Example I: Total energy of Benzene within MP2 approximation

In this example we will calculate the total energy of the benzene using the MP2 approximation.

Let us look at the input file

The first directive "echo" is optional but highly recommended. Its purpose is to write out the contents of your input file into the output file.

```
echo
```

The "title" is also optional. You might want to put a short sentence identifying the nature of your calculation .

```
title "total energy of benzene, MP2/3-21G"
```

The "start" directive is required. It indicates that this is a new calculation and sets up the name of the database to store your results.

```
start c6h6-mp2
```

The name of the database file that you would like to associate with this calculation

```
scratch_dir    ./scratch
permanent_dir  ./perm
```

The location of permanent and scratch directories. The scratch directory contains temporary files. The permanent directory contains essential files which will be required should you wish to restart your calculation

The geometry block specifies the name of the elements that comprise your system as well as their coordinates in the following format:
Name1 x1 y1 z1
Name2 x2 y2 z2
……
Unless indicated otherwise the default units are angstroms, and the system will be centered around the origin.

```
geometry
 C     0.99261000     0.99261000     0.00000000
 C    -1.35593048     0.36332048     0.00000000
 C     0.36332048    -1.35593048     0.00000000
 C    -0.99261000    -0.99261000     0.00000000
 C     1.35593048    -0.36332048     0.00000000
 C    -0.36332048     1.35593048     0.00000000
 H     1.75792000     1.75792000     0.00000000
 H    -2.40136338     0.64344338     0.00000000
 H     0.64344338    -2.40136338     0.00000000
 H    -1.75792000    -1.75792000     0.00000000
 H     2.40136338    -0.64344338     0.00000000
 H    -0.64344338     2.40136338     0.00000000
end
```

The basis block defines which Gaussian basis sets are to be used with the HF calculation.

```
basis
* library 3-21G
end
```

** denotes that all atoms use 3-21G basis. Other basis for atoms can explicitly be defined:*

```
basis
  H library 3-21G
  C library 3-21G
end
```

```
scf
end
```

The scf block contains parameters that define the HF calculation.

```
task scf energy
```

Task directive requests the actual calculation. In this case we are using self-consistent field Hartree-Fock method (scf) and requesting total energy calculation.

Much of the content of the output file is self-explanatory. There is a section in the output file that summarizes the setup of the calculation

....

```
Summary of "ao basis" -> "" (cartesian)
------------------------------------------------------------------------------
      Tag                 Description            Shells   Functions and Types
---------------- ------------------------------  ------  ---------------------
*                           3-21G                   on all atoms


                     Basis "ao basis" -> "ao basis" (cartesian)
                     -----
 C (Carbon)
 ----------
           Exponent  Coefficients
      -------------- ---------------------------------------------------------
 1 S  1.72256000E+02  0.061767
 1 S  2.59109000E+01  0.358794
 1 S  5.53335000E+00  0.700713

 2 S  3.66498000E+00 -0.395897
 2 S  7.70545000E-01  1.215840

 3 P  3.66498000E+00  0.236460
 3 P  7.70545000E-01  0.860619

 4 S  1.95857000E-01  1.000000

 5 P  1.95857000E-01  1.000000

 H (Hydrogen)
 ------------
           Exponent  Coefficients
      -------------- ---------------------------------------------------------
 1 S  5.44717800E+00  0.156285
 1 S  8.24547000E-01  0.904691

 2 S  1.83192000E-01  1.000000


Summary of "ao basis" -> "ao basis" (cartesian)
------------------------------------------------------------------------------
      Tag                 Description            Shells   Functions and Types
---------------- ------------------------------  ------  ---------------------
C                           3-21G                   5        9   3s2p
H                           3-21G                   2        2   2s


                                NWChem SCF Module
                                -----------------


                          total energy of benzene, HF/3-21G


 ao basis        = "ao basis"
 functions       =    66
 atoms           =    12
 closed shells   =    21
 open shells     =     0
 charge          =   0.00
 wavefunction    = RHF
 input vectors   = atomic
```

