

## Example I: Total energy of Benzene within Hartree-Fock approximation

In this example we will calculate the total energy of the benzene using the Hartree-Fock (HF) approximation.

Let us look at the input file

**echo**

*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.*

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

**title** "total energy of benzene, HF/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-scf

*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

alg	7
alu	0
a2g	2
a2u	2
blg	0
blu	7
b2g	2
b2u	2
elg	4
elu	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 alg	2 alu	3 a2g	4 a2u	5 blg
6 blu	7 b2g	8 b2u	9 elg	10 elu
11 e2g	12 e2u			

Orbital symmetries:

1 alg	2 elu	3 elu	4 blu	5 e2g
6 e2g	7 alg	8 elu	9 elu	10 e2g
11 e2g	12 alg	13 blu	14 b2u	15 elu
16 elu	17 a2u	18 e2g	19 e2g	20 elg
21 elg	22 e2u	23 e2u	24 alg	25 b2g
26 elu	27 elu	28 e2g	29 e2g	30 blu
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 ints 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:

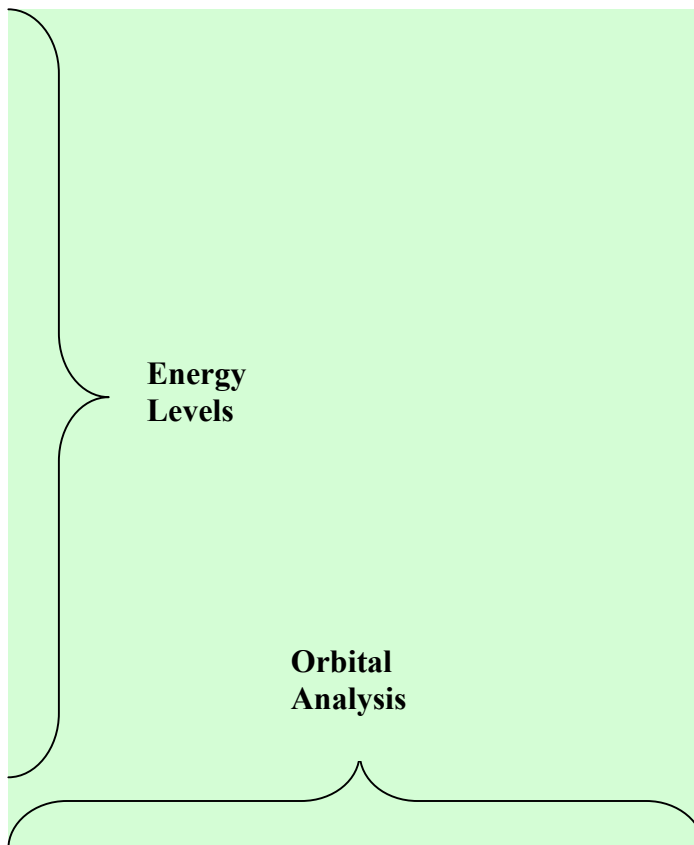
1 a1g	2 a1u	3 a2g	4 a2u	5 b1g
6 b1u	7 b2g	8 b2u	9 e1g	10 e1u
11 e2g	12 e2u			

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  
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Vector	7	Occ=2.000000D+00	E=-1.145005D+00	Symmetry=alg			
		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=elu			
		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=elu			
		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=alg		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=blu		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=elu		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=elu		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=elg					
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=elg					
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=alg					
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=elu					
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=elu					
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=blu  
 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=elu  
 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
```

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

```
scratch_dir ./scratch
```

```
permanent_dir ./perm
```

Previously generated files in permanent directory will be reused

```
driver
```

The driver block defines optimization parameters.

```
maxiter 20
```

Maximum number of iterations is 20

```
xyz benzene
```

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

```
end
```

```
task scf optimize
```

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 ok	0.00009 ok	0.02735	0.05411	15.6

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 HF/3-21G"
```

```
restart c6h6-scf
```

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

```
scratch_dir ./scratch
```

```
permanent_dir ./perm
```

Previously generated files in permanent directory will be reused

```
freq
```

```
animate
```

```
end
```

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

```
task scf freq
```

Task directive to commence frequency calculation using scf 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

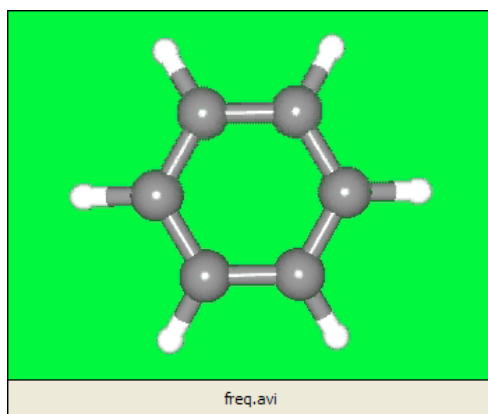
18	0.12001	0.06937	0.00000	0.00000	-0.03280	0.09746
19	0.00000	0.00000	-0.03637	-0.11413	0.00000	0.00000
20	0.00000	0.00000	0.08322	-0.08616	0.00000	0.00000
21	0.00016	-0.31932	0.00000	0.00000	0.39059	-0.22864
22	0.00000	0.00000	-0.08709	-0.11251	0.00000	0.00000
23	0.00000	0.00000	0.08485	-0.03543	0.00000	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 be 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.m7.xyz
```

and load it into your favorite visualization program.



**Above gif movie Created ECCE trajectory toolkit, povray, and ImageMajik:**

- 1) Generate a sequence of \*.pov files using the ECCE trajectory toolkit.
- 2) Generate \*.png files using povray with the following csh script:
 

```
> foreach a (`ls *.pov`)
  povray +W400 +H300 $a
```



end

- 3) Just one command is needed to create a movie from a sequence of gif files:

```
convert -delay 20 *.gif -loop 1 outfile.gif
```

The delay value is the number of milliseconds between frames--Karen found 20 to be OK in her situation at least. The loop value is the number of times it will loop through all images before stopping. The input gif file wildcard specification assumes that a directory listing orders them properly of course, which Ecce will do by appending a frame number on the end. It creates a single output file that can grow quite large depending upon the output size of your gifs and the number of frames of course.

You view these with a standard web browser including mozilla, firefox, and KDE Konqueror. Internet Explorer doesn't seem to be able to handle them though. So you just open the animated gif file like you would any other file and it will start animating.