

How to use G03

User name

IP

- Double click the “CYGWin” icon on desktop, and key in `/usr/X11R6/bin/startxwin.bat`
- It will open a X-term window, then key in `ssh -Y -l tigp01 pcfc2.sinica.edu.tw`
- Key in `passwd “obc&789”`
- Key in “gv &” to open GaussView

password

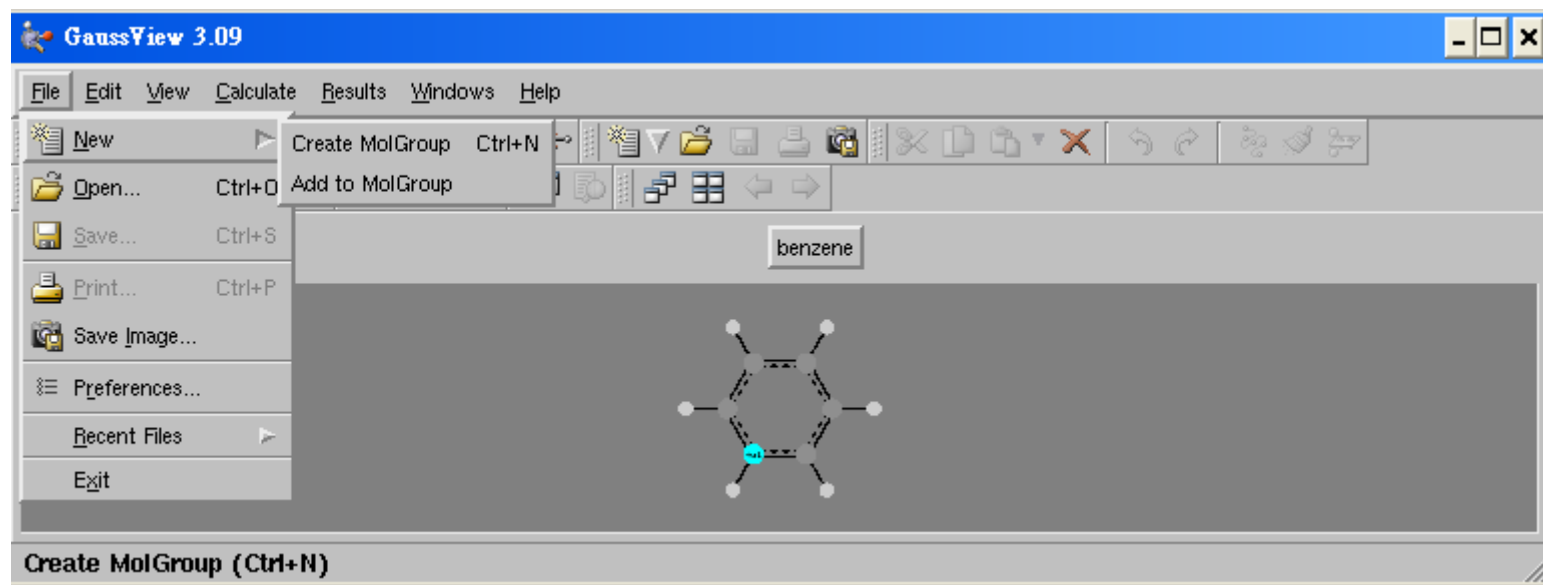
Some Useful Website

Technical Support Information

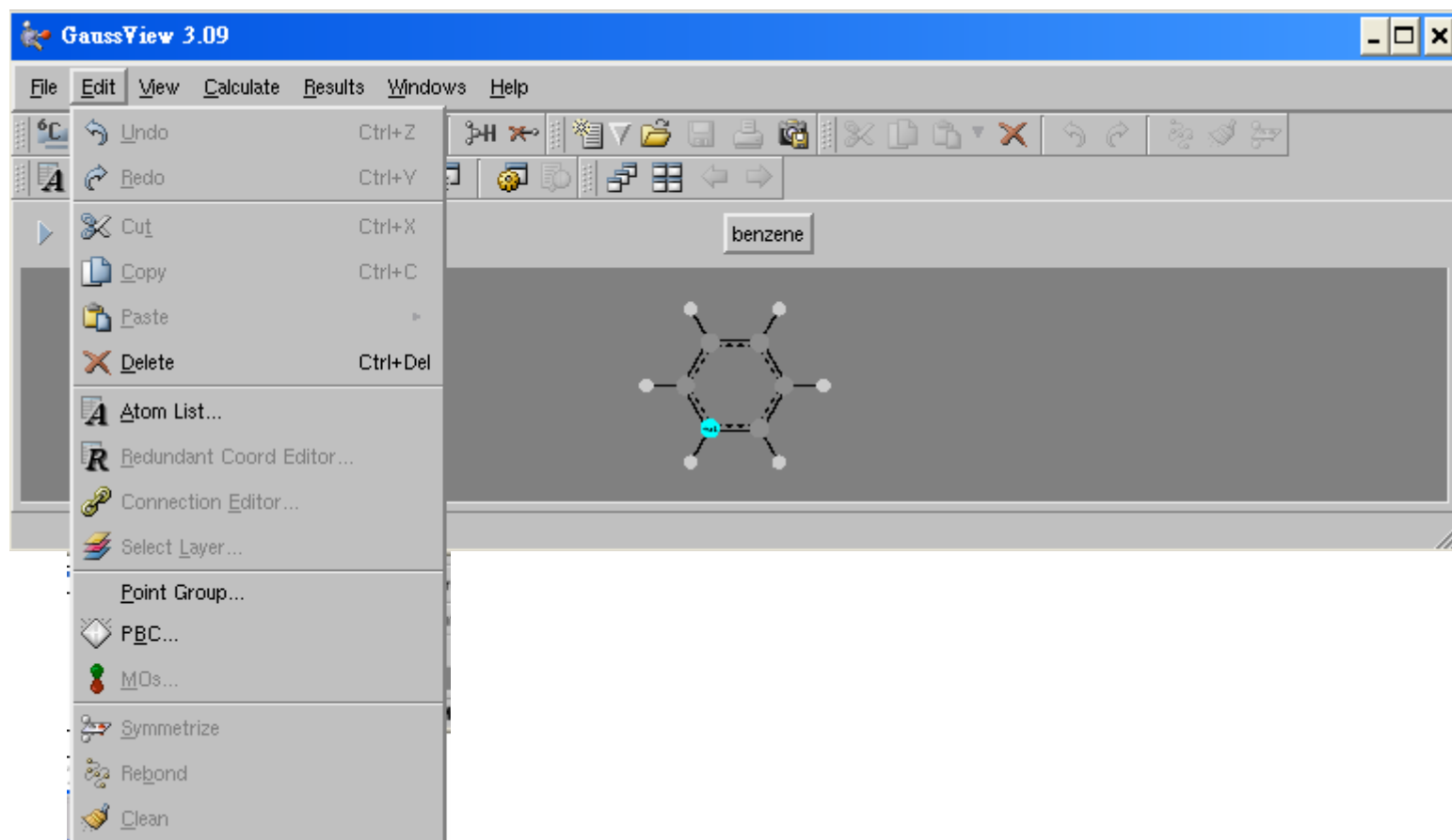
http://www.gaussian.com/tech_top_level.htm

Pull-down menu options:

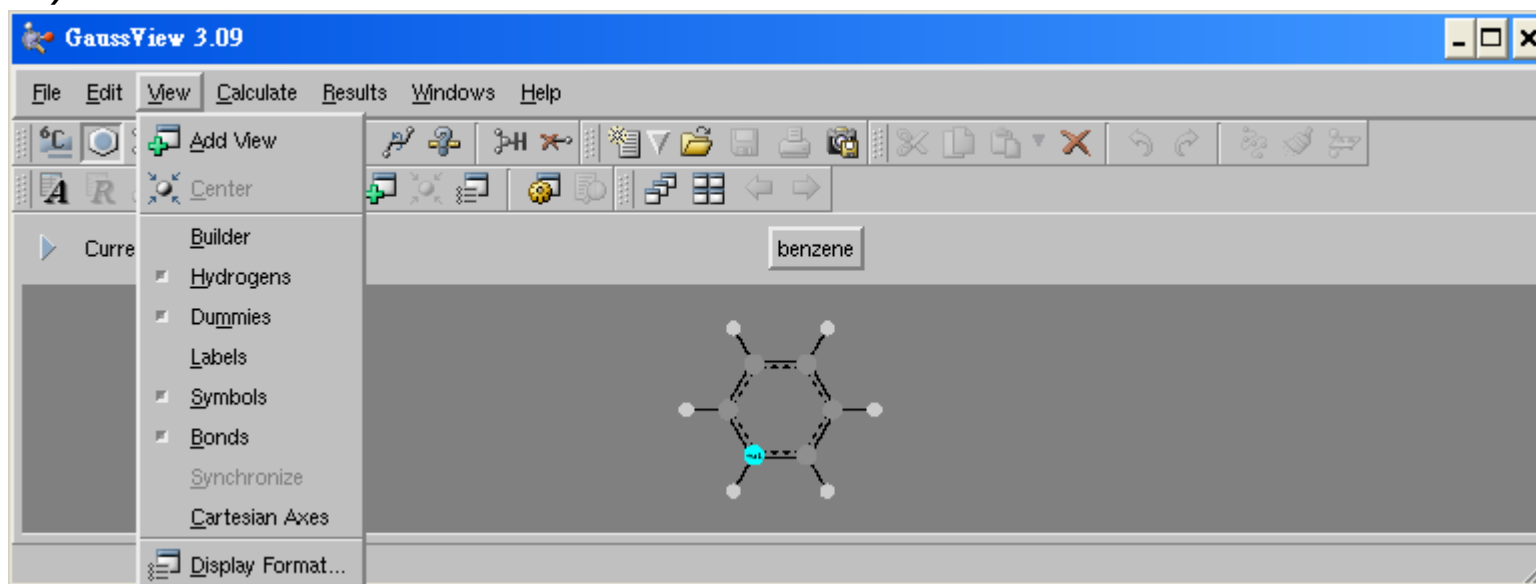
1) File:



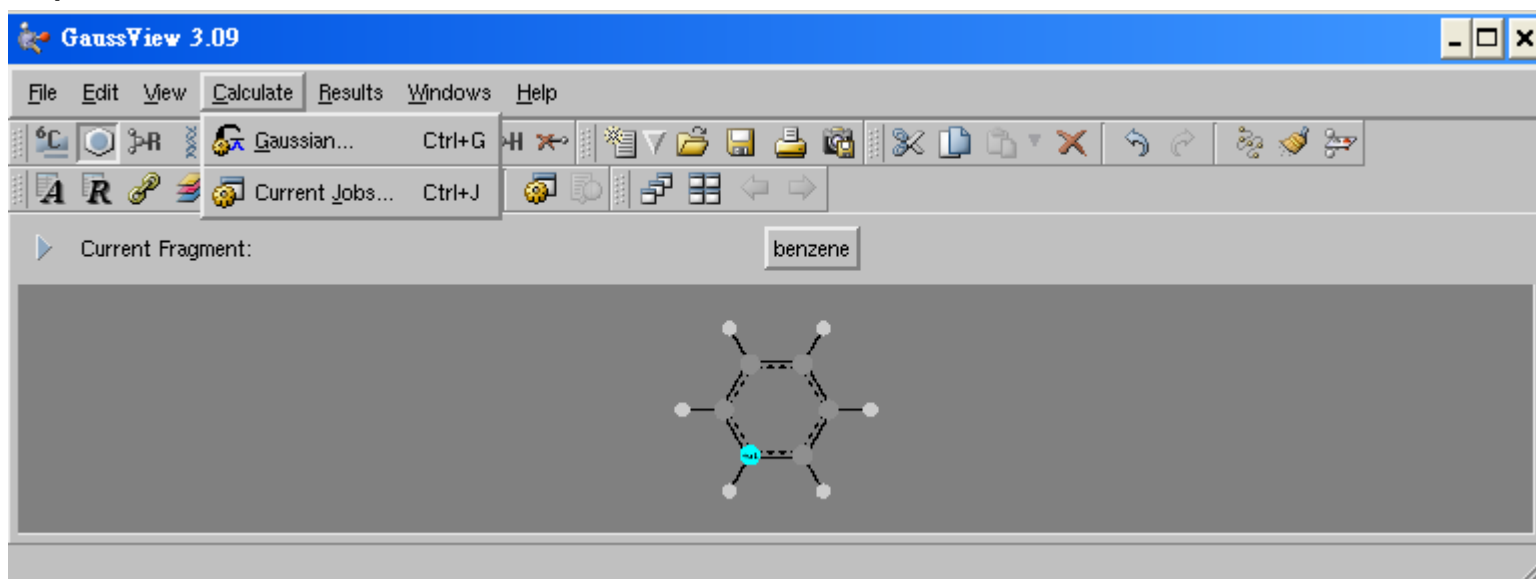
2) Edit:



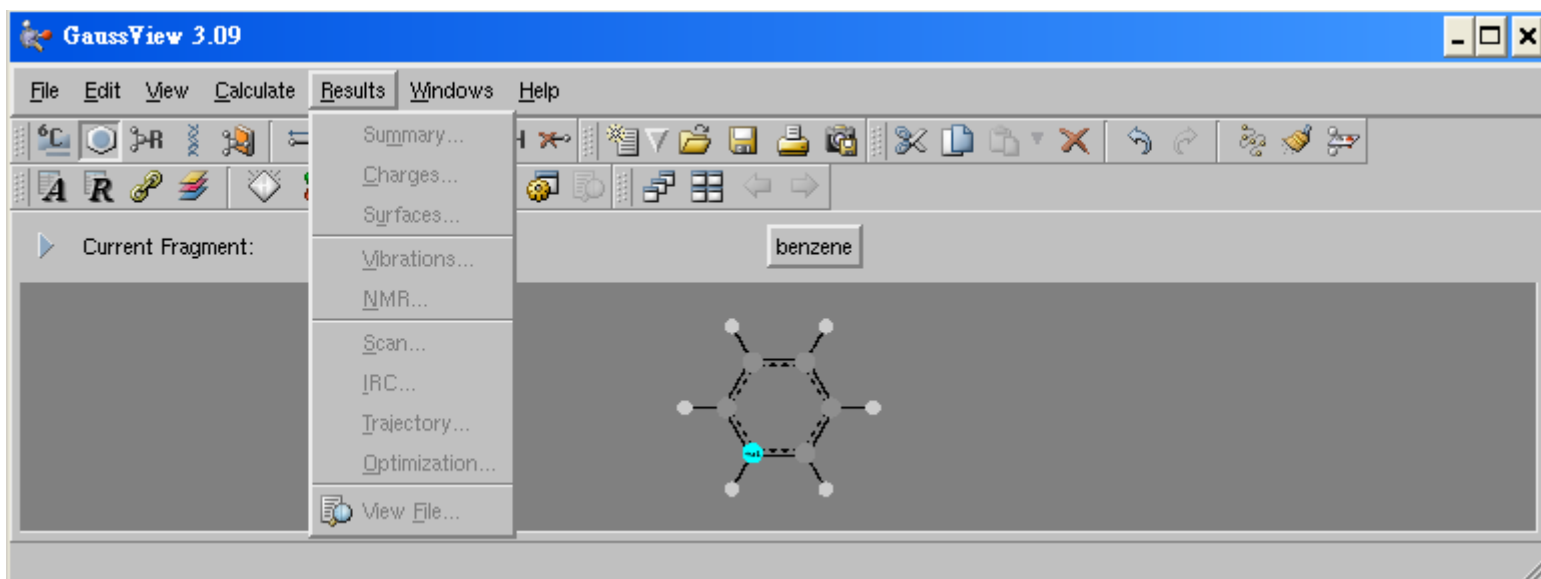
3) View:



