000000
3	O	1	X	0.000000	0.000000	0.502654	0.000000	0.000000
4	O	1	Y	-0.001551	-0.085756	0.000000	0.556998	0.000000
5	O	1	Z	0.000000	0.000000	0.000000	0.000000	0.638051
6	O	1	S	-0.004287	-0.418081	0.000000	-0.336499	0.000000
7	O	1	X	0.000000	0.000000	0.272567	0.000000	0.000000
8	O	1	Y	0.000193	-0.031484	0.000000	0.392719	0.000000
9	O	1	Z	0.000000	0.000000	0.000000	0.000000	0.500508
10	O	1	XX	0.003757	-0.006108	0.000000	-0.000946	0.000000
11	O	1	YY	0.003804	-0.008118	0.000000	0.037023	0.000000
12	O	1	ZZ	0.003946	-0.001333	0.000000	-0.009842	0.000000
13	O	1	XY	0.000000	0.000000	0.033236	0.000000	0.000000
14	O	1	XZ	0.000000	0.000000	0.000000	0.000000	0.000000
15	O	1	YZ	0.000000	0.000000	0.000000	0.000000	0.027592
16	H	2	S	0.000004	-0.148346	0.243557	0.142992	0.000000
17	H	2	S	0.000340	-0.012890	0.127763	0.087827	0.000000
18	H	2	X	-0.000372	0.022032	-0.011606	-0.014912	0.000000
19	H	2	Y	-0.000252	0.013411	-0.018915	0.006307	0.000000
20	H	2	Z	0.000000	0.000000	0.000000	0.000000	0.020794
21	H	3	S	0.000004	-0.148346	-0.243557	0.142992	0.000000
22	H	3	S	0.000340	-0.012890	-0.127763	0.087827	0.000000
23	H	3	X	0.000372	-0.022032	-0.011606	0.014912	0.000000
24	H	3	Y	-0.000252	0.013411	0.018915	0.006307	0.000000
25	H	3	Z	0.000000	0.000000	0.000000	0.000000	0.020794

			6	7	8	9	10	
			0.2153	0.3084	1.0169	1.0930	1.1346	
			A	A	A	A	A	
1	O	1	S	0.101673	0.000000	0.000000	0.051308	-0.000702
2	O	1	S	-0.053763	0.000000	0.000000	-0.017051	0.873792
3	O	1	X	0.000000	0.325542	-0.139019	0.000000	0.000000
4	O	1	Y	-0.208251	0.000000	0.000000	-0.609791	-0.519299
5	O	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
6	O	1	S	-1.458226	0.000000	0.000000	-0.024251	-1.530576
7	O	1	X	0.000000	0.869844	-0.406539	0.000000	0.000000
8	O	1	Y	-0.504147	0.000000	0.000000	0.474197	0.780962
9	O	1	Z	0.000000	0.000000	0.000000	0.000000	0.000000
10	O	1	XX	0.054524	0.000000	0.000000	0.345108	0.196432
11	O	1	YY	0.044225	0.000000	0.000000	0.117644	0.315076
12	O	1	ZZ	0.074332	0.000000	0.000000	-0.106231	0.361605
13	O	1	XY	0.000000	0.039660	0.277341	0.000000	0.000000
14	O	1	XZ	0.000000	0.000000	0.000000	0.000000	0.000000
15	O	1	YZ	0.000000	0.000000	0.000000	0.000000	0.000000
16	H	2	S	0.052623	-0.050635	0.767706	0.552718	-0.486089
17	H	2	S	1.060515	-1.443647	-0.577724	-0.488177	0.398065
18	H	2	X	-0.003854	0.016199	0.055353	0.203965	-0.011229
19	H	2	Y	-0.001625	0.009185	0.107338	0.073174	0.028747
20	H	2	Z	0.000000	0.000000	0.000000	0.000000	0.000000
21	H	3	S	0.052623	0.050635	-0.767706	0.552718	-0.486089
22	H	3	S	1.060515	1.443647	0.577724	-0.488177	0.398065
23	H	3	X	0.003854	0.016199	0.055353	-0.203965	0.011229
24	H	3	Y	-0.001625	-0.009185	-0.107338	0.073174	0.028747
25	H	3	Z	0.000000	0.000000	0.000000	0.000000	0.000000