Gaussian basis sets parameters

```
 output vectors  = ./perm/c6h6-scf.movecs
 use symmetry    = T
 symmetry adapt  = T


Summary of "ao basis" -> "ao basis" (cartesian)
------------------------------------------------------------------------------
      Tag                 Description            Shells   Functions and Types
---------------- ------------------------------  ------  ---------------------
C                            3-21G                  5        9   3s2p
H                            3-21G                  2        2   2s


     Symmetry analysis of basis
     --------------------------

       a1g         7
       a1u         0
       a2g         2
       a2u         2
       b1g         0
       b1u         7
       b2g         2
       b2u         2
       e1g         4
       e1u        18
       e2g        18
       e2u         4


Forming initial guess at       0.6s


     Superposition of Atomic Density Guess
     -------------------------------------

Sum of atomic energies:        -227.75976746

     Non-variational initial energy
     ------------------------------

Total energy =    -231.937013
1-e energy   =    -705.828643
2-e energy   =     271.451090
HOMO         =      -0.283977
LUMO         =       0.017158


     Symmetry analysis of molecular orbitals - initial
     -------------------------------------------------

 Numbering of irreducible representations:

    1 a1g         2 a1u         3 a2g         4 a2u         5 b1g
    6 b1u         7 b2g         8 b2u         9 e1g        10 e1u
   11 e2g        12 e2u

 Orbital symmetries:

    1 a1g         2 e1u         3 e1u         4 b1u         5 e2g
    6 e2g         7 a1g         8 e1u         9 e1u        10 e2g
   11 e2g        12 a1g        13 b1u        14 b2u        15 e1u
   16 e1u        17 a2u        18 e2g        19 e2g        20 e1g
   21 e1g        22 e2u        23 e2u        24 a1g        25 b2g
   26 e1u        27 e1u        28 e2g        29 e2g        30 b1u
   31 e2g


Starting SCF solution at       1.3s
```

```
------------------------------------------------
        Quadratically convergent ROHF

Convergence threshold     :          1.000E-04
Maximum no. of iterations :           20
Final Fock-matrix accuracy:          1.000E-07
------------------------------------------------


Integral file          = ./perm/c6h6-scf.aoints.0
Record size in doubles =  65536        No. of integs per rec  =  43688
Max. records in memory =      6        Max. records in file   = 141042
No. of bits per label  =      8        No. of bits per value  =     64


#quartets = 3.741D+04 #integrals = 1.410D+05 #direct =  0.0% #cached =100.0%


             iter       energy          gnorm     gmax       time
            ----- ------------------ --------- --------- --------
                1     -229.3668943486  7.17D-01  2.50D-01      5.5
                2     -229.4161883416  7.84D-02  2.32D-02      5.8
                3     -229.4167722379  3.49D-03  1.08D-03      6.0
                4     -229.4167733653  1.71D-06  5.91D-07      6.1
```

Usually it takes a few iterations to converge the HF equations

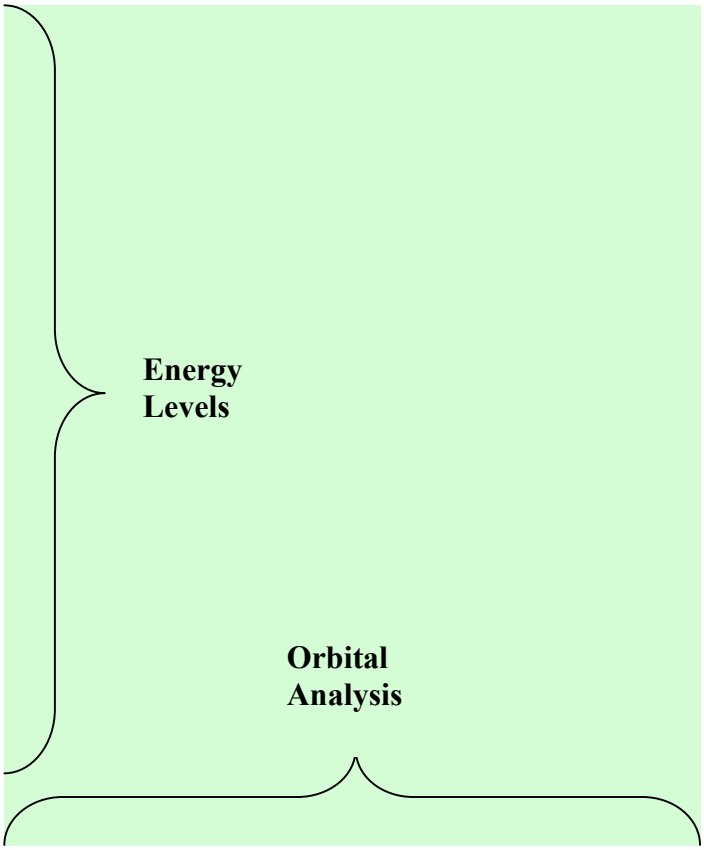
```
      Final RHF  results
      ------------------

        Total SCF energy =   -229.416773365268
     One-electron energy =   -709.316417273146
     Two-electron energy =    277.459104353356
Nuclear repulsion energy =    202.440539554522

       Time for solution =      4.8s
```

Total Energy Analysis

```
      Symmetry analysis of molecular orbitals - final
      -----------------------------------------------

 Numbering of irreducible representations:

    1 a1g         2 a1u         3 a2g         4 a2u         5 b1g
    6 b1u         7 b2g         8 b2u         9 e1g        10 e1u
   11 e2g        12 e2u

 Orbital symmetries:

    1 b1u         2 e2g         3 e2g         4 e1u         5 e1u
    6 a1g         7 a1g         8 e1u         9 e1u        10 e2g
   11 e2g        12 a1g        13 b1u        14 b2u        15 e1u
   16 e1u        17 a2u        18 e2g        19 e2g        20 e1g
   21 e1g        22 e2u        23 e2u        24 a1g        25 e1u
   26 e1u        27 b2g        28 e2g        29 e2g        30 b1u
   31 e2g
```

Final eigenvalues

	1
1	-11.1828
2	-11.1825
3	-11.1825
4	-11.1822
5	-11.1822
6	-11.1816
7	-1.1450
8	-1.0094
9	-1.0094
10	-0.8210
11	-0.8210
12	-0.7116
13	-0.6408
14	-0.6171
15	-0.5885
16	-0.5885
17	-0.5006
18	-0.4902
19	-0.4902
20	-0.3357
21	-0.3357
22	0.1460
23	0.1460
24	0.2546
25	0.3218
26	0.3218
27	0.3644
28	0.3657
29	0.3657
30	0.3683
31	0.4991