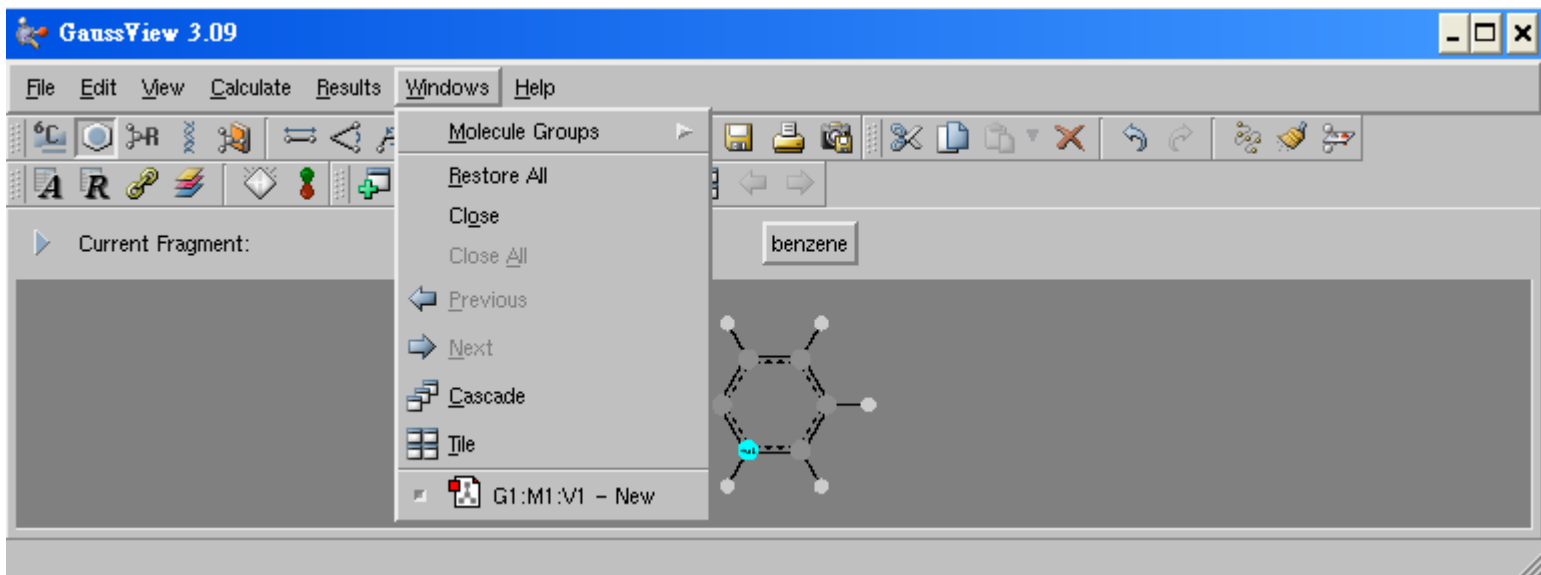
4) Calculate:



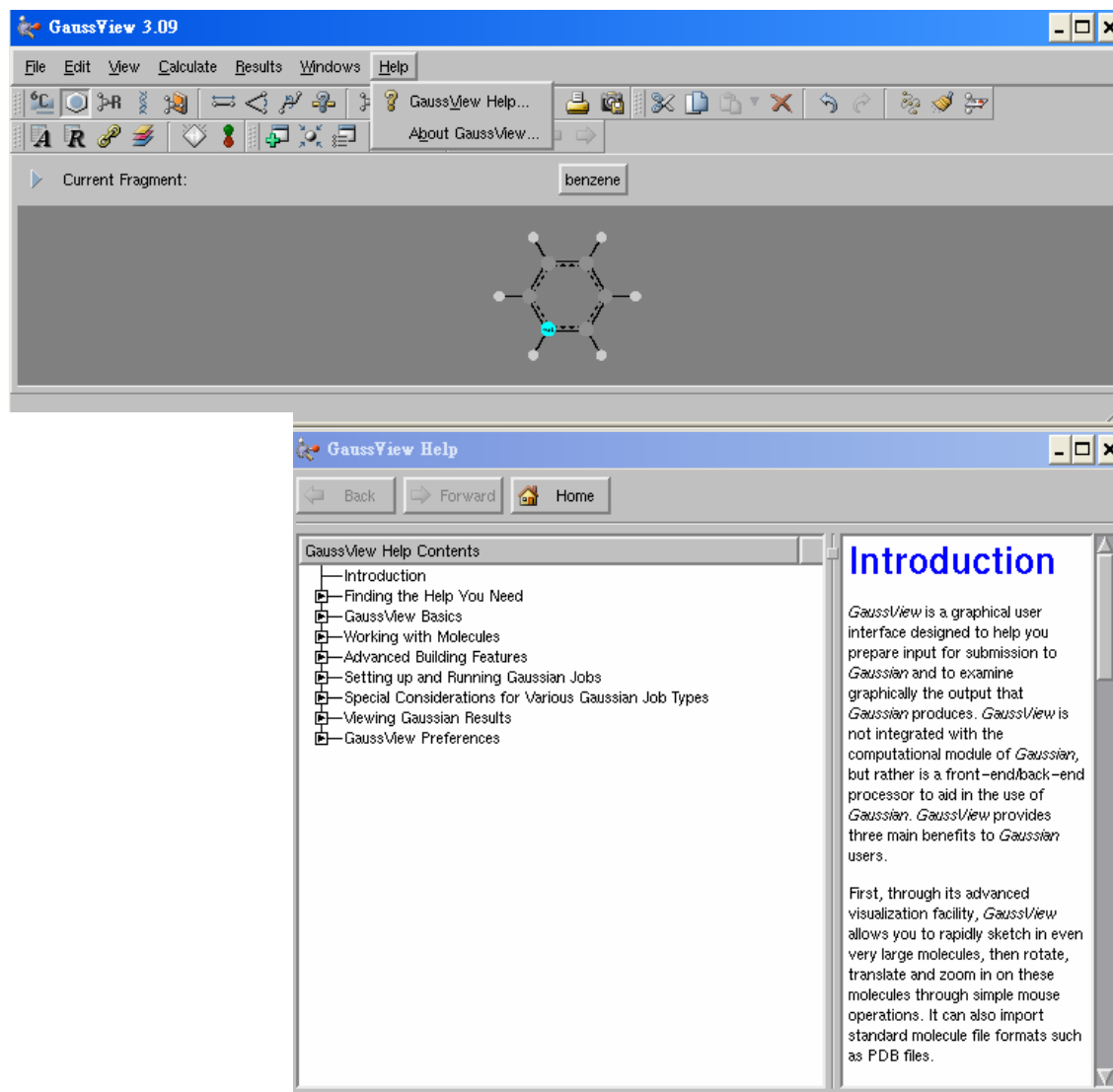
5) Results:



6) Windows:

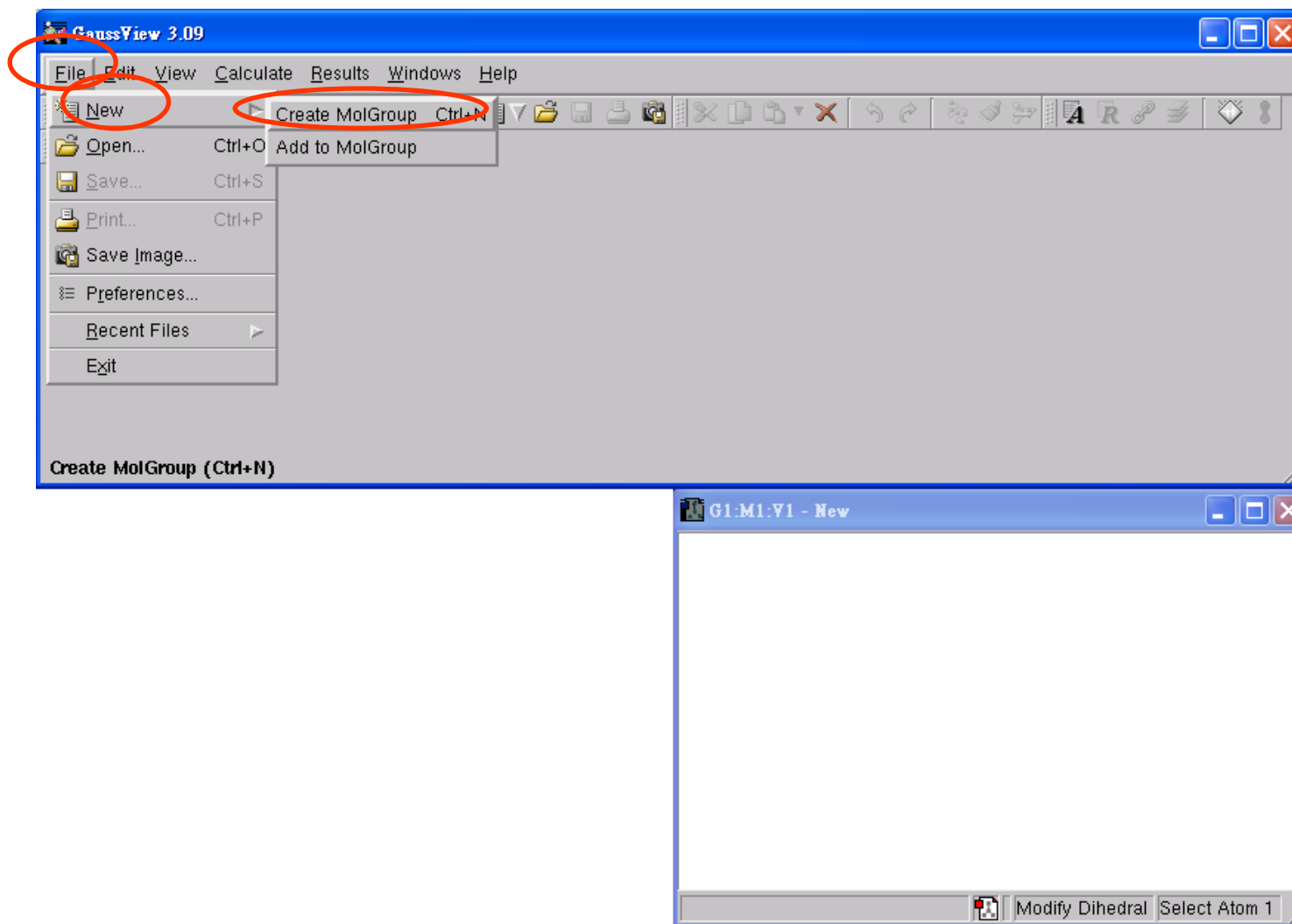


7) Help:



Step1 : Coarse Optimization

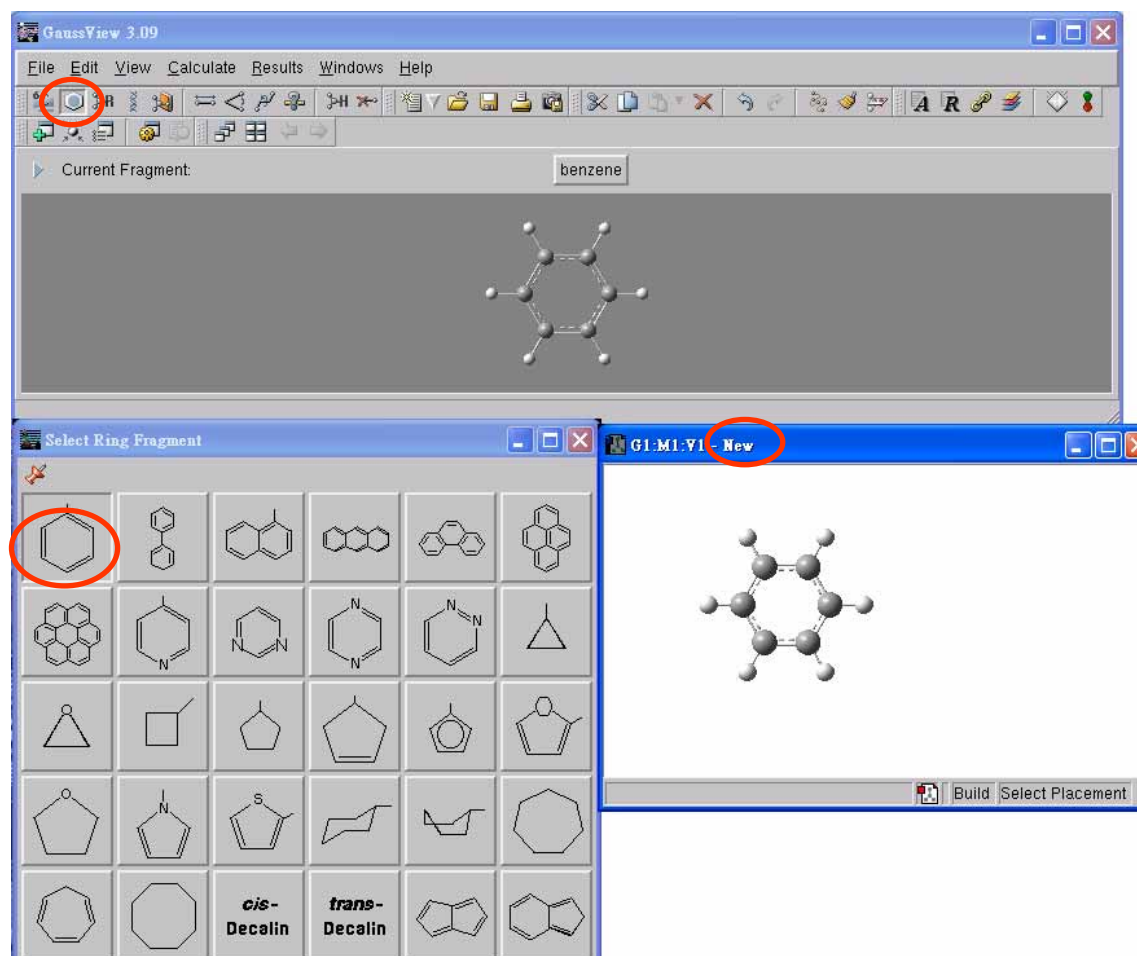
Open new file → File → New → Create MolGroup



