Computational Chemistry: What and Why?

Keywords: Ab initio, computational chemistry, Hartree-Fock theory, energy calculation, dipole moment.

What is all about computational chemistry?

Computational chemistry is simply the application of chemical, mathematical and computing skills to solve chemical problems on a computer. One can calculate molecular geometry (bond length, bond angle and dihedral angle), energy (at equilibrium and transition state), rates (how fast a reaction takes place) and various spectroscopic (IR, UV-Vis, NMR etc) and physical properties of molecules. Computational chemistry has broadly the following components: molecular mechanics, *ab initio* and semi-empirical quantum mechanics, density functional methods, molecular dynamics simulation.

Molecular mechanics or force field calculations are based on a model that treats a molecule as a collection of atoms held together by bonds governed by a set of classical mechanical potential (ball and spring). It is easy to calculate the energy of a collection of atoms and bonds, if one knows the equilibrium bond lengths, angles between them and the energy cost of stretching and bending of bonds. Thus, by varying the geometry of a molecule, one can calculate the structure of the molecule corresponding to the minimum energy (geometry optimization). This method relies on force-field with embedded empirical parameters obtained mainly from experiment. It is computationally least intensive and useful with limited computer resources. Molecular mechanics is quite fast to find the minimum energy structure; a molecule of 100 atoms can be optimized in seconds on a standard PC. It can be used for molecules as large as enzymes. It can handle systems of more than thousand atoms but this technique does not provide information on electronic structure of a molecule.

Ab initio (Latin: 'from the beginning') calculations are based on the Schrodinger equation which describes the behaviour of electrons in a molecule. This method solves Schrodinger equation for a molecule that provides electron distribution and energy of the system considering the values of the fundamental constants and the atomic numbers of the atoms present. However, the Schrodinger equation cannot be solved exactly for a system with more than one electron. Thus, several approximations are adopted for practical purposes. *Ab inito* calculations are computationally demanding; needs good computer resource and applicable for small size molecules. It is mathematically rigorous and useful for a broad range of systems with no input from experiment. On the other hand, semi-empirical calculations are based on Schrodinger equation but parameterized with experimental values. It is computationally less demanding than *ab initio* method and it can handle systems of 100 atoms easily. Density functional theory (DFT) is a quantum mechanical modelling method which uses electron density to calculate energy often fitting the functional with empirical data. DFT is computationally more demanding than semi-empirical methods but faster than *ab initio* correlated (post HF) methods. While electronic structure calculations (*Ab initio*, semi-empirical or DFT) describe the motions of electrons and generate energy surface, molecular dynamics simulation describes the motions of the atoms within a molecule and in presence of surrounding molecules.

How to proceed for calculation?

In the following sections we will discuss how to calculate structure, energy and other properties of a molecule (with examples) at the basic level using a quantum chemistry program. There are many open source programs with academic license designed for quantum chemical calculations. GAMESS is one such program having the capacity to perform almost all sorts of modern quantum chemical calculations.
available at http://www.msg.ameslab.gov/gamess for academic purpose. One has to first register to download the program. This program has hardware dependent components. Depending on the availability of type of computational resource, one may like to download the whole source code or precompiled executable file suitable for 32 or 64 bit processor on a LINUX box. GAMESS is well documented with manual and a few test examples.

The first task is to decide the type of calculations required for a molecule. GAMESS controls the type of calculations by keywords which are required to provide at the beginning of an INPUT file, known as header. So, depending on the requirement of specific type of calculations, one has to provide certain keywords. A typical header which starts with a '$GROUP NAME' and ends with '$END' for calculation of energy of a molecule given in an input file is as follows:

```
********************

$SYSTEM  TIMLIM=600.0  MWORDS=10  MEMDDI=40  $END
$CONTRL  SCFTYP=RHF  ICHARG=0  MULT=1  RUNTYP=ENERGY  COORD=ZMT  $END
$BASIS  GBASIS=N31  NGAUSS=6  NDFUNC=1  NPFUNC=1  $END
$DATA


$END

********************
```

The group ‘SYSTEM’ is for system related input and provides control information for your computer's operation.