ROHF Final Molecular Orbital Analysis

Vector 7 Occ=2.000000D+00 E=-1.145005D+00 Symmetry=a1g
MO Center= -4.1D-17, -1.7D-18, -8.9D-36, r^2= 2.1D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
42	0.184587	5 C s	33	0.184587	4 C s
15	0.184587	2 C s	51	0.184587	6 C s
24	0.184587	3 C s	6	0.184587	1 C s

Vector 8 Occ=2.000000D+00 E=-1.009436D+00 Symmetry=e1u
MO Center= 3.6D-17, -2.8D-16, 1.1D-18, r^2= 2.9D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
24	0.299828	3 C s	51	-0.299828	6 C s
33	0.253459	4 C s	6	-0.253459	1 C s

Vector 9 Occ=2.000000D+00 E=-1.009436D+00 Symmetry=e1u
MO Center= -2.6D-16, 1.8D-16, -1.2D-18, r^2= 2.9D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
42	0.319441	5 C s	15	-0.319441	2 C s
33	-0.199877	4 C s	6	0.199877	1 C s

Vector 10 Occ=2.000000D+00 E=-8.210207D-01 Symmetry=e2g
MO Center= -3.0D-16, 2.8D-17, -2.1D-21, r^2= 3.7D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
51	0.342851	6 C s	24	0.342851	3 C s
33	-0.201167	4 C s	6	-0.201167	1 C s
13	0.153965	2 C py	40	-0.153965	5 C py

Vector 11 Occ=2.000000D+00 E=-8.210207D-01 Symmetry=e2g
MO Center= 9.3D-17, -6.1D-17, -3.8D-21, r^2= 3.7D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
15	0.314089	2 C s	42	0.314089	5 C s
33	-0.279746	4 C s	6	-0.279746	1 C s
21	0.172949	3 C px	48	-0.172949	6 C px

Vector 12 Occ=2.000000D+00 E=-7.116373D-01 Symmetry=a1g
MO Center= -1.0D-17, -3.5D-17, -2.6D-35, r^2= 4.2D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
39	0.163127	5 C px	12	-0.163127	2 C px
49	0.163127	6 C py	22	-0.163127	3 C py

Vector 13 Occ=2.000000D+00 E=-6.408308D-01 Symmetry=b1u
MO Center= -9.0D-17, -9.0D-17, 2.8D-34, r^2= 5.3D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
6	0.195323	1 C s	33	-0.195323	4 C s
15	0.195323	2 C s	42	-0.195323	5 C s
24	0.195323	3 C s	51	-0.195323	6 C s

Vector 14 Occ=2.000000D+00 E=-6.171063D-01 Symmetry=b2u
MO Center= -1.2D-16, -6.3D-17, 1.0D-36, r^2= 2.8D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
40	0.235666	5 C py	13	0.235666	2 C py
21	-0.235666	3 C px	48	-0.235666	6 C px
30	0.172519	4 C px	31	-0.172519	4 C py
4	-0.172519	1 C py	3	0.172519	1 C px

Vector 15 Occ=2.000000D+00 E=-5.885335D-01 Symmetry=e1u
MO Center= -2.4D-17, 1.2D-16, 6.0D-37, r^2= 4.1D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
49	0.222550	6 C py	22	0.222550	3 C py
26	0.176377	3 C py	53	0.176377	6 C py
3	0.175644	1 C px	30	0.175644	4 C px

Vector 16 Occ=2.000000D+00 E=-5.885335D-01 Symmetry=e1u
MO Center= 2.8D-16, 8.3D-17, -2.2D-35, r^2= 4.1D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
39	0.243564	5 C px	12	0.243564	2 C px
43	0.191748	5 C px	16	0.191748	2 C px
4	0.152308	1 C py	31	0.152308	4 C py
57	-0.151768	8 H s	63	0.151768	11 H s

Vector 17 Occ=2.000000D+00 E=-5.006215D-01 Symmetry=a2u
MO Center= 5.2D-17, 1.4D-17, 4.8D-32, r^2= 2.8D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
5	0.179936	1 C pz	14	0.179936	2 C pz
23	0.179936	3 C pz	32	0.179936	4 C pz
41	0.179936	5 C pz	50	0.179936	6 C pz
27	0.176567	3 C pz	45	0.176567	5 C pz
9	0.176567	1 C pz	54	0.176567	6 C pz

Vector 18 Occ=2.000000D+00 E=-4.902455D-01 Symmetry=e2g
MO Center= 2.2D-16, 1.3D-15, 1.5D-19, r^2= 4.1D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
26	0.229054	3 C py	53	-0.229054	6 C py
13	0.222131	2 C py	40	-0.222131	5 C py
4	0.210241	1 C py	31	-0.210241	4 C py
49	-0.191293	6 C py	22	0.191293	3 C py
8	0.186988	1 C py	35	-0.186988	4 C py

Vector 19 Occ=2.000000D+00 E=-4.902455D-01 Symmetry=e2g
MO Center= 2.2D-16, 4.7D-17, -1.3D-33, r^2= 4.1D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function