Create Molecule : CN-PPV

Double Click at **Ring Fragment** →

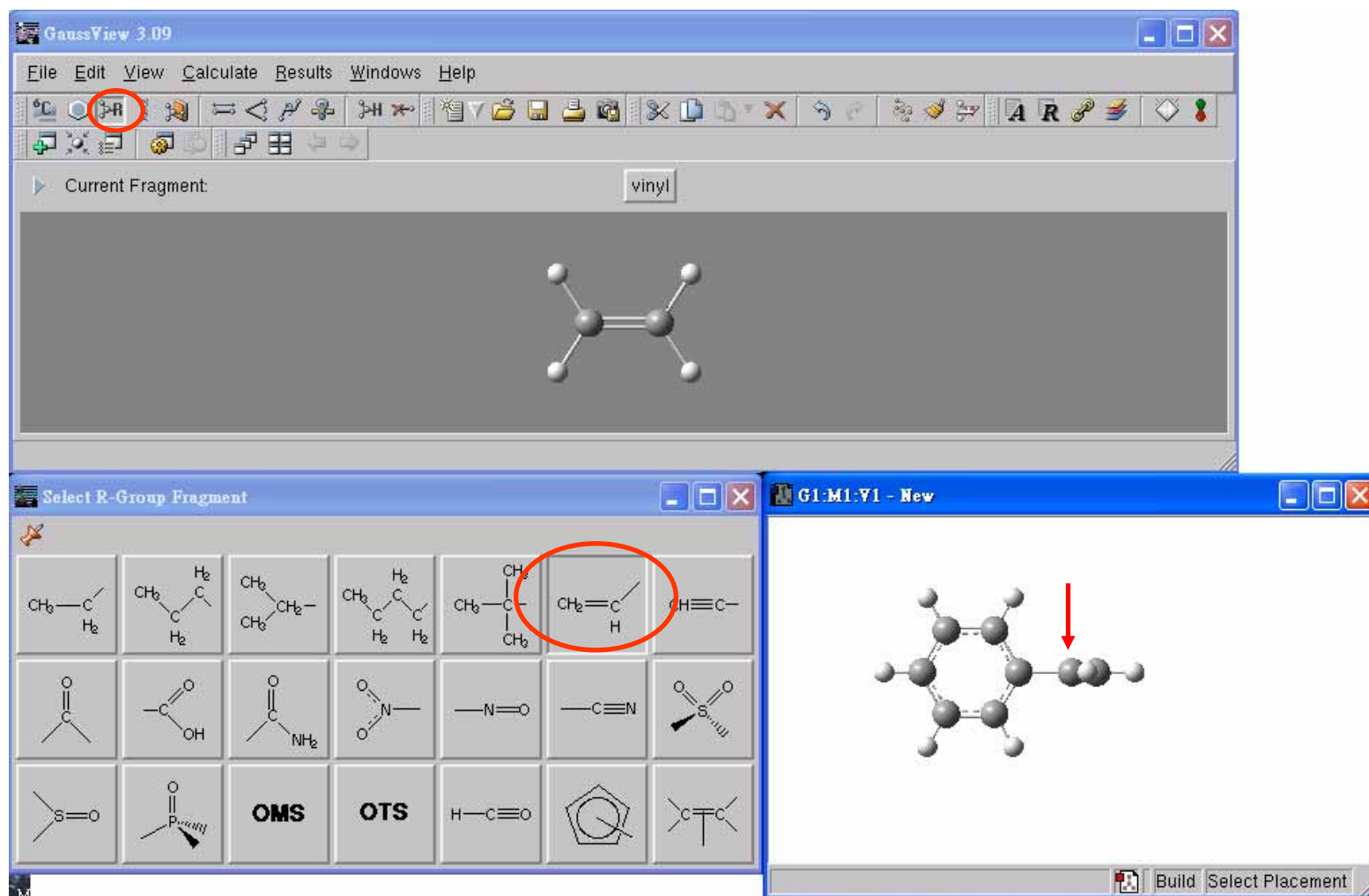
Select **Benzene** → Click at **new** window