TIMLIM = Time limit to stop the job in minutes (600 minutes= 10 hrs).

MWORDS = Maximum replicated memory which your job can use on every node. This is given in units of 1,000,000 words, where a word is defined as 64 bits or 8 bytes.

MEMDDI = Total memory needed for the distributed data interface (DDI) storage, given in units of 1,000,000 words.

So, total memory allotted per core (or processor) = $10 \times 10^6 \times 8$ bytes + $1/n(10 \times 10^6 \times 8$ bytes)

(n = number of core or processor) = 100 MB for n=4 (for a quad core LINUX box).

Total memory requested in the quad core LINUX box is 400 MB.

If your request of total memory is more than the physical memory (RAM) of the computer, the job will not run! To decide on the right amount of memory requirement for a particular job, one may give a ‘CHECK’ run. See the keyword in group ‘CONTRL’ .

****

The group ‘CONTRL’ specifies the level of theory, type of calculations, input coordinate choices, charge and multiplicity of the molecule. The program converts them to internal parameters which then control the execution.

The keyword ‘SCFTYP’ refers to the type of wave function requested for the calculation. At this point, we will restrict ourselves to the following few cases only.

SCFTYP = RHF, Restricted Hartree Fock calculation for closed shell system with even number of electrons.
= UHF, Unrestricted Hartree Fock calculation for open shell systems with odd number of electrons.
= ROHF, Restricted open shell Hartree Fock calculation for open shell system with odd number of electrons.

ICHARG=0 if the molecule is neutral, for a uninegatively charged system it is -1 and for a unipositively charged system it is 1 and so on.

MULT=1 if the electronic state is Singlet, it is 2 for a Doublet system and 3 for Triplet electronic state. One has to provide right type of ‘SCFTYP’ for different electronic state.

RUNTYP=ENERGY if you want to calculate only energy of the system with the supplied geometrical input. If you want to calculate the minimum energy structure, you have to give RUNTYP=OPTIMIZE.

If you want to check the INPUT and MEMORY requirement for your INPUT, add a keyword to ‘CONTRL’ group as EXETYP=CHECK. This will not do actual calculation but will do an assessment of MEMORY requirement for your job and check the INPUT if it is given correctly or not. See the output of the check run and modify the MEMORY requirement of your job.

The keyword 'COORD' controls the way of initial geometrical parameters of the INPUT molecule to be supplied in 'DATA' group. COORD=CART specifies the INPUT of the molecule to be given in Cartesian Co-ordinate only. COORD=ZMT requires the INPUT specification should be provided in Z-Matrix format. We will now discuss this aspect for INPUT specification of H_2O and H_2CO molecules.

The following three rows show the INPUT specification of H_2O molecule in Cartesian Co-ordinate. The first column is for the atom followed by atomic number. The next three columns are for the values of X, Y and Z co-ordinates. One has to start with the central atom as the number one atom and heavier atoms should be at the beginning rows.

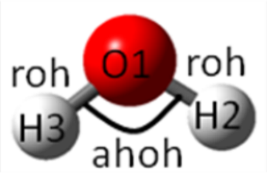
```
 O            8.0     0.0000000000        -0.1313355536         0.0000000000
 H            1.0     1.6697650855         1.0421950037         0.0000000000
 H            1.0    -1.6697650855         1.0421950037         0.0000000000
```

With the same INPUT philosophy in Cartesian Co-ordinate (COORD=CART), it is given for H2CO molecule.

```
 C            6.0     0.0000000000         0.0000000000        -1.2407939767
 O            8.0     0.0000000000         0.0000000000         1.2158498073
 H            1.0     1.7674747685         0.0000000000        -2.2612460101
 H            1.0    -1.7674747685         0.0000000000        -2.2612460101
```

