Example I: Total energy, geometry optimization, and frequency calculation of Benzene within B3LYP using the DFT module

In this example we will calculate the total energy of the benzene using the B3LYP 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, B3LYP/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-b3lyp
```

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
```

```
dft
  xc b3lyp
end
```

The dft block contains parameters that define the HF calculation.
-xc defines the exchange correlation potential

```
task dft energy
```

Task directive requests the actual calculation. In this case we are using DFT module (dft) and requesting total energy calculation. NOTE-this calculation isn't really needed since this is done by task dft optimize

```
task dft optimize
```

Task directive requests the actual calculation. In this case we are using DFT module (dft) and requesting a geometry optimization calculation.

```
task dft freq
```

Task directive requests the actual calculation. In this case we are using DFT module (dft) and requesting a frequency calculation.

The output file is self-explanatory and follows that of the hf-session1.doc.

Example II: Total energy, geometry optimization, and frequency calculation of Benzene within B3LYP using the DFT module