Create Molecule : CN-PPV

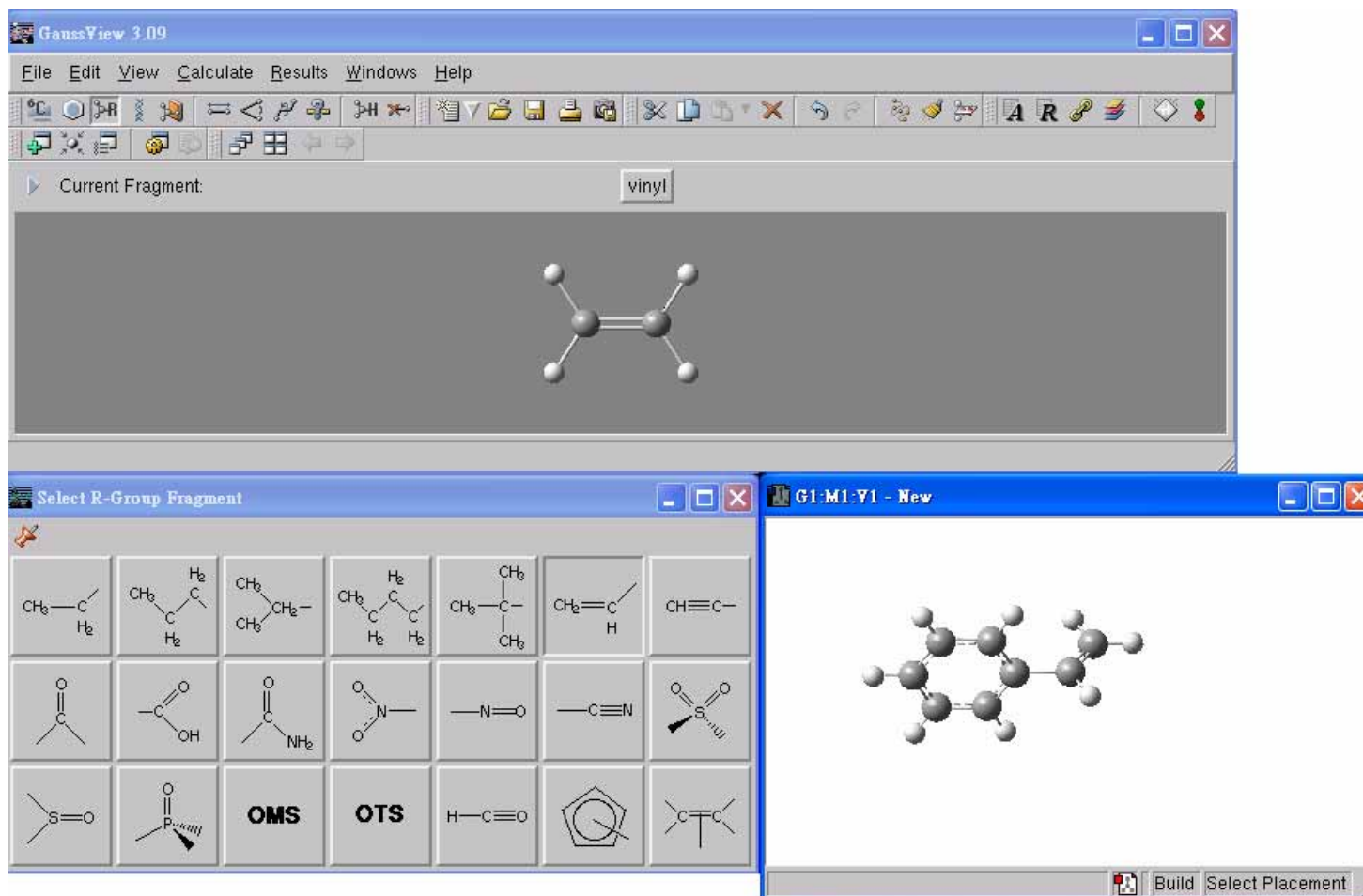
Double Click at **R-Group Fragment** →

Select **vinyl** → Click at **H** atom



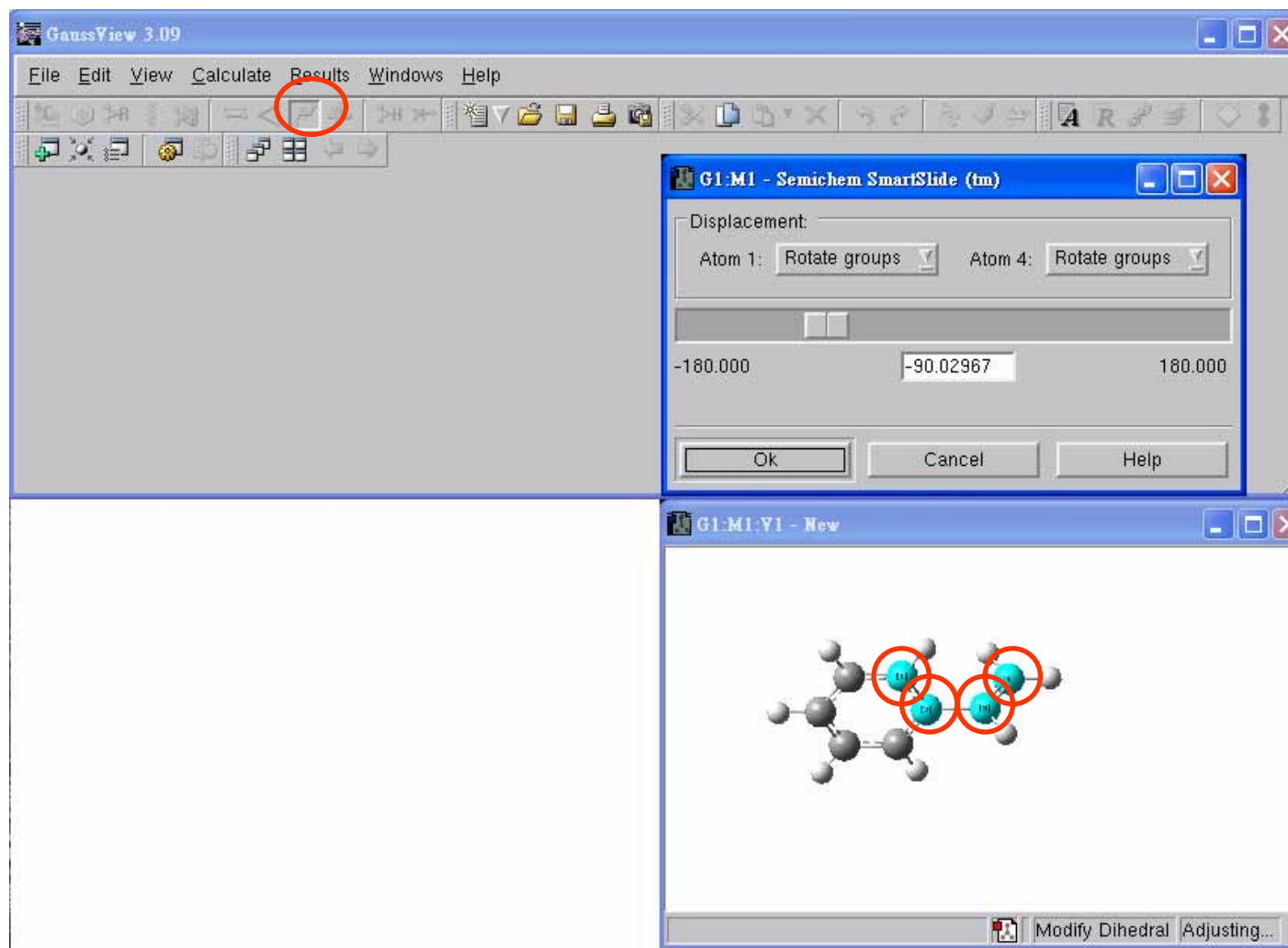