A different way of defining geometrical parameters of a molecule is by Z-Matrix (COORD=ZMT) which is intuitively simpler to a chemist. The first set of data is made for an INPUT of H_2O molecule. Oxygen atom (central and heavier) is considered as the first atom. One H atom is considered as the second atom which is connected to the first atom by a bond distance, roh. The third atom, another H atom is connected to the first atom by bond distance, roh and the second atom (H) by a bond angle, ahoh. This is a three atom system and this Z-Matrix defines the molecule uniquely. The value of bond distance and bond angle variables are given after a blank line. So, in the present Z-Matrix of 3 rows and 5 columns, the first column refers to atom name, second and forth columns specify the bond distance and bond angle connectivity respectively. Third and fifth columns refer to bond distance and bond angle variables. Note that only one bond distance variable is given in this case as the molecule is symmetric and two bond distances are same.

```
O
H    1    roh
H    1    roh    2    ahoh
```

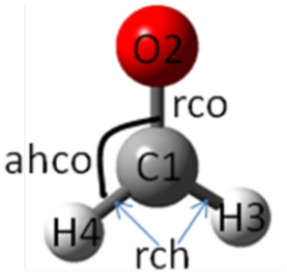


```
roh=1.08
ahoh=109.5
```

Now, we will consider a molecule of atoms where we need to include another variable (dihedral angle) to define the molecule uniquely. Dihedral angle is the angle between two planes. To explain this point, we consider formaldehyde (H_2CO) molecule. We have two heavy atoms and the central atom is C. So it is now atom number 1. We put O as the second atom which is connected to the atom1 (C) by a bond (2-1). One of the two H atoms is taken as atom number 3 and it is connected to atom1 by a bond (3-1) and atom3 by an angle (3-1-2). Atoms 1, 2 & 3 are in a plane. For atom4, apart from bond and angle, we need to include another parameter to define its orientation in space uniquely. This is done by the variable dihedral angle, dhcoh (see the following Z-Matrix) which is the angle between planes 4-1-2 and 1-2-3. If the 4th atom is in the same plane of atoms 1, 2, 3 and in the same side of the bond 1-2 with respect to atom3, dihedral angle should be zero and it is in the other side of the bond 1-2, dihedral angle should be 180. If it is not in the same plane, one has to give appropriate angle for its spatial orientation.

```
C
O     1     rco
H     1     rch     2     ahco
H     1     rch     2     ahco     3     dhcoh

rco=1.3
rch=1.08
ahco=120.0
dhcoh=180.0
```

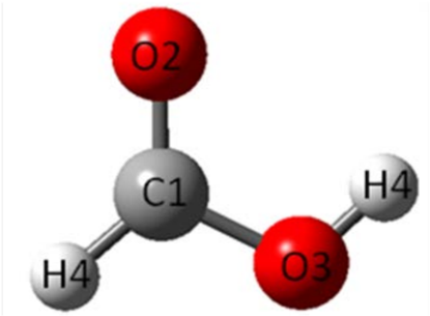


dhcoh is the angle between H3C1O2 & H4C1O2 planes

For a molecule with more than 4 atoms, one has to follow the same INPUT philosophy in Z-Matrix format based on the connectivity of atom5 and others. To illustrate this aspect for your convenience, we now give the Z-Matrix of formic acid (HCOOH), a molecule of five atoms.

```
C
O     1     rco1
O     1     rco2     2     aoco
H     1     rch      2     ahco     3     dhcoo
H     3     roh      1     ahoc     2     dhoco

rco1=1.3
```



```
rco2=1.3
rch=1.08
roh=1.0
aoco=120.0
ahoc=109.5
dhcoo=180.0
dhoco=0.0
```

****

The group ‘BASIS’ decides on a mathematical basis function to describe electronic wave function of the molecule. A sum of atom centres Gaussian functions is the most common approach, $\Psi = \sum C_i e^{-\alpha_i r^2}$. Large basis sets have more freedom to properly describe the electronic state of the molecule. At the same time, large basis sets can drastically increase the cost of a calculation. At present we will use an atomic basis function which is most commonly used, namely, 6-31G(d,p) and this is also expressed as 6-31G**. This particular basis set is equivalent to the following basis set in keywords of GAMESS. We will discuss different types of basis sets available and also on how to decide a particular basis set for a particular type of calculation later.

```
$BASIS  GBASIS=N31  NGAUSS=6  NDFUNC=1  NPFUNC=1  $END
```

****

After deciding on a particular basis set and providing the appropriate keywords for it, one has to work on the group ‘DATA’.

