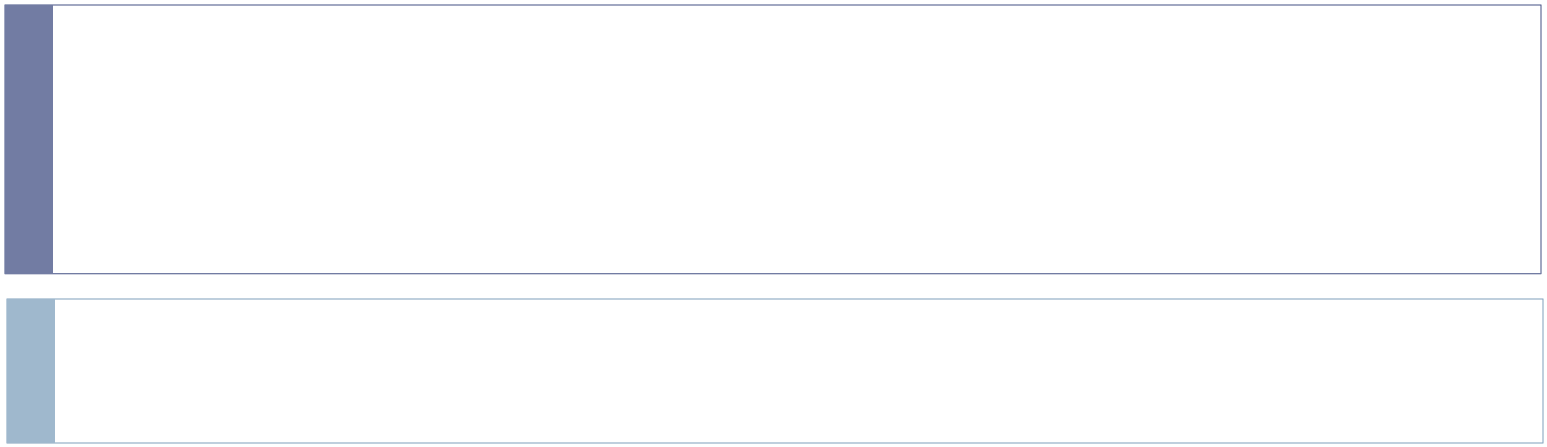
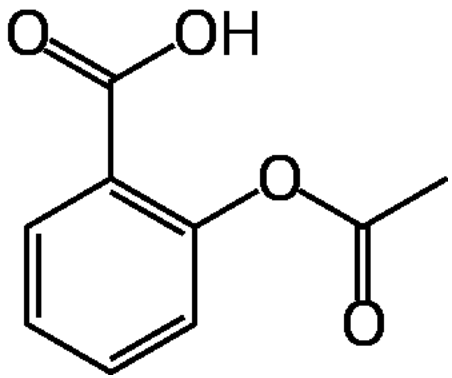
Gaussian tutorial