21	-0.224484	3 C	px	48	0.224484	6 C	px
43	0.223830	5 C	px	16	-0.223830	2 C	px
3	-0.205535	1 C	px	30	0.205535	4 C	px
34	0.197435	4 C	px	7	-0.197435	1 C	px
12	-0.193646	2 C	px	39	0.193646	5 C	px

Vector 20 Occ=2.000000D+00 E=-3.357365D-01 Symmetry=e1g
MO Center= -4.5D-17, -9.7D-17, -3.5D-18, r^2= 3.1D+00

Bfn.	Coefficient	Atom+Function		Bfn.	Coefficient	Atom+Function	
9	0.323596	1 C	pz	36	-0.323596	4 C	pz
32	-0.265577	4 C	pz	5	0.265577	1 C	pz
27	-0.197327	3 C	pz	54	0.197327	6 C	pz
23	-0.161947	3 C	pz	50	0.161947	6 C	pz

Vector 21 Occ=2.000000D+00 E=-3.357365D-01 Symmetry=e1g
MO Center= -6.9D-17, -5.6D-17, 3.7D-18, r^2= 3.1D+00

Bfn.	Coefficient	Atom+Function		Bfn.	Coefficient	Atom+Function	
18	0.300755	2 C	pz	45	-0.300755	5 C	pz
27	-0.259730	3 C	pz	54	0.259730	6 C	pz
14	0.246831	2 C	pz	41	-0.246831	5 C	pz
50	0.213161	6 C	pz	23	-0.213161	3 C	pz

Vector 22 Occ=0.000000D+00 E= 1.459825D-01 Symmetry=e2u
MO Center= 8.3D-17, -1.1D-16, -3.1D-19, r^2= 3.5D+00

Bfn.	Coefficient	Atom+Function		Bfn.	Coefficient	Atom+Function	
27	0.531815	3 C	pz	54	0.531815	6 C	pz
36	-0.499907	4 C	pz	9	-0.499907	1 C	pz
50	0.240042	6 C	pz	23	0.240042	3 C	pz
5	-0.225639	1 C	pz	32	-0.225639	4 C	pz

Vector 23 Occ=0.000000D+00 E= 1.459825D-01 Symmetry=e2u
MO Center= -1.3D-16, -1.4D-17, 1.7D-19, r^2= 3.5D+00

Bfn.	Coefficient	Atom+Function		Bfn.	Coefficient	Atom+Function	
18	0.595665	2 C	pz	45	0.595665	5 C	pz
9	-0.325466	1 C	pz	36	-0.325466	4 C	pz
27	-0.270199	3 C	pz	54	-0.270199	6 C	pz
14	0.268861	2 C	pz	41	0.268861	5 C	pz

Vector 24 Occ=0.000000D+00 E= 2.546186D-01 Symmetry=a1g
MO Center= 2.8D-16, -2.8D-16, -7.8D-34, r^2= 8.1D+00

Bfn.	Coefficient	Atom+Function		Bfn.	Coefficient	Atom+Function	
56	0.733362	7 H	s	58	0.733362	8 H	s
60	0.733362	9 H	s	62	0.733362	10 H	s
64	0.733362	11 H	s	66	0.733362	12 H	s
6	-0.534084	1 C	s	15	-0.534084	2 C	s
24	-0.534084	3 C	s	33	-0.534084	4 C	s

Vector 25 Occ=0.000000D+00 E= 3.217568D-01 Symmetry=e1u
MO Center= -1.5D-15, 8.9D-16, -3.9D-35, r^2= 8.6D+00

Bfn.	Coefficient	Atom+Function		Bfn.	Coefficient	Atom+Function	
58	-1.046788	8 H	s	64	1.046788	11 H	s
66	-1.016830	12 H	s	60	1.016830	9 H	s
15	0.702058	2 C	s	42	-0.702058	5 C	s
51	0.681966	6 C	s	24	-0.681966	3 C	s
16	-0.567722	2 C	px	43	-0.567722	5 C	px

Vector 26 Occ=0.000000D+00 E= 3.217568D-01 Symmetry=e1u
MO Center= -1.9D-16, 3.9D-16, -2.2D-34, r^2= 8.6D+00

Bfn.	Coefficient	Atom+Function		Bfn.	Coefficient	Atom+Function	
56	1.191430	7 H	s	62	-1.191430	10 H	s
6	-0.799066	1 C	s	33	0.799066	4 C	s
60	-0.621660	9 H	s	66	0.621660	12 H	s
64	0.569771	11 H	s	58	-0.569771	8 H	s
34	-0.468654	4 C	px	7	-0.468654	1 C	px

Vector 27 Occ=0.000000D+00 E= 3.644467D-01 Symmetry=b2g
            MO Center= 3.0D-16, -2.8D-17, -9.9D-20, r^2= 3.8D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
45	0.620218	5 C pz	27	-0.620218	3 C pz
54	0.620218	6 C pz	18	-0.620218	2 C pz
9	-0.620218	1 C pz	36	0.620218	4 C pz
23	-0.210799	3 C pz	14	-0.210799	2 C pz
41	0.210799	5 C pz	50	0.210799	6 C pz