In this group, the first line is reserved for the title of your calculation. Title should be brief but should carry the information on the type of calculations. In the following example, the title is “Water-Energy//RHF/6-31G(d,p)”. This implies that it is an energy calculation is for water molecule at ‘Restricted Hartree Fock’ level of theory with 6-31G(d,p) atomic basis set.

The next line is to give information on symmetry of the molecule. One may give a proper point group of the system or give geometrical data in such a way that the molecule belongs to a particular symmetry with C_1 point group as given in the following example. After this information, a blank line should be added before providing actual geometrical parameters. In this example, geometrical information is provided to the program in Z-Matrix format. So, INPUT of water molecule is ready for single point energy calculation based on electronic structure theory as follows:

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

O
H    1    roh
H    1    roh    2    ahoh

roh=1.08
ahoh=109.5
$END
```

****

This input information should be saved in a file with filename extension 'inp' on the LINUX machine where you want to run this job eg. at present this file is saved as 'water-eng-hf.inp'. The next step is to run GAMESS with this input file.

18.3 How to run a job?

If you have downloaded and installed the LINUX version of games program suitable for your machine, you will find a document is provided for the steps to follow to run GAMESS. First thing is to modify the 'script' provided to run games on your machine. This essentially needs to give the path of your 'working directory', path for the location of 'games executive file' and path of a 'scratch' directory. You need to create a directory named as 'scratch' with enough disk space. The program keeps some necessary files while running a job in this directory. Once the job is completed, these files will be removed. You may modify your 'script' to do this operation once the calculation is over. GAMESS runs under sequential as well as parallel environment. Data communication in this program is done through 'distributed data interface' or 'ddi'. The pre-compiled version of games comes with ddi executive file 'ddi.exe' also. You have to give right path for the location of 'ddi.exe' in the script. Finally you may submit the job from your working directory typing the following syntax.

```
./rungms  water-eng-hf  >  water-eng-hf.log
```

Note that 'rungms' is the appropriately modified script to run games on your LINUX box. The input file is water-eng-hf.inp having different group with keywords and geometrical information. The output data will be saved in a file named as water-eng-hf.log. The following few pages will display the output of this run.

How to analyze output?

```
********************


----- GAMESS execution script -----
This job is running on host dkm103.barc.gov.in
under operating system Linux at Fri Mar 16 13:45:42 EDT 2012
Available scratch disk space (Kbyte units) at beginning of the job is
The generated host list is
dkm103:cpus=8

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

          ******************************************************
          *         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.DUPUIS, 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,
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DUDLEY,
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     GRANT MERRILL, NORIYUKI MINEZAWA, JONATHAN MULLIN, TAKESHI NAGATA,
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  ADDITIONAL CODE HAS BEEN PROVIDED BY COLLABORATORS IN OTHER GROUPS:
     IOWA STATE UNIVERSITY:
          JOE IVANIC, LAIMUTIS BYTAUTAS, KLAUS RUEDENBERG
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          KIYOSHI YAGI, MAHITO CHIBA, SEIKEN TOKURA, NAOAKI KAWAKAMI
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     UNIVERSITY OF PISA: BENEDETTA MENNUCCI, JACOPO TOMASI
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     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
```

This job was running on a LINUX machine with 8 cpu

```
          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 13:45:43 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=ENERGY 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>
   10000000 WORDS OF MEMORY AVAILABLE

     BASIS OPTIONS
     -------------
     GBASIS=N31          IGAUSS=       6      POLAR=POPN31
     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
```

INPUT

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

 ATOM        ATOMIC                       COORDINATES  (BOHR)
             CHARGE          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
```

INPUT in Z-Matrix format is converted to Cartesian coordinate. Note that all the calculations are carried out in Cartesian coordinate only.

```
         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
```

Input on basis set has been converted to internal parameters based on program data library on 6-31G** basis set requested for H_2O molecule.

```
     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

      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
```