-Infrared spectra calculation

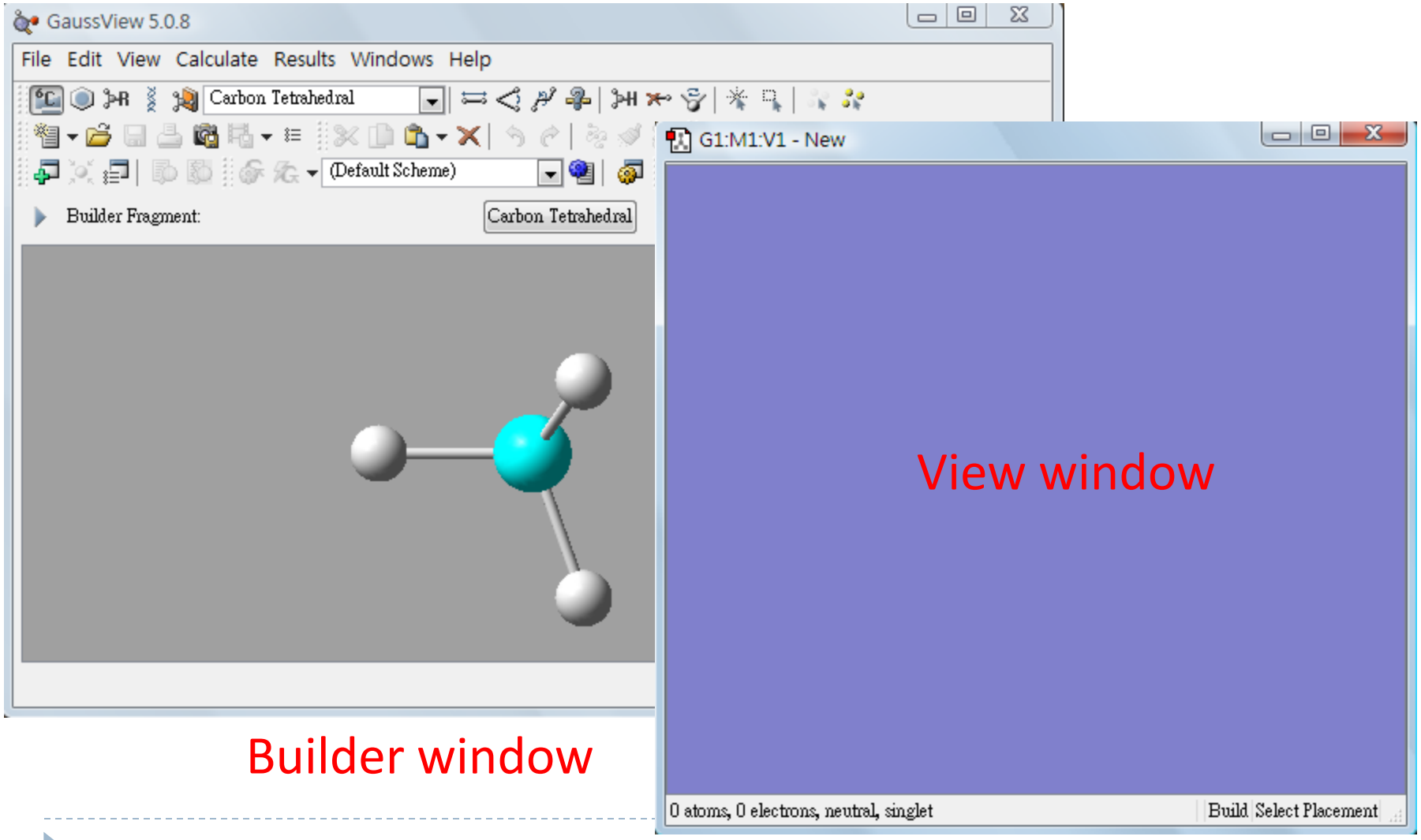


In this tutorial

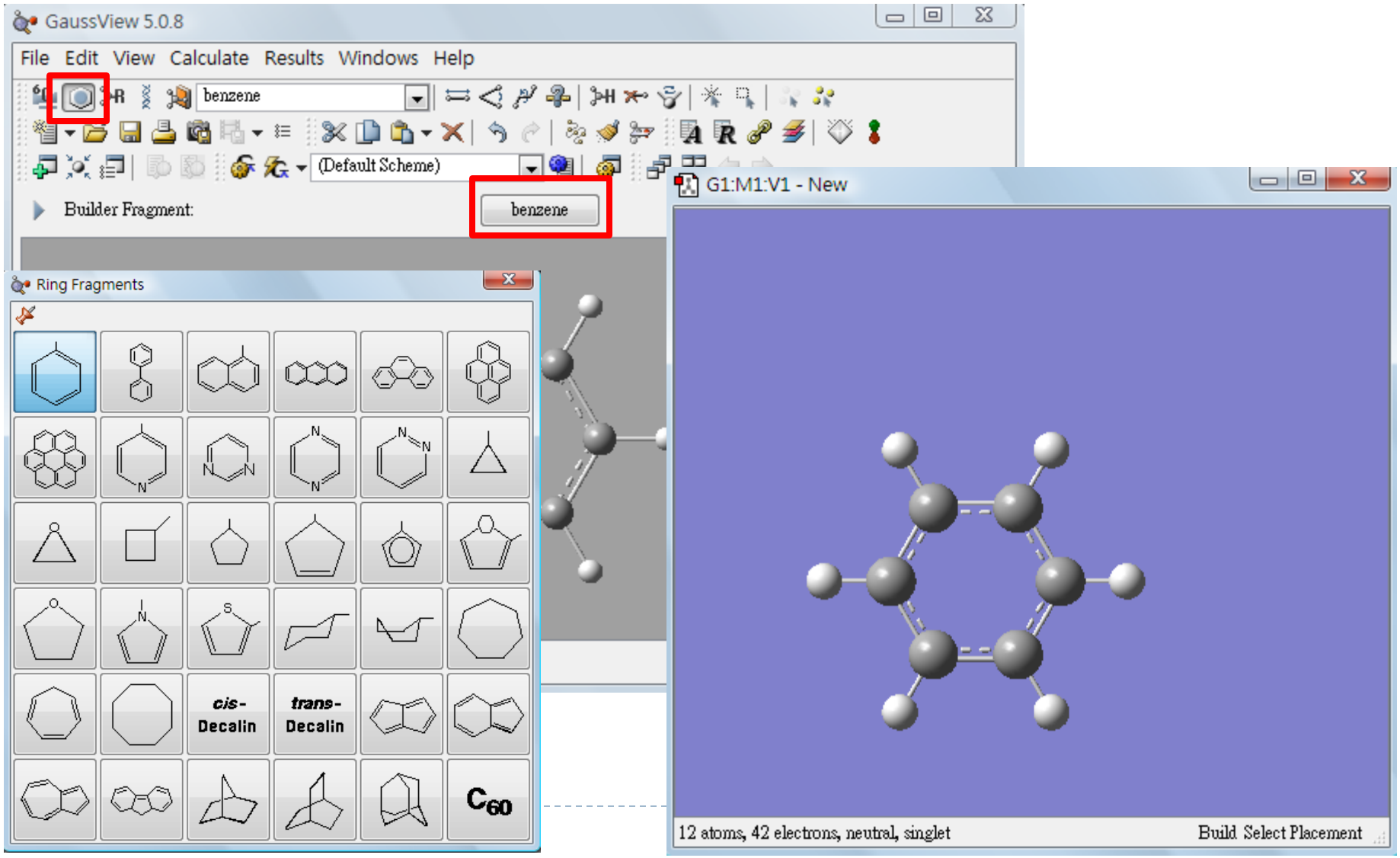
- Gaussian 03 program was used to perform the calculation.
- GaussView 5.0 was used to prepare the input file for Gaussian.
- Exampled compound: Aspirin