Vector 28 Occ=0.000000D+00 E= 3.656570D-01 Symmetry=e2g
            MO Center= -1.9D-15, -1.1D-15, -3.2D-21, r^2= 8.5D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
51	1.473477	6 C s	24	1.473477	3 C s
66	-1.195656	12 H s	60	-1.195656	9 H s
33	-0.769710	4 C s	6	-0.769710	1 C s
15	-0.703767	2 C s	42	-0.703767	5 C s
62	0.624583	10 H s	56	0.624583	7 H s

Vector 29 Occ=0.000000D+00 E= 3.656570D-01 Symmetry=e2g
            MO Center= 3.8D-16, -1.4D-15, -6.3D-22, r^2= 8.5D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
42	1.295104	5 C s	15	1.295104	2 C s
33	-1.257032	4 C s	6	-1.257032	1 C s
64	-1.050915	11 H s	58	-1.050915	8 H s
62	1.020021	10 H s	56	1.020021	7 H s
43	0.506509	5 C px	16	-0.506509	2 C px

Vector 30 Occ=0.000000D+00 E= 3.682704D-01 Symmetry=b1u
            MO Center= -3.2D-15, -1.6D-15, -8.5D-21, r^2= 9.5D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
60	1.077887	9 H s	58	1.077887	8 H s
66	-1.077887	12 H s	62	-1.077887	10 H s
64	-1.077887	11 H s	56	1.077887	7 H s
26	0.933938	3 C py	16	0.933938	2 C px
53	0.933938	6 C py	43	0.933938	5 C px

Vector 31 Occ=0.000000D+00 E= 4.990941D-01 Symmetry=e2g
            MO Center= 4.1D-16, 8.7D-16, 2.2D-20, r^2= 4.9D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
33	1.715775	4 C s	6	1.715775	1 C s
7	-1.077045	1 C px	34	1.077045	4 C px
8	-1.038433	1 C py	35	1.038433	4 C py
51	-0.908863	6 C s	24	-0.908863	3 C s
56	0.866184	7 H s	62	0.866184	10 H s

Vector 32 Occ=0.000000D+00 E= 4.990941D-01 Symmetry=e2g
            MO Center= 2.1D-15, -1.2D-15, 3.2D-21, r^2= 4.9D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
15	1.515336	2 C s	42	1.515336	5 C s
24	-1.456474	3 C s	51	-1.456474	6 C s
43	-1.372974	5 C px	16	1.372974	2 C px
26	-1.335645	3 C py	53	1.335645	6 C py
64	0.764995	11 H s	58	0.764995	8 H s

Vector 33 Occ=0.000000D+00 E= 5.131039D-01 Symmetry=e1u
            MO Center= 1.8D-15, 1.4D-15, 6.1D-34, r^2= 4.9D+00

Bfn.	Coefficient	Atom+Function	Bfn.	Coefficient	Atom+Function
51	1.596055	6 C s	24	-1.596055	3 C s
42	-1.359989	5 C s	15	1.359989	2 C s
8	-1.317120	1 C py	35	-1.317120	4 C py
7	1.275548	1 C px	34	1.275548	4 C px
17	-1.141368	2 C py	44	-1.141368	5 C py

center of mass
----
x =   0.00000000 y =   0.00000000 z =   0.00000000

moments of inertia (a.u.)

        320.062201089014   0.000000000000   0.000000000000
          0.000000000000   320.062201089014   0.000000000000
          0.000000000000   0.000000000000   640.124402178029

 Mulliken analysis of the total density

   Atom   Charge   Shell Charges
-----------   ------   ---
   1 C   6   6.24   1.99 0.40 1.59 0.89 1.37
   2 C   6   6.24   1.99 0.40 1.59 0.89 1.37
   3 C   6   6.24   1.99 0.40 1.59 0.89 1.37
   4 C   6   6.24   1.99 0.40 1.59 0.89 1.37
   5 C   6   6.24   1.99 0.40 1.59 0.89 1.37
   6 C   6   6.24   1.99 0.40 1.59 0.89 1.37
   7 H   1   0.76   0.47 0.29
   8 H   1   0.76   0.47 0.29
   9 H   1   0.76   0.47 0.29
  10 H   1   0.76   0.47 0.29
  11 H   1   0.76   0.47 0.29
  12 H   1   0.76   0.47 0.29

Mulliken and Multipole Analysis

      Multipole analysis of the density wrt the origin

    L   x y z   total   open   nuclear
    -   - - -   -----   ----   -------
    0   0 0 0   0.000000   0.000000   42.000000

    1   1 0 0   0.000000   0.000000   0.000000
    1   0 1 0   0.000000   0.000000   0.000000
    1   0 0 1   0.000000   0.000000   0.000000

    2   2 0 0   -23.337595   0.000000   192.878835
    2   1 1 0   0.000000   0.000000   0.000000
    2   1 0 1   0.000000   0.000000   0.000000
    2   0 2 0   -23.337595   0.000000   192.878835
    2   0 1 1   0.000000   0.000000   0.000000
    2   0 0 2   -30.731480   0.000000   0.000000

Example II: Structural optimization of benzene within the Hartree-Fock approximation

In this example we will optimize the structure of benzene using results generated from prior energy calculation. Since most of the parameters are already stored in the database the input is very simple.