Rotate the molecule

Rotate the molecule using left button



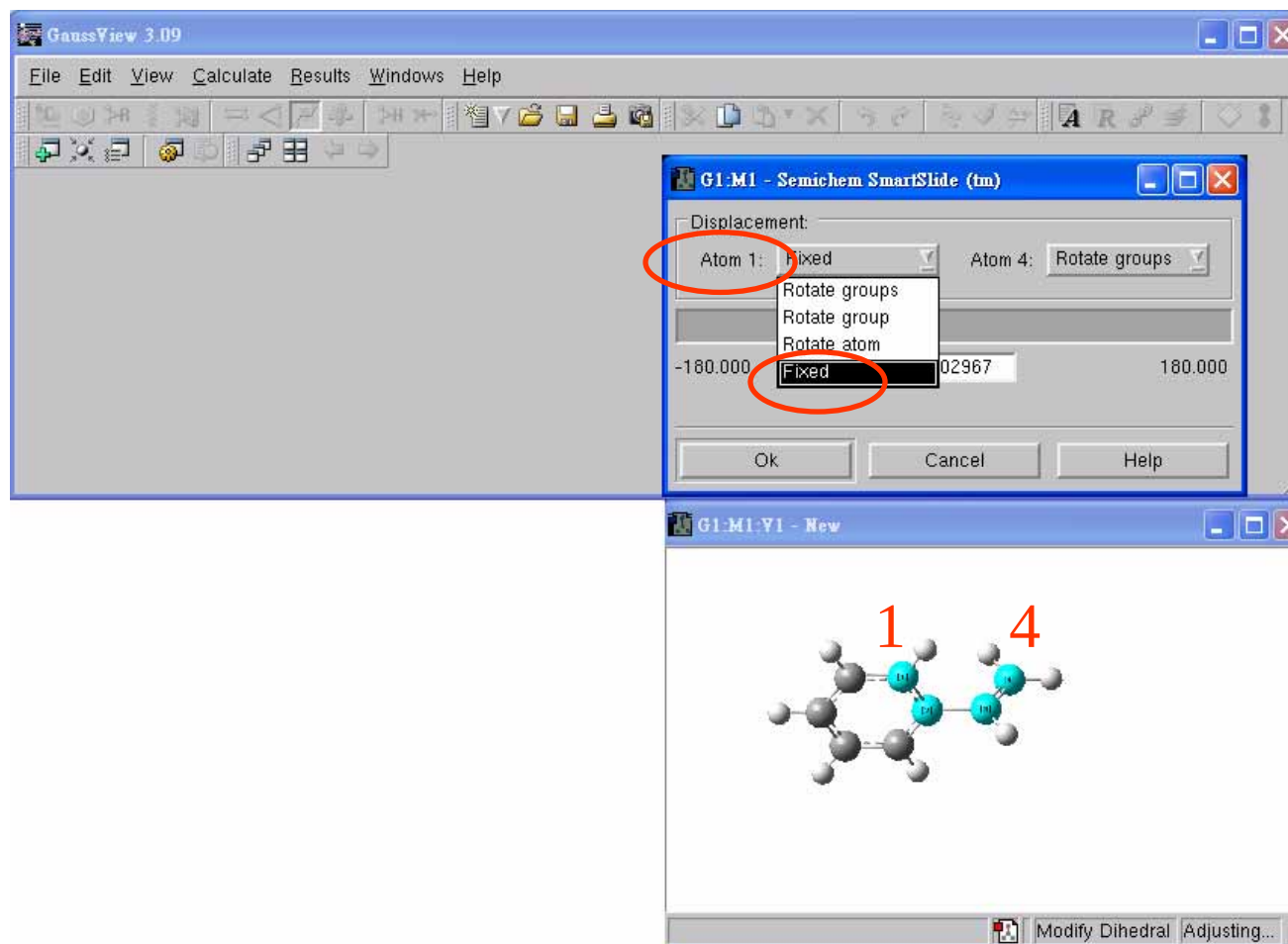
Modify Dihedral Angle

Click **Modify dihedral** → Select atoms



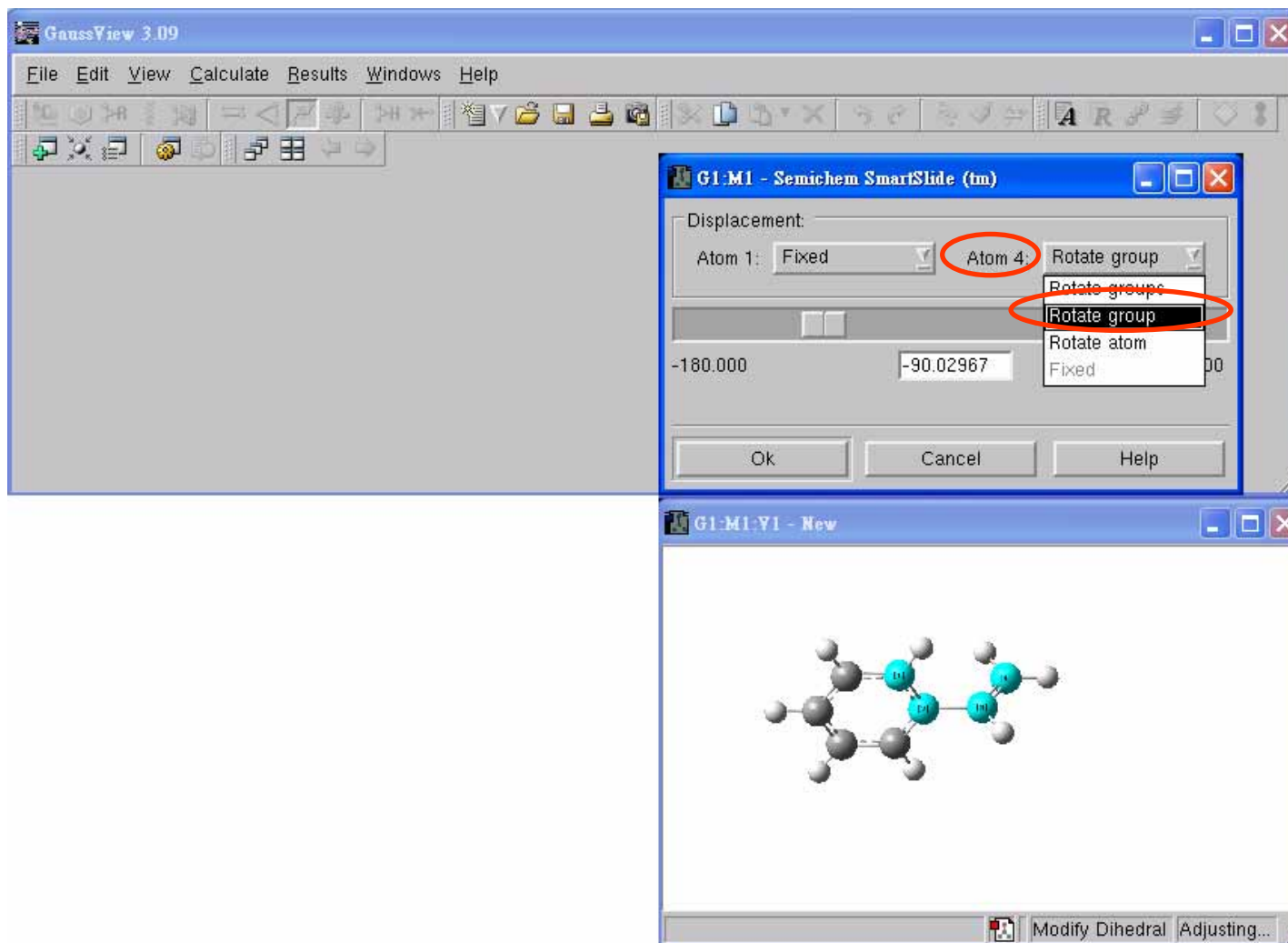