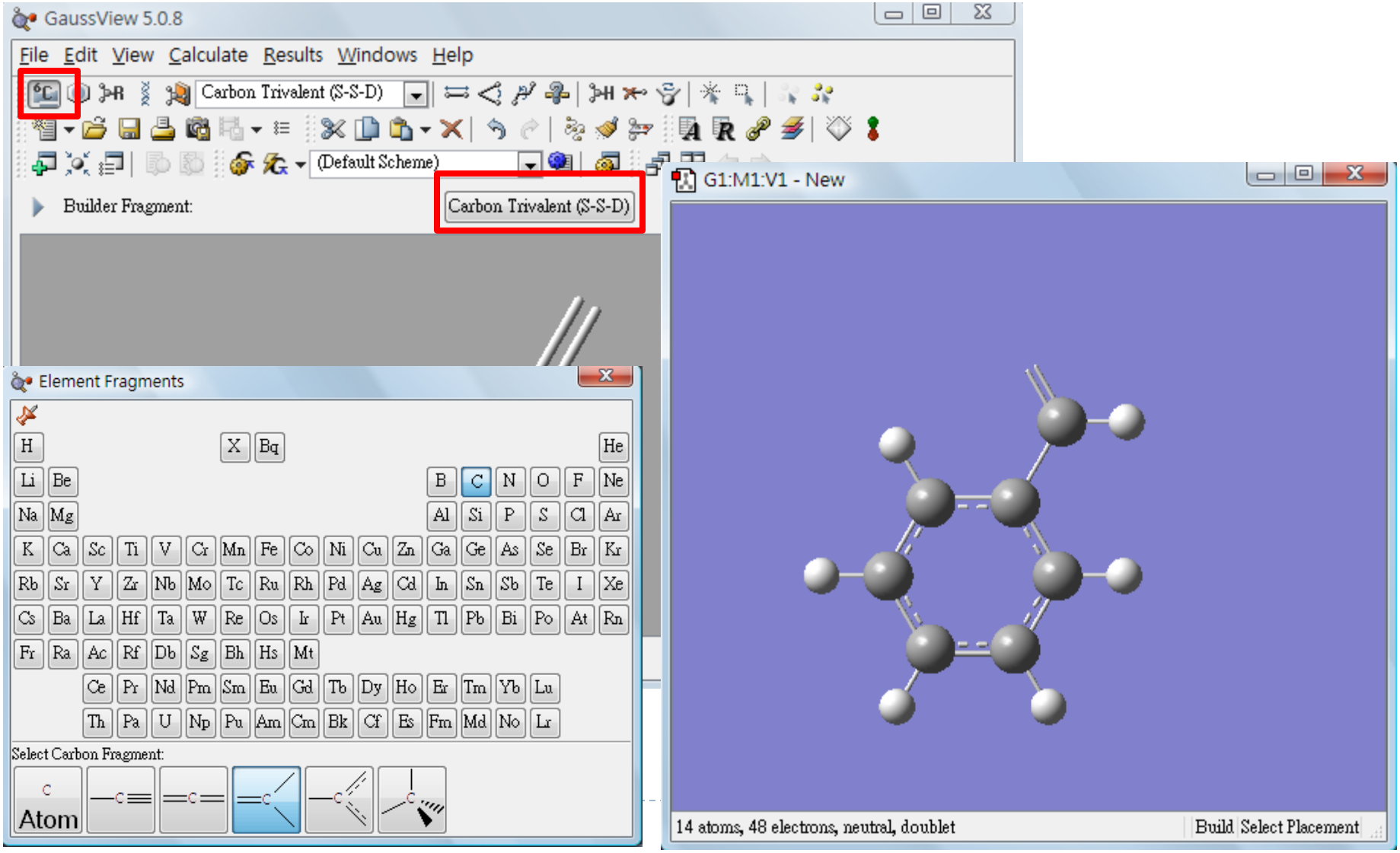
Drawing the compound by GaussView



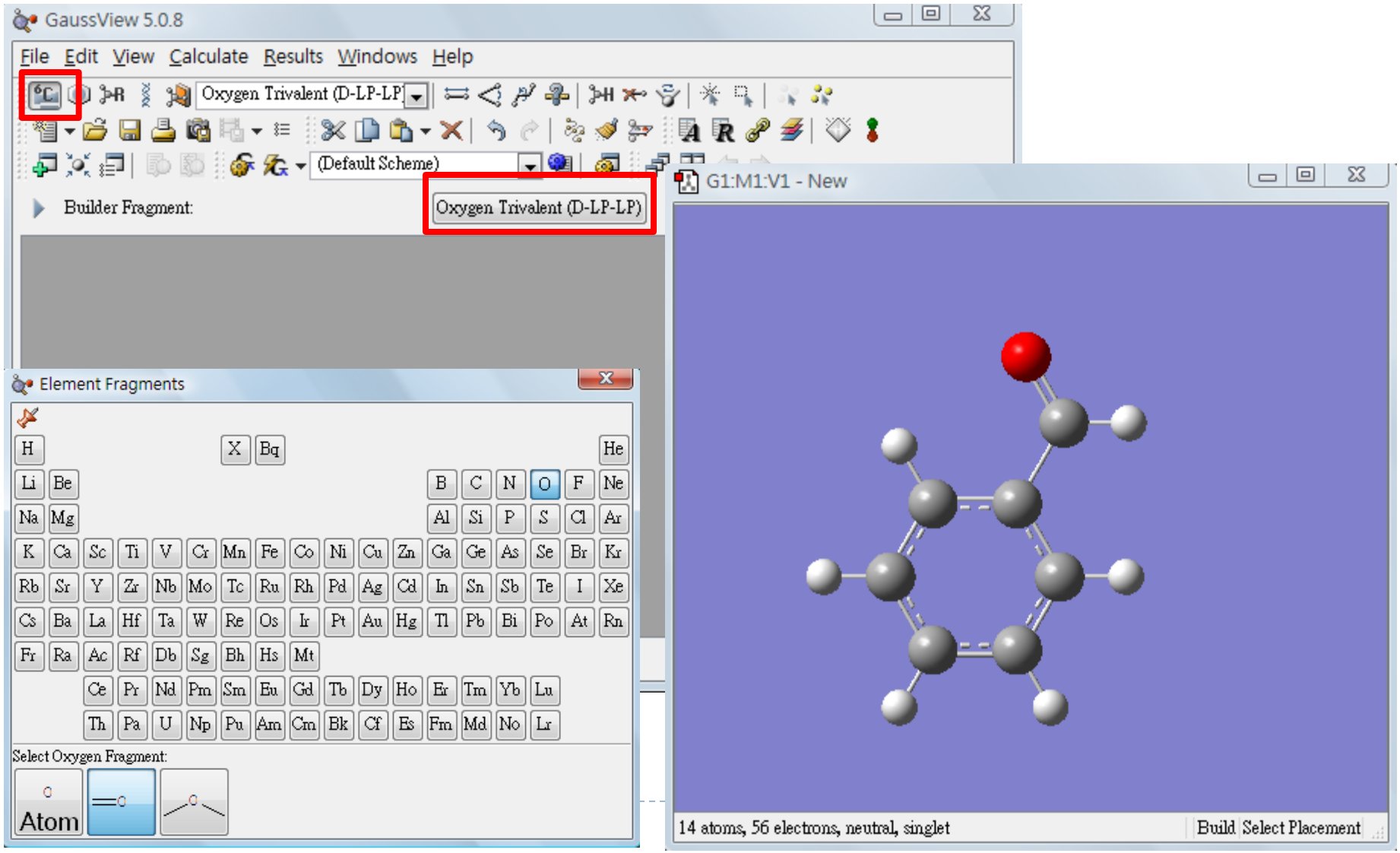
Drawing the compound by GaussView



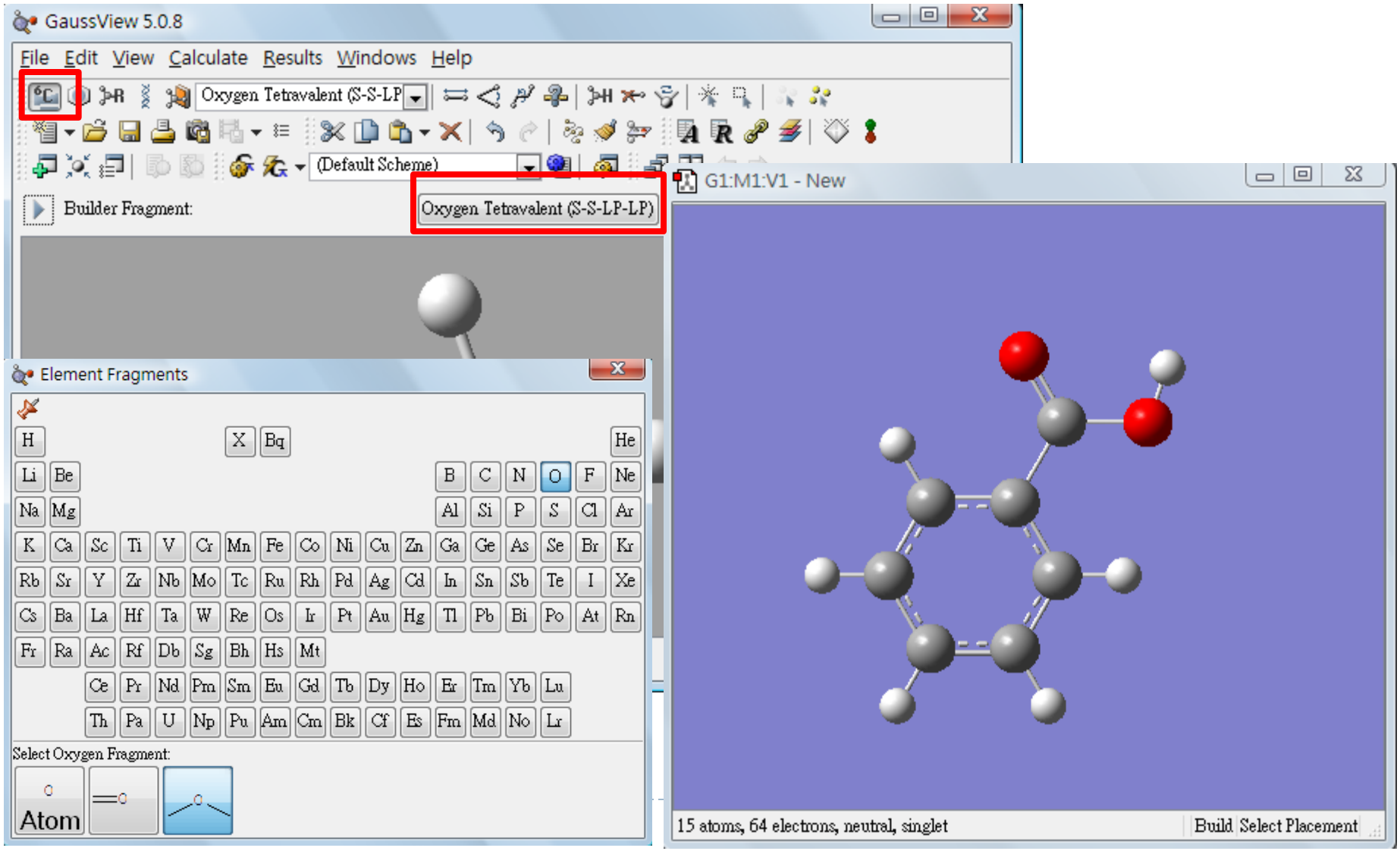
Drawing the compound by GaussView



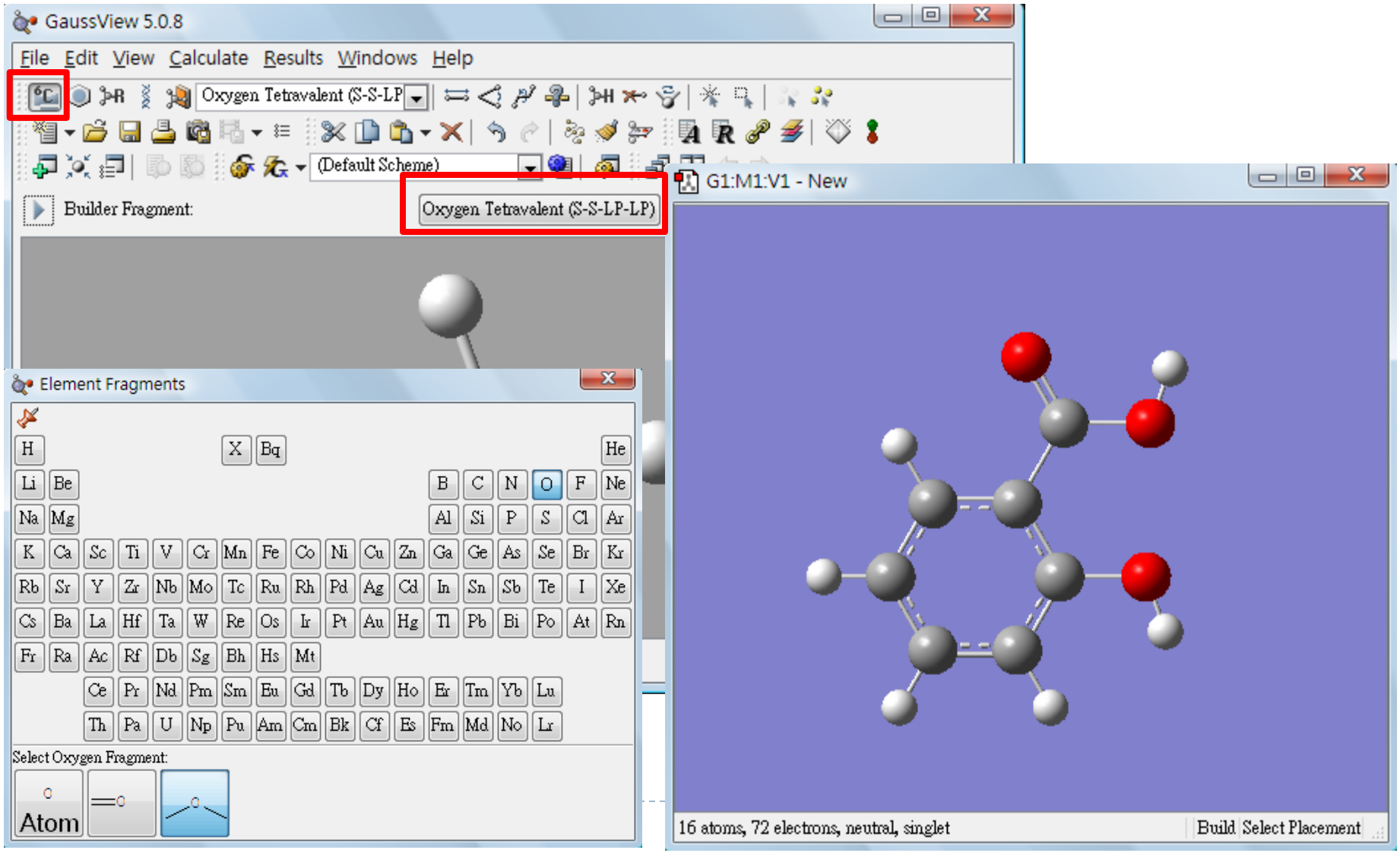
Drawing the compound by GaussView



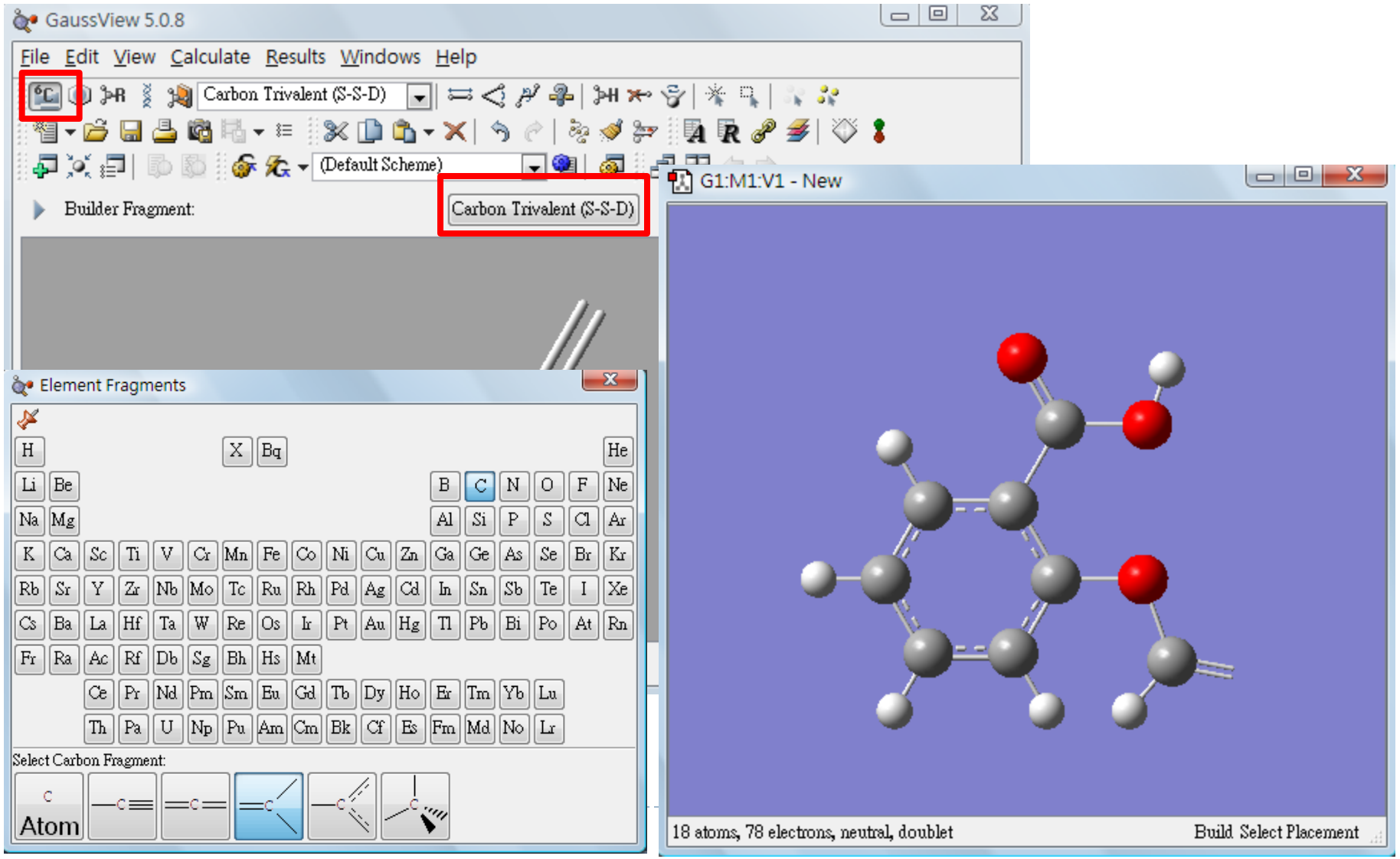
Drawing the compound by GaussView



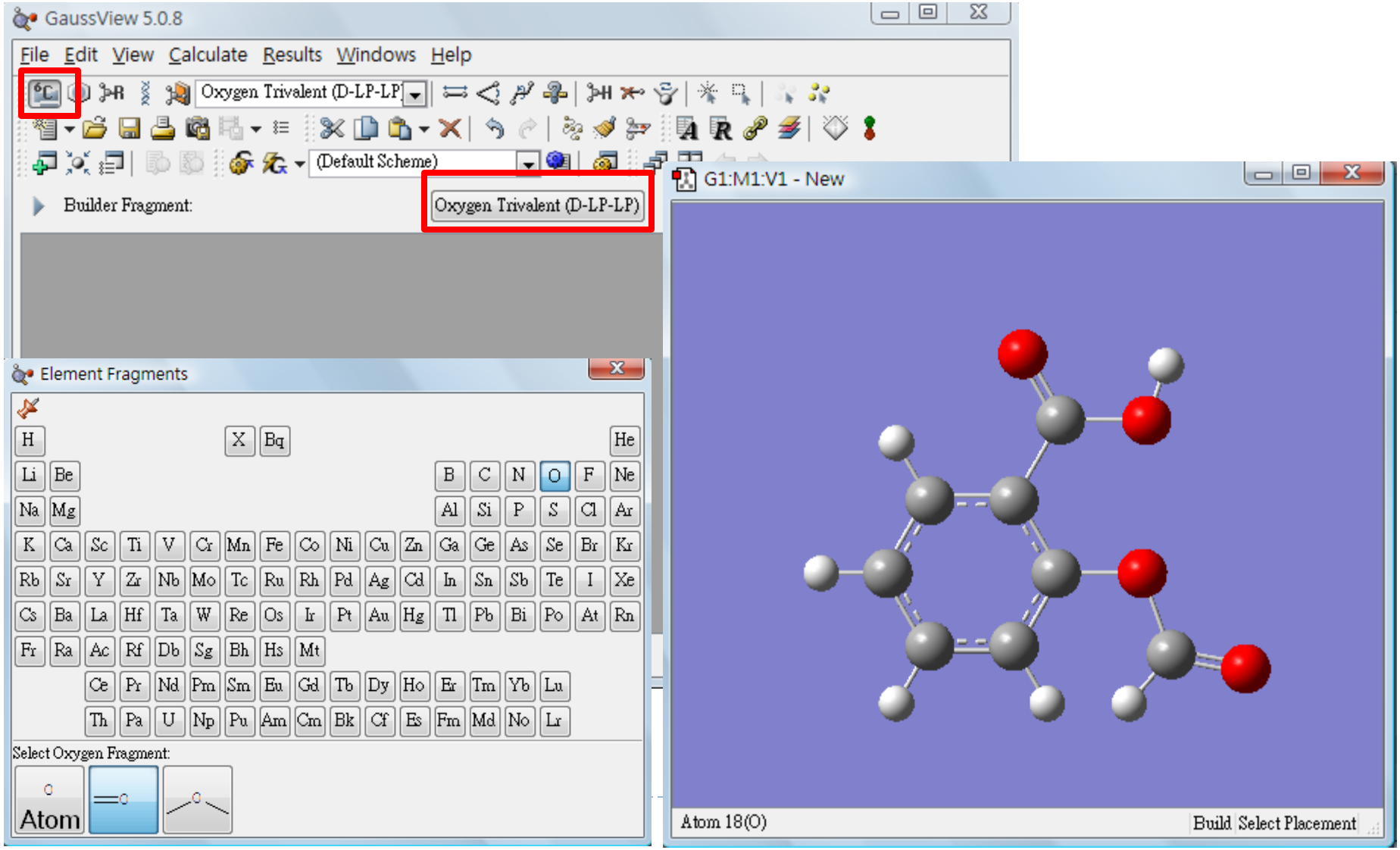