11

12

13

14

15

COMPUTATIONAL CHEMISTRY II

			1.1690	1.2955	1.4117	1.8025	1.8295	
			A	A	A	A	A	
1	O	1	S	0.000000	0.000000	-0.082135	0.000000	-0.028357
2	O	1	S	0.000000	0.000000	-1.411793	0.000000	-0.285825
3	O	1	X	0.000000	0.869021	0.000000	0.000000	0.000000
4	O	1	Y	0.000000	0.000000	-0.413211	0.000000	-0.035058
5	O	1	Z	-0.962345	0.000000	0.000000	0.000000	0.000000
6	O	1	S	0.000000	0.000000	3.616014	0.000000	0.829784
7	O	1	X	0.000000	-1.798682	0.000000	0.000000	0.000000
8	O	1	Y	0.000000	0.000000	1.061244	0.000000	0.473996
9	O	1	Z	1.044143	0.000000	0.000000	0.000000	0.000000
10	O	1	XX	0.000000	0.000000	-0.595907	0.000000	0.235035
11	O	1	YY	0.000000	0.000000	-0.351179	0.000000	-0.787985
12	O	1	ZZ	0.000000	0.000000	-0.313089	0.000000	0.277118
13	O	1	XY	0.000000	-0.165252	0.000000	0.000000	0.000000
14	O	1	XZ	0.000000	0.000000	0.000000	-0.668960	0.000000
15	O	1	YZ	0.013812	0.000000	0.000000	0.000000	0.000000
16	H	2	S	0.000000	0.132753	-0.327489	0.000000	-0.228937
17	H	2	S	0.000000	0.998108	-0.804958	0.000000	-0.137229
18	H	2	X	0.000000	-0.182238	-0.001543	0.000000	0.171622
19	H	2	Y	0.000000	-0.130530	0.111868	0.000000	-0.259593
20	H	2	Z	-0.014815	0.000000	0.000000	-0.351410	0.000000
21	H	3	S	0.000000	-0.132753	-0.327489	0.000000	-0.228937
22	H	3	S	0.000000	-0.998108	-0.804958	0.000000	-0.137229
23	H	3	X	0.000000	-0.182238	0.001543	0.000000	-0.171622
24	H	3	Y	0.000000	0.130530	0.111868	0.000000	-0.259593
25	H	3	Z	-0.014815	0.000000	0.000000	0.351410	0.000000

PROPERTY VALUES FOR THE RHF SELF-CONSISTENT FIELD WAVEFUNCTION

ENERGY COMPONENTS

WAVEFUNCTION NORMALIZATION = 1.0000000000

ONE ELECTRON ENERGY = -123.3383142209
TWO ELECTRON ENERGY = 37.9856765767
NUCLEAR REPULSION ENERGY = 9.3290226296

TOTAL ENERGY = -76.0236150146

ELECTRON-ELECTRON POTENTIAL ENERGY = 37.9856765767
NUCLEUS-ELECTRON POTENTIAL ENERGY = -199.2027162181
NUCLEUS-NUCLEUS POTENTIAL ENERGY = 9.3290226296

TOTAL POTENTIAL ENERGY = -151.8880170118
TOTAL KINETIC ENERGY = 75.8644019972
VIRIAL RATIO (V/T) = 2.0020986525

..... PI ENERGY ANALYSIS

ENERGY ANALYSIS:
FOCK ENERGY= -47.3669344502
BARE H ENERGY= -123.3383142209
ELECTRONIC ENERGY = -85.3526243355

COMPUTATIONAL CHEMISTRY II

```

KINETIC ENERGY=      75.8644019972
N-N REPULSION=       9.3290226296
TOTAL ENERGY=      -76.0236017059
SIGMA PART(1+2)=    -77.7508242633
(K,V1,2)=          71.3235765047   -180.4534985083
31.3790977404
PI PART(1+2)=      -7.6018000723
(K,V1,2)=          4.5408254925   -18.7492177098
6.6065921450
SIGMA SKELETON, ERROR=  -68.4218016337   0.0000000000
MIXED PART= 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
..... END OF PI ENERGY ANALYSIS .....

```

MULLIKEN AND LOWDIN POPULATION ANALYSES

ATOMIC MULLIKEN POPULATION IN EACH MOLECULAR ORBITAL

	1	2	3	4	5
	2.000000	2.000000	2.000000	2.000000	2.000000
1	2.000225	1.638496	1.284456	1.769699	1.977825
2	-0.000113	0.180752	0.357772	0.115150	0.011088
3	-0.000113	0.180752	0.357772	0.115150	0.011088

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

				MULLIKEN	LOWDIN
1	O	1	S	1.99539	1.97726
2	O	1	S	0.89422	0.68158
3	O	1	X	0.80330	0.71539
4	O	1	Y	0.95122	0.88697
5	O	1	Z	1.14259	1.10724
6	O	1	S	0.88680	0.46339
7	O	1	X	0.46697	0.54948
8	O	1	Y	0.66474	0.70661
9	O	1	Z	0.83314	0.82118
10	O	1	XX	0.00852	0.18026
11	O	1	YY	0.00236	0.16668
12	O	1	ZZ	0.00518	0.16428
13	O	1	XY	0.01419	0.02197
14	O	1	XZ	0.00000	0.00000
15	O	1	YZ	0.00209	0.00079
16	H	2	S	0.49500	0.44957
17	H	2	S	0.12632	0.21550
18	H	2	X	0.01844	0.04273
19	H	2	Y	0.01380	0.03526
20	H	2	Z	0.01109	0.03539
21	H	3	S	0.49500	0.44957
22	H	3	S	0.12632	0.21550
23	H	3	X	0.01844	0.04273
24	H	3	Y	0.01380	0.03526
25	H	3	Z	0.01109	0.03539