Input file:

```
echo

title "optimization of benzene HF/3-21G

restart c6h6-scf

scratch_dir ./scratch
permanent_dir ./perm


driver

  maxiter 20

  xyz benzene

end


task scf optimize
```

The "restart" directive indicates that we will reusing the results from our previous calculation. Notice the name of the database file

Previously generated files in permanent directory will be reused

The driver block defines optimization parameters.

Maximum number of iterations is 20

The structural snapshots of the system will be generated at each step in xyz format with file prefix s2 (e.g. s2-001.xyz, ...)

Task directive to commence structural optimization using scf method

As the optimization process consists of series of total energy evaluations the contents of the output file are very much similar to that in Example I. At each step the total energy and force information will be outputted as follows

```
  Step         Energy      Delta E   Gmax     Grms     Xrms     Xmax   Walltime
  ---- ---------------- -------- -------- -------- -------- -------- --------
@    1   -229.41944507 -2.7D-03  0.00026  0.00009  0.02735  0.05411     15.6
                                     ok       ok
```

Step number

Total Energy and its Change with respect to last step

Maximum value of the force and its RMS average

The best way to keep track of the optimization calculation is to run the following command on the output file:

```
grep @  outputfile
```

Example III: Frequency calculation of benzene within the Hartree-Fock approximation

In this example we will calculate the vibrational frequency of benzene for the optimized geometry calculated in Example II.

Input file:

```
echo

title "frequency generation of benzene 3-21G"

restart c6h6-scf

scratch_dir ./scratch
permanent_dir ./perm


freq
 animate
end


task scf freq
```

The "restart" directive indicates that we will reusing the results from our previous geometry optimization calculation.

Previously generated files in permanent directory will be reused

The frequency block is optional. The animation keyword directs the program to generate XYZ files to animate vibrational modes.

Task directive to commence frequency calculation using pspw method

Output file:

Raw Frequencies including rotational and translation degrees of freedom

....

```
          -------------------------------------------------
          NORMAL MODE EIGENVECTORS IN CARTESIAN COORDINATES
          -------------------------------------------------
                 (Frequencies expressed in cm-1)

                       1           2           3           4           5           6

 Frequency         -1.39        0.01        1.39        2.86        2.90        3.12
```

1	0.09804	0.00000	-0.05659	0.00000	0.00000	-0.07411
2	0.05658	0.00000	0.09804	0.00000	0.00000	0.07410
3	0.00000	0.11319	0.00000	-0.00035	-0.14822	0.00000
4	0.09804	0.00000	-0.05658	0.00000	0.00000	-0.02712
5	0.05658	0.00000	0.09803	0.00000	0.00000	-0.10124
6	0.00000	0.11319	0.00000	0.12853	0.07381	0.00000
7	0.09804	0.00000	-0.05658	0.00000	0.00000	0.10124
8	0.05658	0.00000	0.09804	0.00000	0.00000	0.02712
9	0.00000	0.11319	0.00000	-0.12819	0.07441	0.00000
10	0.09804	0.00000	-0.05658	0.00000	0.00000	0.07411
11	0.05658	0.00000	0.09803	0.00000	0.00000	-0.07411
12	0.00000	0.11319	0.00000	0.00035	0.14822	0.00000
13	0.09804	0.00000	-0.05658	0.00000	0.00000	0.02713
14	0.05658	0.00000	0.09804	0.00000	0.00000	0.10123
15	0.00000	0.11319	0.00000	-0.12853	-0.07381	0.00000
16	0.09804	0.00000	-0.05659	0.00000	0.00000	-0.10123
17	0.05658	0.00000	0.09804	0.00000	0.00000	-0.02713
18	0.00000	0.11319	0.00000	0.12819	-0.07441	0.00000
19	0.09804	0.00000	-0.05659	0.00000	0.00000	-0.13149
20	0.05658	0.00000	0.09805	0.00000	0.00000	0.13149
21	0.00000	0.11319	0.00000	-0.00062	-0.26300	0.00000
22	0.09804	0.00000	-0.05658	0.00000	0.00000	-0.04813
23	0.05658	0.00000	0.09803	0.00000	0.00000	-0.17963
24	0.00000	0.11319	0.00000	0.22808	0.13096	0.00000
25	0.09804	0.00000	-0.05657	0.00000	0.00000	0.17963
26	0.05658	0.00000	0.09804	0.00000	0.00000	0.04813
27	0.00000	0.11319	0.00000	-0.22746	0.13204	0.00000
28	0.09804	0.00000	-0.05657	0.00000	0.00000	0.13150
29	0.05658	0.00000	0.09803	0.00000	0.00000	-0.13150
30	0.00000	0.11319	0.00000	0.00062	0.26300	0.00000
31	0.09804	0.00000	-0.05658	0.00000	0.00000	0.04814
32	0.05658	0.00000	0.09805	0.00000	0.00000	0.17962
33	0.00000	0.11319	0.00000	-0.22808	-0.13096	0.00000
34	0.09804	0.00000	-0.05659	0.00000	0.00000	-0.17962
35	0.05658	0.00000	0.09804	0.00000	0.00000	-0.04814
36	0.00000	0.11319	0.00000	0.22746	-0.13204	0.00000