Drawing the compound by GaussView



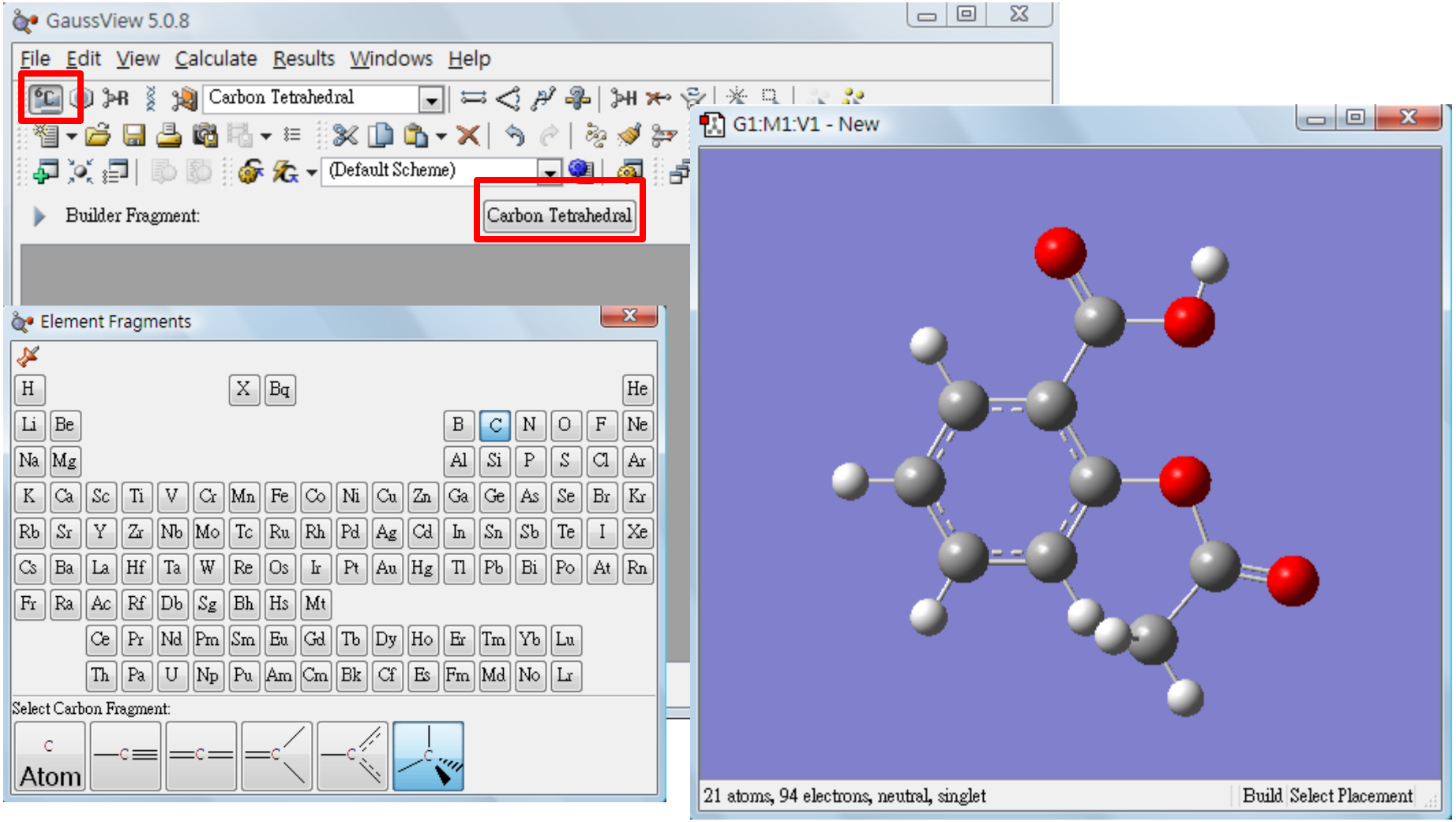
Drawing the compound by GaussView



Drawing the compound by GaussView

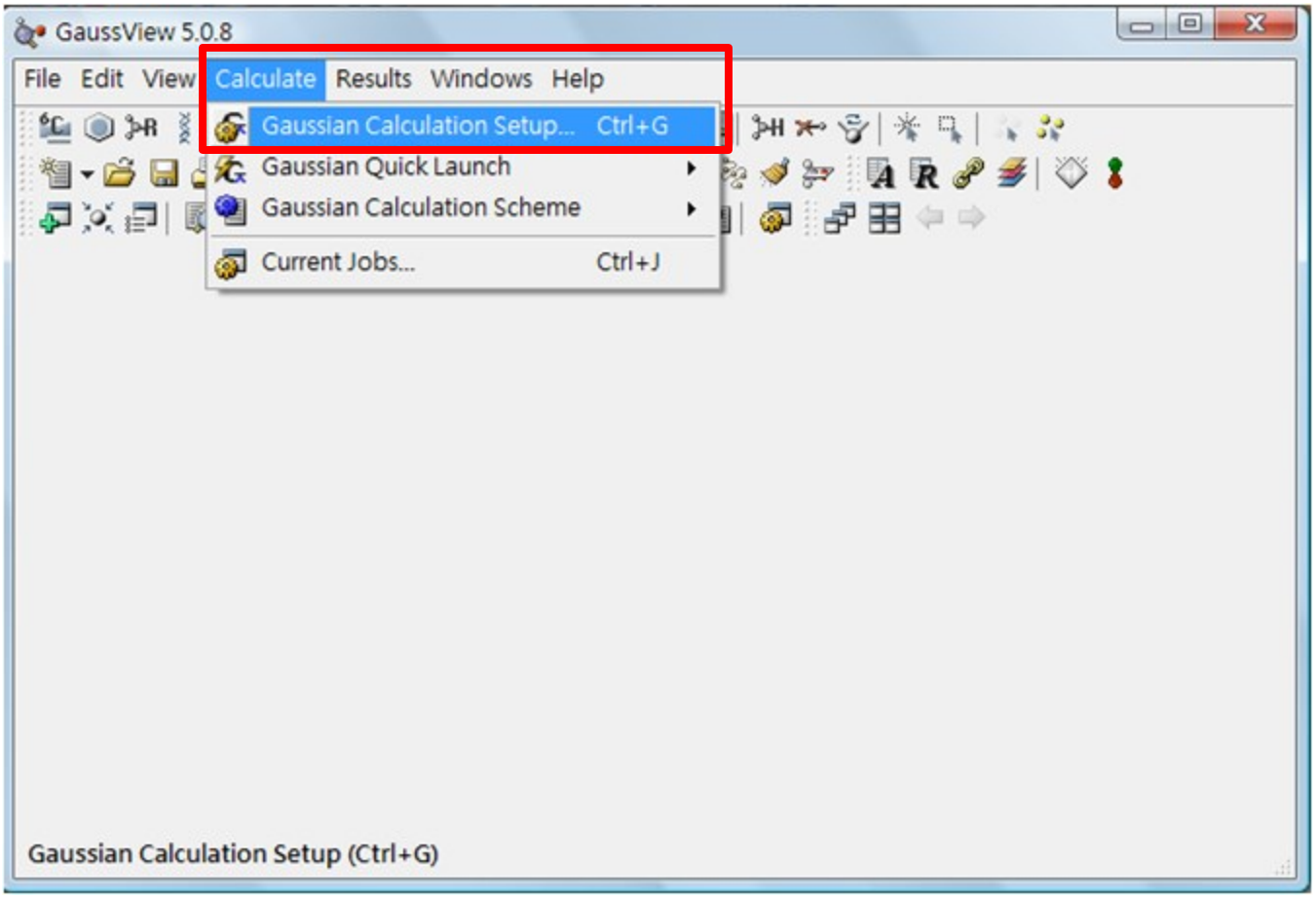


Drawing the compound by GaussView

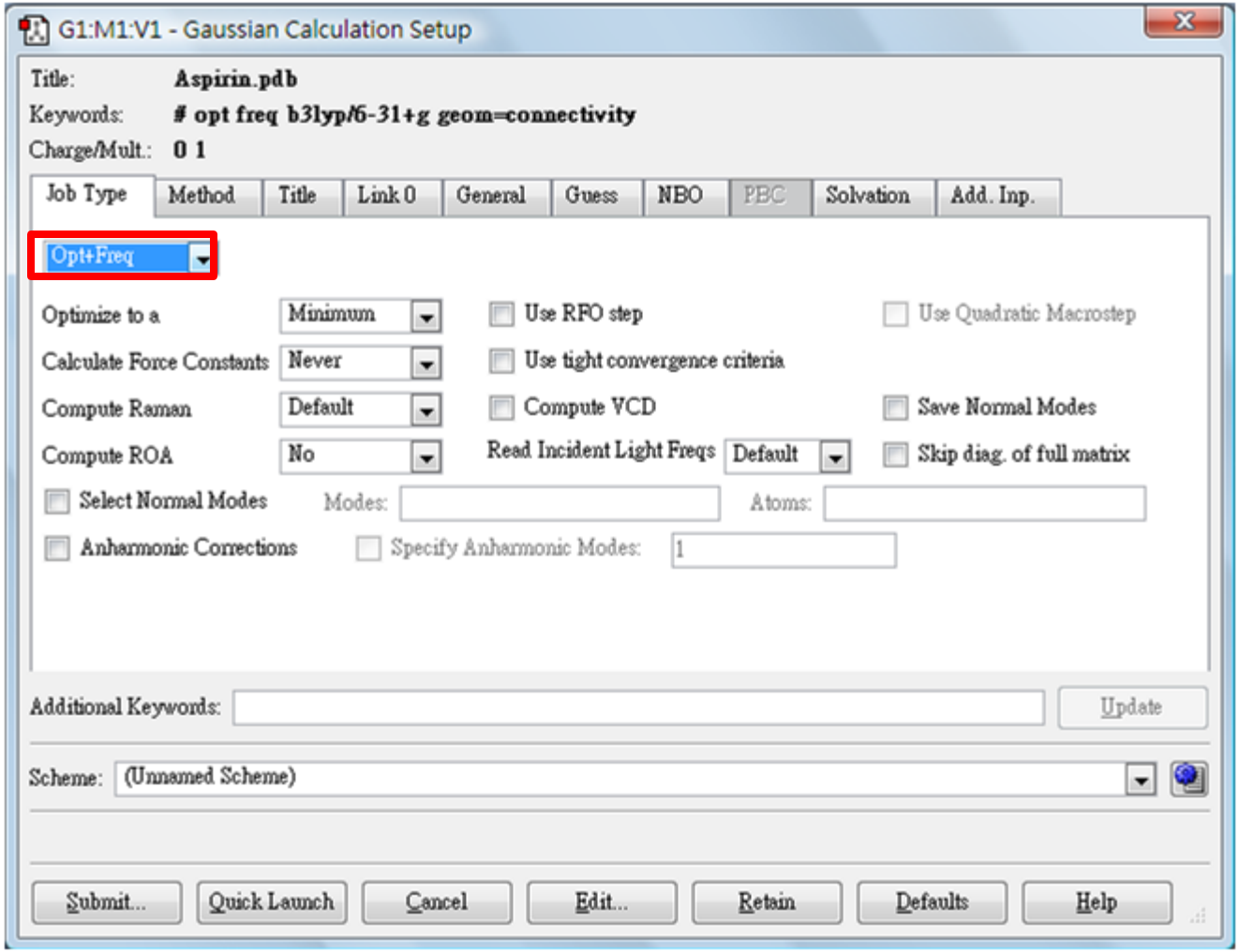


- File → Save → aspirin.pdb

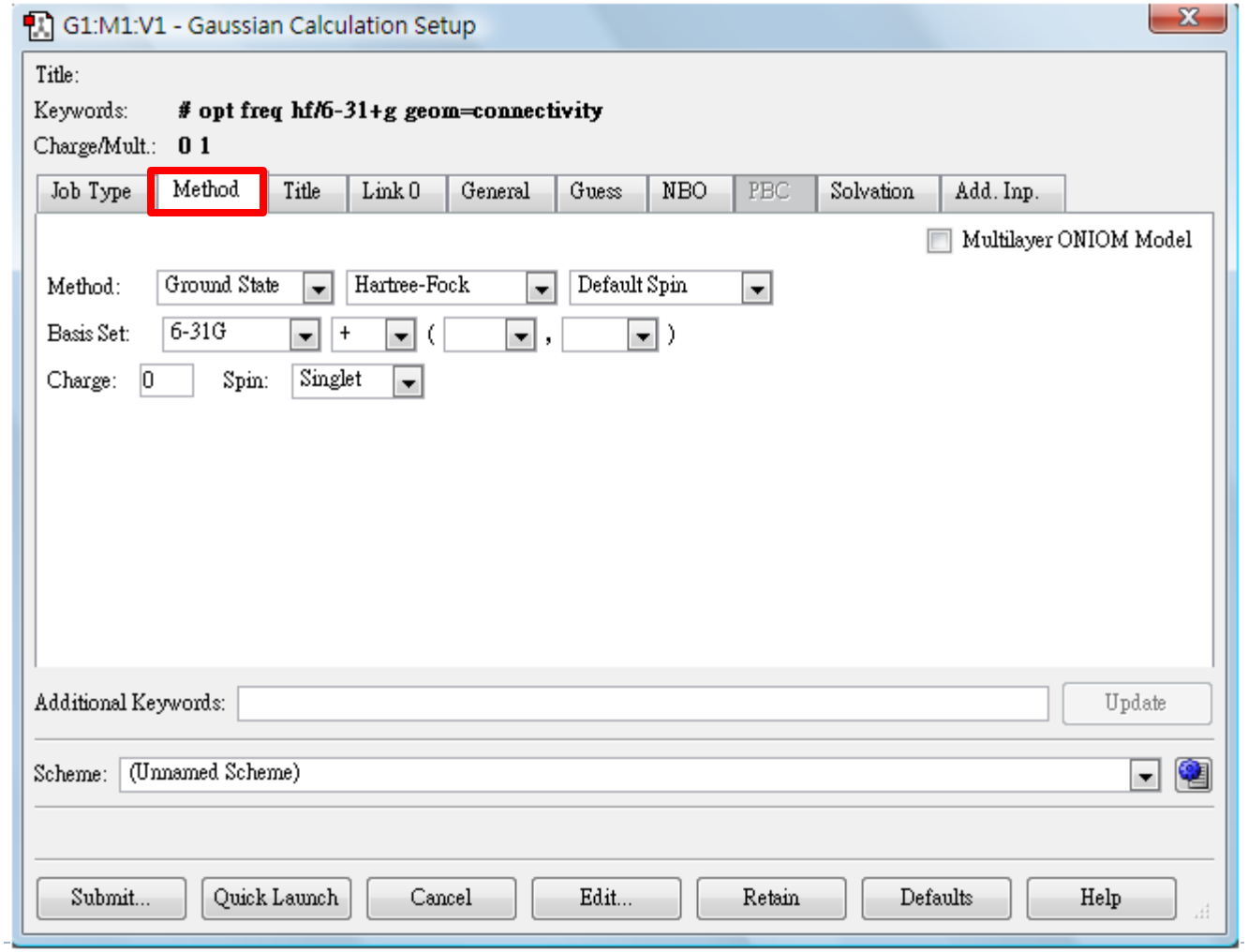
Calculation setup



Calculation setup



Calculation setup



Calculation setup

- Save → aspirin.gjf (Gaussian input file)