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

COMPUTATIONAL CHEMISTRY II

	1	2	3
1	8.0430384		
2	0.3138313	0.3756996	
3	0.3138313	-0.0248814	0.3756996

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 O	8.670701	-0.670701	8.443090	-0.443090
2 H	0.664650	0.335350	0.778455	0.221545
3 H	0.664650	0.335350	0.778455	0.221545

 BOND ORDER AND VALENCE ANALYSIS BOND ORDER THRESHOLD=0.050

BOND			BOND		
ATOM PAIR	DIST	ORDER	ATOM PAIR	DIST	ORDER
1 2	0.943	0.884	1 3	0.943	0.884

ATOM	TOTAL VALENCE	BONDED VALENCE	FREE VALENCE
1 O	1.768	1.768	0.000
2 H	0.882	0.882	0.000
3 H	0.882	0.882	0.000

 ELECTROSTATIC MOMENTS

POINT	1	X	Y	Z (BOHR)	CHARGE
		0.000000	0.058192	0.000000	0.00 (A.U.)
		DX	DY	DZ	/D/ (DEBYE)
		0.000000	2.147721	0.000000	2.147721

..... END OF PROPERTY EVALUATION

CPU 0: STEP CPU TIME= 0.01 TOTAL CPU TIME= 0.2 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 3.3 SECONDS, CPU UTILIZATION IS 4.60%
 \$VIB

IVIB= 0 IATOM= 0 ICOORD= 0 E= -76.0236150146
 0.000000000E+00-6.892379892E-05 0.000000000E+00 3.777530295E-05
 3.446189952E-05
 0.000000000E+00-3.777530300E-05 3.446189931E-05 0.000000000E+00
 4.234583861E-12 2.147721190E+00 3.259519769E-17

.....END OF GEOMETRY SEARCH.....

CPU 0: STEP CPU TIME= 0.00 TOTAL CPU TIME= 0.2 (0.0 MIN)
 TOTAL WALL CLOCK TIME= 3.4 SECONDS, CPU UTILIZATION IS 4.36%
 1047322 WORDS OF DYNAMIC MEMORY USED

EXECUTION OF GAMESS TERMINATED NORMALLY Fri Mar 16 13:45:51 2012
 DDI: 263624 bytes (0.3 MB / 0 MWords) used by master data server.

 CPU timing information for all processes
 =====

0: 0.60 + 0.96 = 0.157
 1: 0.42 + 0.63 = 0.106
 2: 0.41 + 0.74 = 0.116
 3: 0.37 + 0.62 = 0.100
 4: 0.44 + 0.67 = 0.112

5: 0.37 + 0.43 = 0.81
 6: 0.44 + 0.57 = 0.102
 7: 0.36 + 0.35 = 0.72

```
-----
ddikick.x: exited gracefully.
----- accounting info -----
Files used on the master node dkml03.barc.gov.in were:
-rw-rw-r-- 1 dilip dilip 180016 Mar 16 13:45 /scratch/dkmaity/water-hf-opt.F08
-rw-rw-r-- 1 dilip dilip 180016 Mar 16 13:45 /scratch/dkmaity/water-hf-opt.F08.001
-rw-rw-r-- 1 dilip dilip 180016 Mar 16 13:45 /scratch/dkmaity/water-hf-opt.F08.002
-rw-rw-r-- 1 dilip dilip 180016 Mar 16 13:45 /scratch/dkmaity/water-hf-opt.F08.003
-rw-rw-r-- 1 dilip dilip 180016 Mar 16 13:45 /scratch/dkmaity/water-hf-opt.F08.004
-rw-rw-r-- 1 dilip dilip 180016 Mar 16 13:45 /scratch/dkmaity/water-hf-opt.F08.005
-rw-rw-r-- 1 dilip dilip 180016 Mar 16 13:45 /scratch/dkmaity/water-hf-opt.F08.006
-rw-rw-r-- 1 dilip dilip 180016 Mar 16 13:45 /scratch/dkmaity/water-hf-opt.F08.007
-rw-rw-r-- 1 dilip dilip 1341520 Mar 16 13:45 /scratch/dkmaity/water-hf-opt.F10
Fri Mar 16 13:45:54 EDT 2012
0.243u 0.114s 0:06.98 5.0% 0+0k 0+16io 0pf+0w
```

The output ends here. Since the INPUT requested geometry optimization, the program does calculations to locate the minimum energy structure followed by property calculations with the optimized geometrical parameters. Refer the flow chat of geometry optimization supplied at the beginning of this calculation.

Conclusions: This chapter deals with geometry optimization procedure at HF level of theory. Results are discussed in detail with an example. We will now move to examples in the next chapters where calculations are carried out applying electron correlated post HF as well as DFT methods for more accurate results.