	7	8	9	10	11	12
Frequency	466.30	466.30	698.30	698.30	784.48	819.80
1	0.00000	0.00000	0.06758	-0.09010	0.00000	0.00000
2	0.00000	0.00000	-0.02059	-0.11072	0.00000	0.00000
3	0.00007	-0.13862	0.00000	0.00000	-0.03280	0.09746
4	0.00000	0.00000	-0.11408	-0.08429	0.00000	0.00000
5	0.00000	0.00000	-0.01478	0.07093	0.00000	0.00000
6	-0.12008	0.06925	0.00000	0.00000	-0.03280	0.09746
7	0.00000	0.00000	-0.01822	0.07013	0.00000	0.00000
8	0.00000	0.00000	0.13963	-0.02493	0.00000	0.00000
9	0.12001	0.06937	0.00000	0.00000	-0.03280	0.09746
10	0.00000	0.00000	-0.06758	0.09010	0.00000	0.00000
11	0.00000	0.00000	0.02059	0.11072	0.00000	0.00000
12	0.00007	-0.13862	0.00000	0.00000	-0.03280	-0.09746
13	0.00000	0.00000	0.11408	0.08428	0.00000	0.00000
14	0.00000	0.00000	0.01478	-0.07093	0.00000	0.00000
15	-0.12008	0.06925	0.00000	0.00000	-0.03280	-0.09746

16	0.00000	0.00000	0.01822	-0.07013	0.00000	0.00000
17	0.00000	0.00000	-0.13963	0.02493	0.00000	0.00000
18	0.12001	0.06937	0.00000	0.00000	-0.03280	-0.09746
19	0.00000	0.00000	-0.03637	-0.11413	0.00000	0.00000
20	0.00000	0.00000	0.08322	-0.08616	0.00000	0.00000
21	0.00016	-0.31932	0.00000	0.00000	0.39059	0.22864
22	0.00000	0.00000	-0.08709	-0.11251	0.00000	0.00000
23	0.00000	0.00000	0.08485	-0.03543	0.00000	0.00000
24	-0.27661	0.15952	0.00000	0.00000	0.39059	0.22864
25	0.00000	0.00000	-0.06032	-0.06939	0.00000	0.00000
26	0.00000	0.00000	0.12797	-0.06220	0.00000	0.00000
27	0.27646	0.15979	0.00000	0.00000	0.39059	0.22864
28	0.00000	0.00000	0.03637	0.11413	0.00000	0.00000
29	0.00000	0.00000	-0.08322	0.08616	0.00000	0.00000
30	0.00016	-0.31932	0.00000	0.00000	0.39059	-0.22864
31	0.00000	0.00000	0.08709	0.11251	0.00000	0.00000
32	0.00000	0.00000	-0.08485	0.03543	0.00000	0.00000
33	-0.27661	0.15952	0.00000	0.00000	0.39059	-0.22864
34	0.00000	0.00000	0.06032	0.06939	0.00000	0.00000
35	0.00000	0.00000	-0.12797	0.06220	0.00000	0.00000
36	0.27646	0.15979	0.00000	0.00000	0.39059	-0.22864

.....

Thermodynamics stuff

Temperature = 298.15K

Zero-Point correction to Energy = 68.245 kcal/mol (0.108755 au)
Thermal correction to Energy = 70.750 kcal/mol (0.112748 au)
Thermal correction to Enthalpy = 71.342 kcal/mol (0.113691 au)

Total Entropy = 62.837 cal/mol-K
- Translational = 38.962 cal/mol-K (mol. weight = 78.0469)
- Rotational = 20.660 cal/mol-K (symmetry # = 12)
- Vibrational = 3.216 cal/mol-K

Cv (constant volume heat capacity) = 14.830 cal/mol-K
- Translational = 2.979 cal/mol-K
- Rotational = 2.979 cal/mol-K
- Vibrational = 8.871 cal/mol-K

Note if symmetry not found in input then this might have to be adjusted

Projected Frequencies

NORMAL MODE EIGENVECTORS IN CARTESIAN COORDINATES

(Projected Frequencies expressed in cm-1)

	1	2	3	4	5	6
P.Frequency	0.00	0.00	0.00	0.00	0.00	0.00
1	0.00000	0.00634	0.00000	0.00000	0.13471	0.01089