```
%chk=D:\GaussianTutorial_IR\aspirin.chk
# opt freq hf/6-31+g geom=connectivity

Aspirin.pdb

0 1
 C                 -1.07170000    0.20620000    0.00000000
 C                 -1.78620000   -0.20620000    0.00000000
 C                 -1.78620000   -1.03130000    0.00000000
 C                 -1.07170000   -1.44380000    0.00000000
 C                 -0.35720000   -1.03130000    0.00000000
 C                 -0.35720000   -0.20620000    0.00000000
 C                 -1.07170000    1.03130000    0.00000000
 O                  0.35720000    0.20620000    0.00000000
 O                 -1.78620000    1.44380000    0.00000000
 O                 -0.35720000    1.44380000    0.00000000
 C                  1.07170000   -0.20620000    0.00000000
 O                  1.07170000   -1.03130000    0.00000000
 C                  1.78620000    0.20630000    0.00000000
 H                 -2.71281439    0.32885679    0.00000000
 H                 -2.71284247   -1.56630815    0.00000000
 H                 -1.07170000   -2.51380000    0.00000000
 H                  0.56944247   -1.56630815    0.00000000
 H                 -0.53260360    2.38763981    0.00000000
 H                  1.59069807    1.25828812    0.00000000
 H                  2.34727926   -0.05220221    0.87365134
 H                  2.34727926   -0.05220221   -0.87365134
```