Note that there are 25 Cartesian Gaussian Basis Functions....Schrodinger equation will be solved to calculate electronic energy and added to this to find the total energy of the system.

```
     $CONTRL OPTIONS
     ---------------
 SCFTYP=RHF          RUNTYP=ENERGY       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.
 PARALL= T  BALTYP=  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: NPREO=     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=     0.02 TOTAL CPU TIME=        0.0 (    0.0 MIN)
TOTAL WALL CLOCK TIME=        0.4 SECONDS, CPU UTILIZATION IS   5.41%

         ********************
         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=        0.4 SECONDS, CPU UTILIZATION IS   4.55%

         -------------
         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...this is by default!
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
...... END OF INITIAL ORBITAL SELECTION ......
CPU     0: STEP CPU TIME=     0.00 TOTAL CPU TIME=        0.0 (    0.0 MIN)
TOTAL WALL CLOCK TIME=        0.6 SECONDS, CPU UTILIZATION IS   3.57%

                   ----------------------
                   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 =    2
II,JST,KST,LST =  5  1  1  1 NREC =         1 INTLOC =    5
II,JST,KST,LST =  6  1  1  1 NREC =         1 INTLOC =    5
II,JST,KST,LST =  7  1  1  1 NREC =         1 INTLOC =  194
II,JST,KST,LST =  8  1  1  1 NREC =         1 INTLOC = 2757
II,JST,KST,LST =  9  1  1  1 NREC =         1 INTLOC = 2757
II,JST,KST,LST = 10  1  1  1 NREC =         1 INTLOC = 2757
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=        0.7 SECONDS, CPU UTILIZATION IS   6.06%
```

Actual calculation starts here.......

```
         --------------------------
                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
   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
```

SCF converges as the energy change in two consecutive iteration cycles (9 & 10) is within the preset limit.

```
          -----------------
          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
          ------------
```

This 25 X 25 Matrix as there are 25 Cartesian Gaussian Basis Functions!

```
                      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
    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
    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=        1.1 SECONDS, CPU UTILIZATION IS   3.64%

     ----------------------------------------------------------------
     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
```

Calculated
Total
Energy

```
                  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
              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
```

Calculated Atomic Charge

```
          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
 ATOM PAIR DIST        ORDER     ATOM PAIR DIST    ORDER

   1    2  1.080       0.864       1    3  1.080   0.864
```

Calculated Bond Order

```
                          TOTAL       BONDED        FREE
     ATOM                VALENCE     VALENCE     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.)
         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=          0.0 (    0.0 MIN)
 TOTAL WALL CLOCK TIME=         1.2 SECONDS, CPU UTILIZATION IS   4.10%
               580000  WORDS OF DYNAMIC MEMORY USED
 EXECUTION OF GAMESS TERMINATED NORMALLY Fri Mar 16 13:45:44 2012
 DDI: 263624 bytes (0.3 MB / 0 MWords) used by master data server.

 ----------------------------------------
 CPU timing information for all processes
 ========================================
 0: 0.17 + 0.45 = 0.63
 1: 0.07 + 0.32 = 0.40
 2: 0.11 + 0.31 = 0.43
 3: 0.08 + 0.26 = 0.35
 4: 0.11 + 0.33 = 0.45
 5: 0.06 + 0.23 = 0.30
 6: 0.05 + 0.27 = 0.33
 7: 0.09 + 0.22 = 0.32
 ----------------------------------------
 ddikick.x: exited gracefully.
Fri Mar 16 13:45:47 EDT 2012
0.218u 0.128s 0:04.93 6.6%   0+0k 8+24io 0pf+0w
```

Calculated Dipole Moment

The output ends here. Since the INPUT requested only for energy calculation, the program does energy and property calculations only with the supplied geometrical parameters.

****

18.5 Conclusions

This chapter introduces a reader about several components of computational chemistry with its advantages and drawbacks. It also talks on preparing an INPUT file for an *ab initio* HF calculation applying GAMESS suit of electron structure theory program. Finally, it also interprets data in the OUTPUT file.