2	0.00000	0.12607	0.00000	0.00000	-0.04766	0.01181
3	-0.08683	0.00000	0.12547	0.10724	0.00000	0.00000
4	0.00000	0.01969	0.00000	0.00000	0.10546	0.04515
5	0.00000	0.07624	0.00000	0.00000	0.06149	-0.11605
6	0.13082	0.00000	0.12975	-0.02884	0.00000	0.00000
7	0.00000	0.05617	0.00000	0.00000	0.02556	0.13875
8	0.00000	0.11272	0.00000	0.00000	-0.01841	-0.02245
9	0.09609	0.00000	-0.04898	0.15215	0.00000	0.00000
10	0.00000	0.04846	0.00000	0.00000	0.04245	0.11897
11	0.00000	0.08395	0.00000	0.00000	0.04460	-0.09627
12	0.18022	0.00000	0.01203	0.04646	0.00000	0.00000
13	0.00000	0.03511	0.00000	0.00000	0.07169	0.08471
14	0.00000	0.13378	0.00000	0.00000	-0.06454	0.03159
15	-0.03743	0.00000	0.00774	0.18254	0.00000	0.00000
16	0.00000	-0.00137	0.00000	0.00000	0.15159	-0.00890
17	0.00000	0.09730	0.00000	0.00000	0.01536	-0.06201
18	-0.00270	0.00000	0.18647	0.00155	0.00000	0.00000
19	0.00000	-0.00997	0.00000	0.00000	0.17043	-0.03096
20	0.00000	0.14238	0.00000	0.00000	-0.08338	0.05366
21	-0.19022	0.00000	0.16939	0.13077	0.00000	0.00000
22	0.00000	0.01372	0.00000	0.00000	0.11854	0.02983
23	0.00000	0.05396	0.00000	0.00000	0.11028	-0.17322
24	0.19596	0.00000	0.17699	-0.11067	0.00000	0.00000
25	0.00000	0.07845	0.00000	0.00000	-0.02323	0.19592
26	0.00000	0.11869	0.00000	0.00000	-0.03149	-0.00713
27	0.13434	0.00000	-0.14013	0.21046	0.00000	0.00000
28	0.00000	0.06477	0.00000	0.00000	0.00673	0.16082
29	0.00000	0.06764	0.00000	0.00000	0.08032	-0.13812
30	0.28361	0.00000	-0.03189	0.02293	0.00000	0.00000
31	0.00000	0.04108	0.00000	0.00000	0.05862	0.10003
32	0.00000	0.15606	0.00000	0.00000	-0.11334	0.08876
33	-0.10257	0.00000	-0.03949	0.26438	0.00000	0.00000
34	0.00000	-0.02365	0.00000	0.00000	0.20039	-0.06606
35	0.00000	0.09133	0.00000	0.00000	0.02843	-0.07733
36	-0.04095	0.00000	0.27763	-0.05675	0.00000	0.00000

	7	8	9	10	11	12
P.Frequency	466.30	466.30	698.30	698.30	784.48	819.80
1	0.00000	0.00000	0.06758	-0.09010	0.00000	0.00000
2	0.00000	0.00000	-0.02059	-0.11072	0.00000	0.00000
3	0.00007	-0.13862	0.00000	0.00000	-0.03280	-0.09746
4	0.00000	0.00000	-0.11408	-0.08428	0.00000	0.00000
5	0.00000	0.00000	-0.01478	0.07093	0.00000	0.00000
6	-0.12008	0.06925	0.00000	0.00000	-0.03280	-0.09746
7	0.00000	0.00000	-0.01822	0.07013	0.00000	0.00000
8	0.00000	0.00000	0.13963	-0.02493	0.00000	0.00000
9	0.12001	0.06937	0.00000	0.00000	-0.03280	-0.09746
10	0.00000	0.00000	-0.06758	0.09010	0.00000	0.00000
11	0.00000	0.00000	0.02059	0.11072	0.00000	0.00000
12	0.00007	-0.13862	0.00000	0.00000	-0.03280	0.09746
13	0.00000	0.00000	0.11408	0.08428	0.00000	0.00000
14	0.00000	0.00000	0.01478	-0.07093	0.00000	0.00000
15	-0.12008	0.06925	0.00000	0.00000	-0.03280	0.09746
16	0.00000	0.00000	0.01822	-0.07013	0.00000	0.00000
17	0.00000	0.00000	-0.13963	0.02493	0.00000	0.00000

18	0.12001	0.06937	0.00000	0.00000	-0.03280	0.09746
19	0.00000	0.00000	-0.03637	-0.11413	0.00000	0.00000
20	0.00000	0.00000	0.08322	-0.08616	0.00000	0.00000
21	0.00016	-0.31932	0.00000	0.00000	0.39059	-0.22864
22	0.00000	0.00000	-0.08709	-0.11251	0.00000	0.00000
23	0.00000	0.00000	0.08485	-0.03543	0.00000	0.00000
24	-0.27661	0.15952	0.00000	0.00000	0.39059	-0.22864
25	0.00000	0.00000	-0.06032	-0.06939	0.00000	0.00000
26	0.00000	0.00000	0.12797	-0.06220	0.00000	0.00000
27	0.27646	0.15979	0.00000	0.00000	0.39059	-0.22864
28	0.00000	0.00000	0.03637	0.11413	0.00000	0.00000
29	0.00000	0.00000	-0.08322	0.08616	0.00000	0.00000
30	0.00016	-0.31932	0.00000	0.00000	0.39059	0.22864
31	0.00000	0.00000	0.08709	0.11251	0.00000	0.00000
32	0.00000	0.00000	-0.08485	0.03543	0.00000	0.00000
33	-0.27661	0.15952	0.00000	0.00000	0.39059	0.22864
34	0.00000	0.00000	0.06032	0.06939	0.00000	0.00000
35	0.00000	0.00000	-0.12797	0.06220	0.00000	0.00000
36	0.27646	0.15979	0.00000	0.00000	0.39059	0.22864

.....

The animation frames will saved into your permanent directory. To view the animation corresponding to mode 7 (the true vibrational mode in this particular case) you can concatenate all animation frames into a single file,

```
cat freq.m-007.s-0*xyz > freq.m6.xyz
```

and load it into your favorite visualization program.