Route section

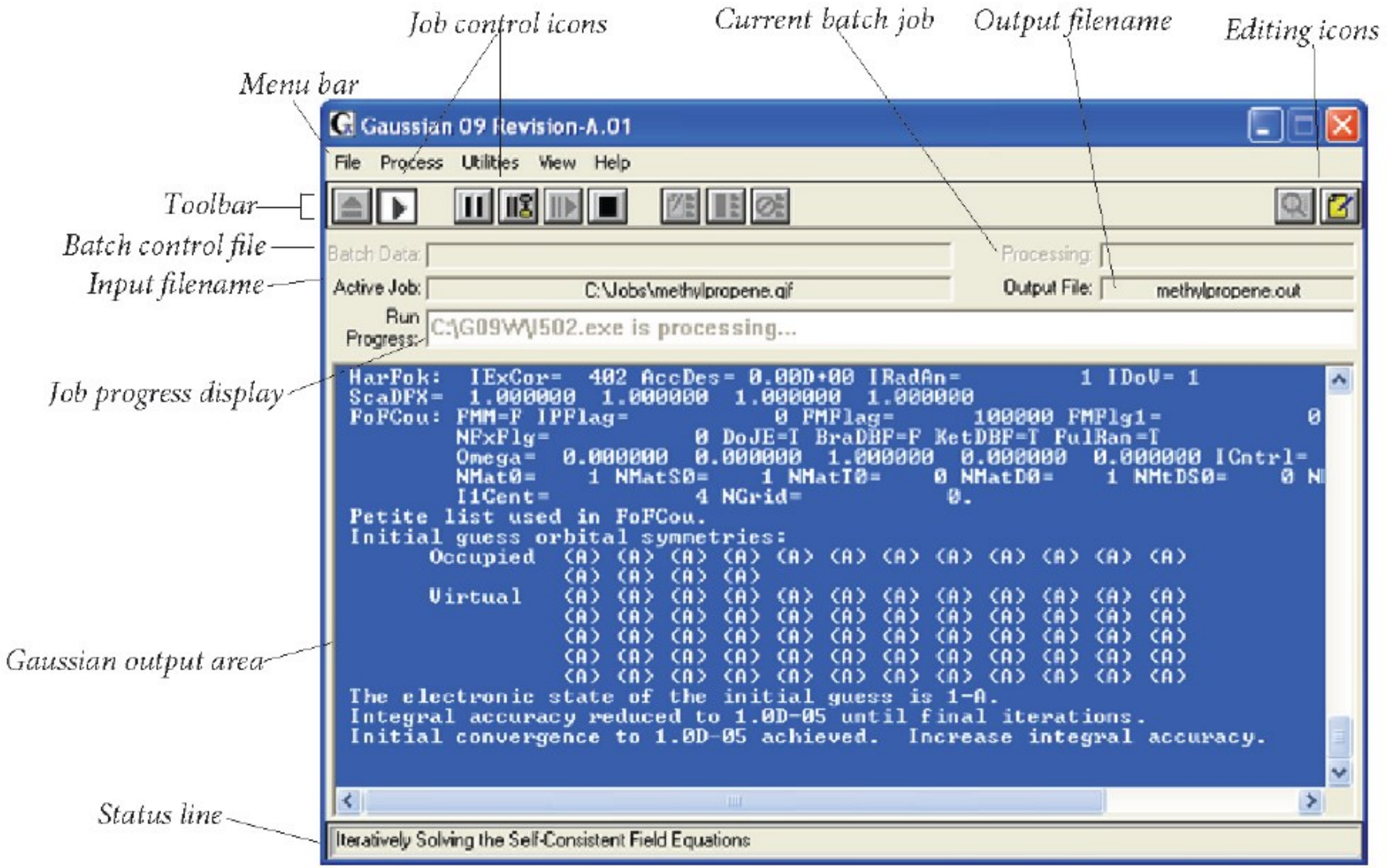
Title section

Molecular specification

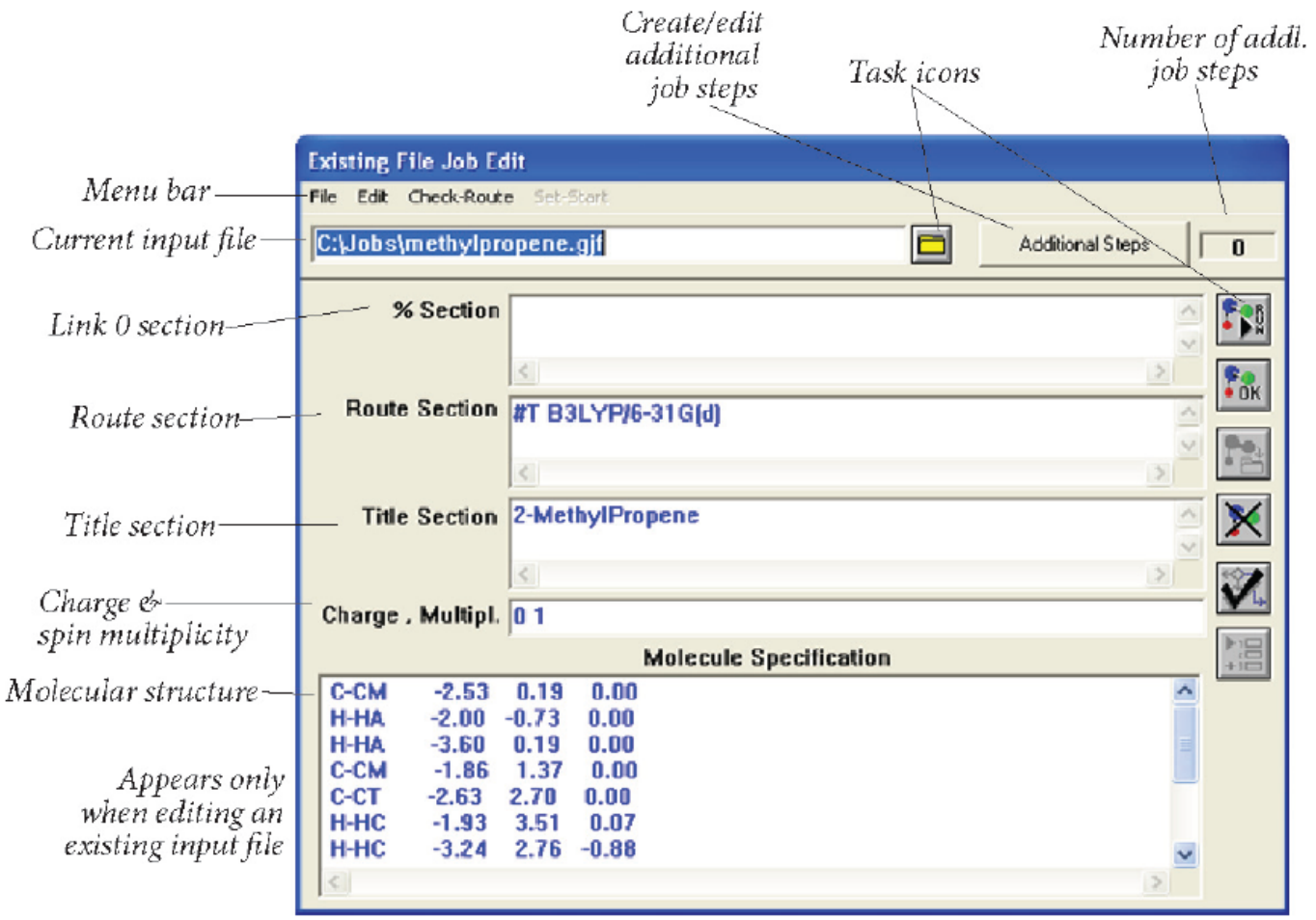
```
1 2 2.0 6 1.0 7 1.0
2 3 1.0 14 1.0
3 4 2.0 15 1.0
4 5 1.0 16 1.0
5 6 2.0 17 1.0
6 8 1.0
7 9 2.0 10 1.0
8 11 1.0
9
10 18 1.0
11 12 2.0 13 1.0
12
13 19 1.0 20 1.0 21 1.0
14
15
16
17
18
19
20
21
```

- Submit job

Job processing window

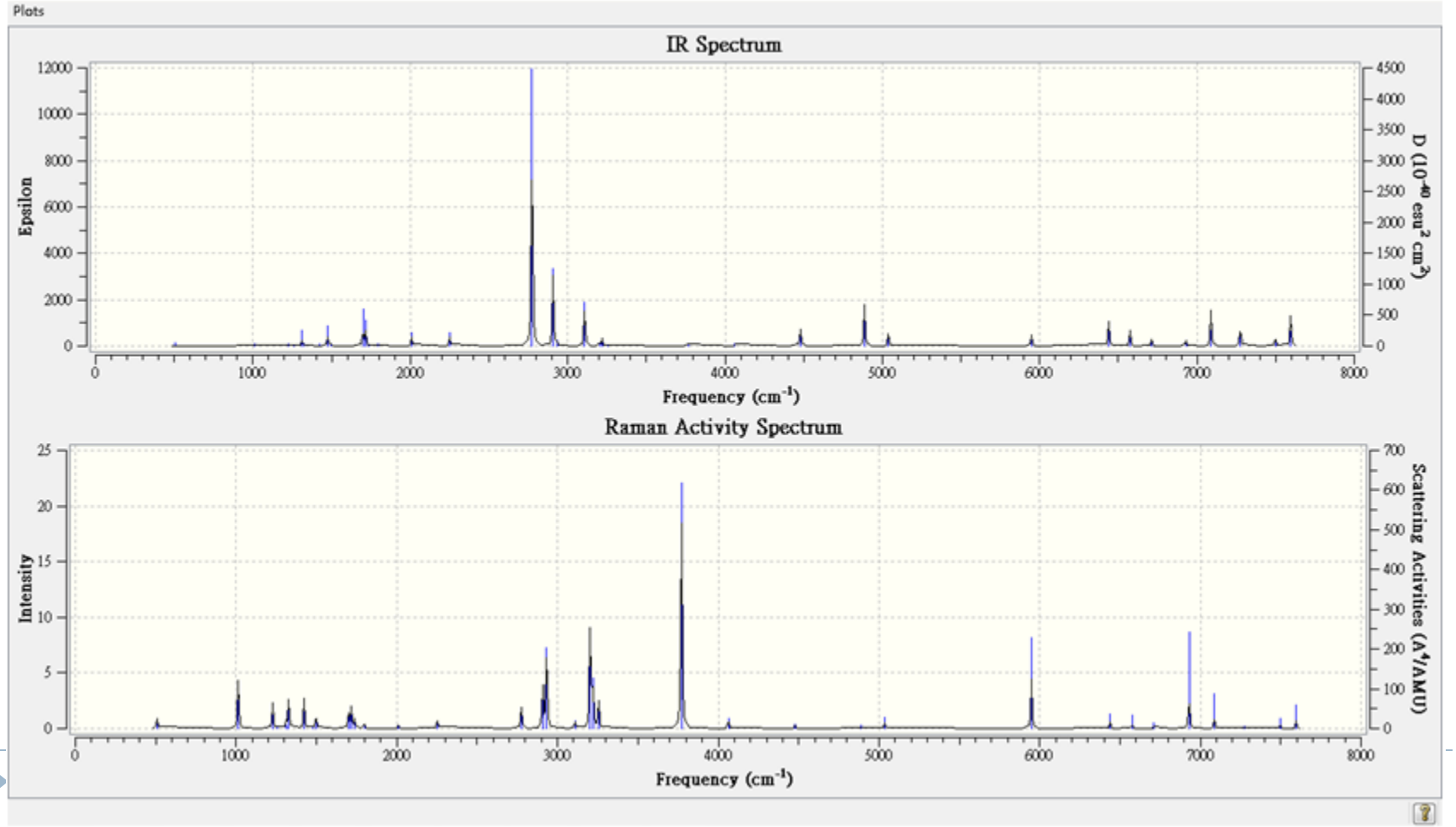


Job edit window



Viewing vibrational frequencies in GaussView

- File → Open → aspirin.out
- Results → Vibrations



Viewing vibrational frequencies in GaussView