Coplanarity

Fixed atom1



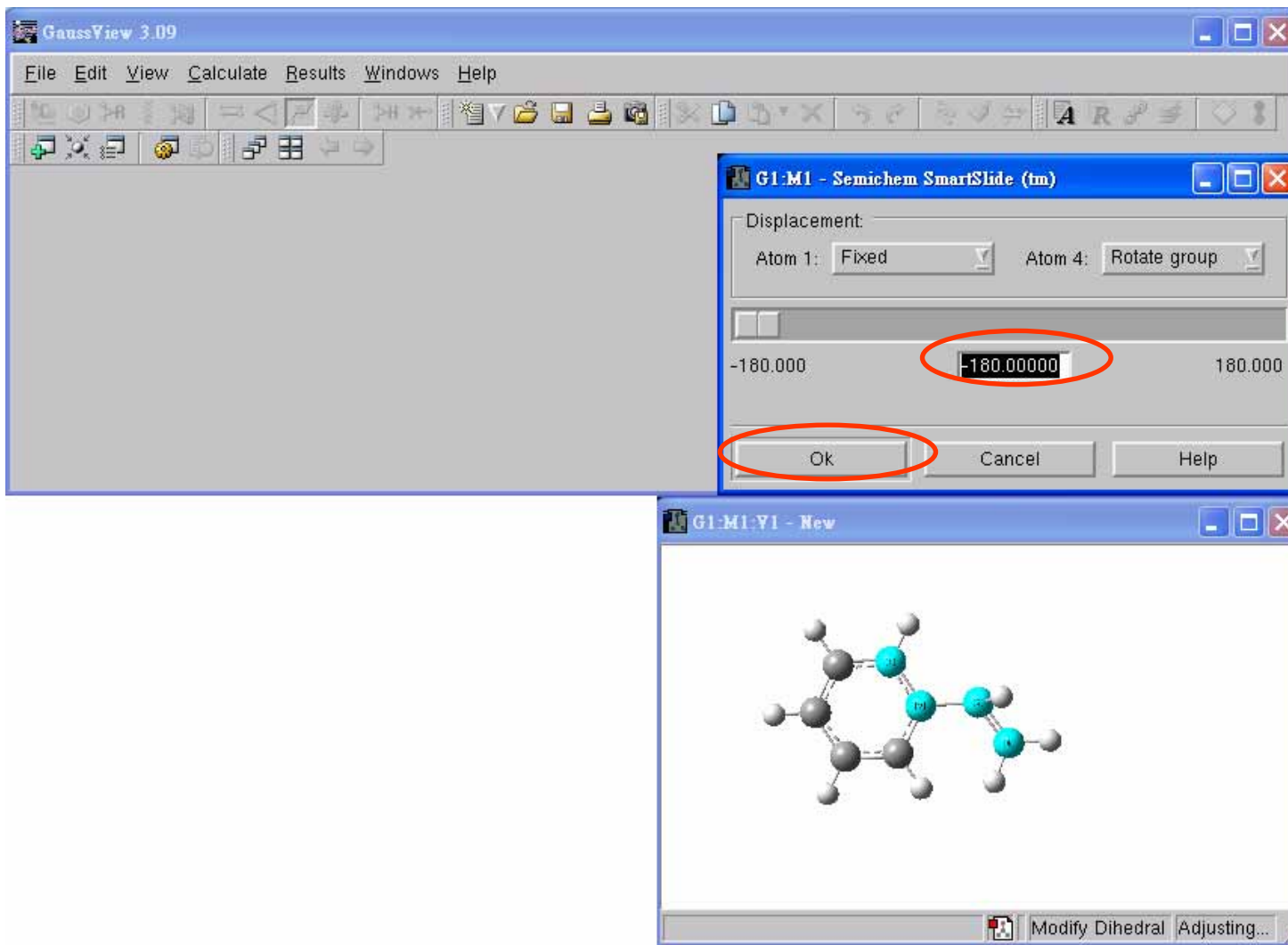
Coplanarity

Rotate atom4 → select **Rotate group**

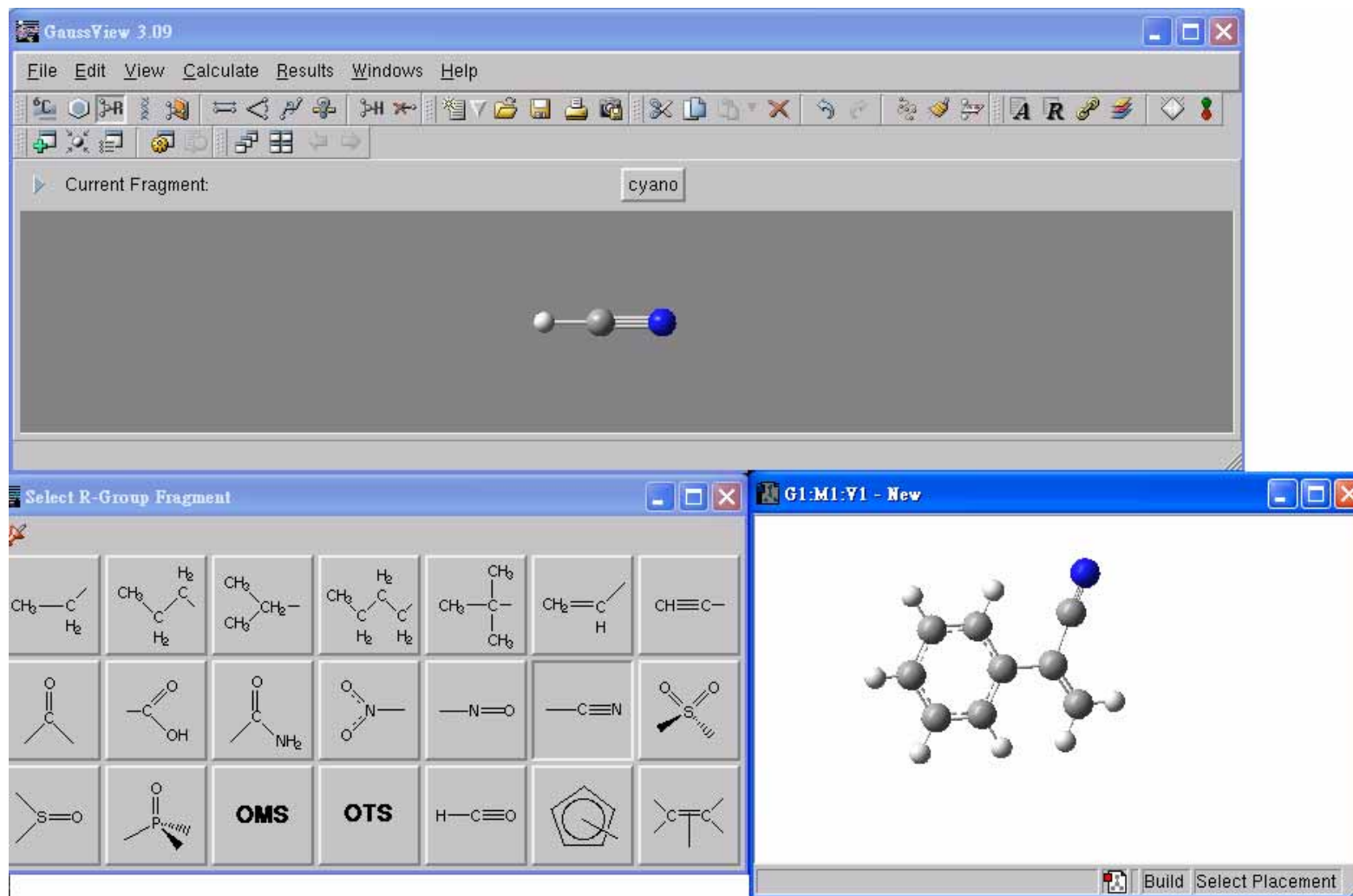


Coplanarity

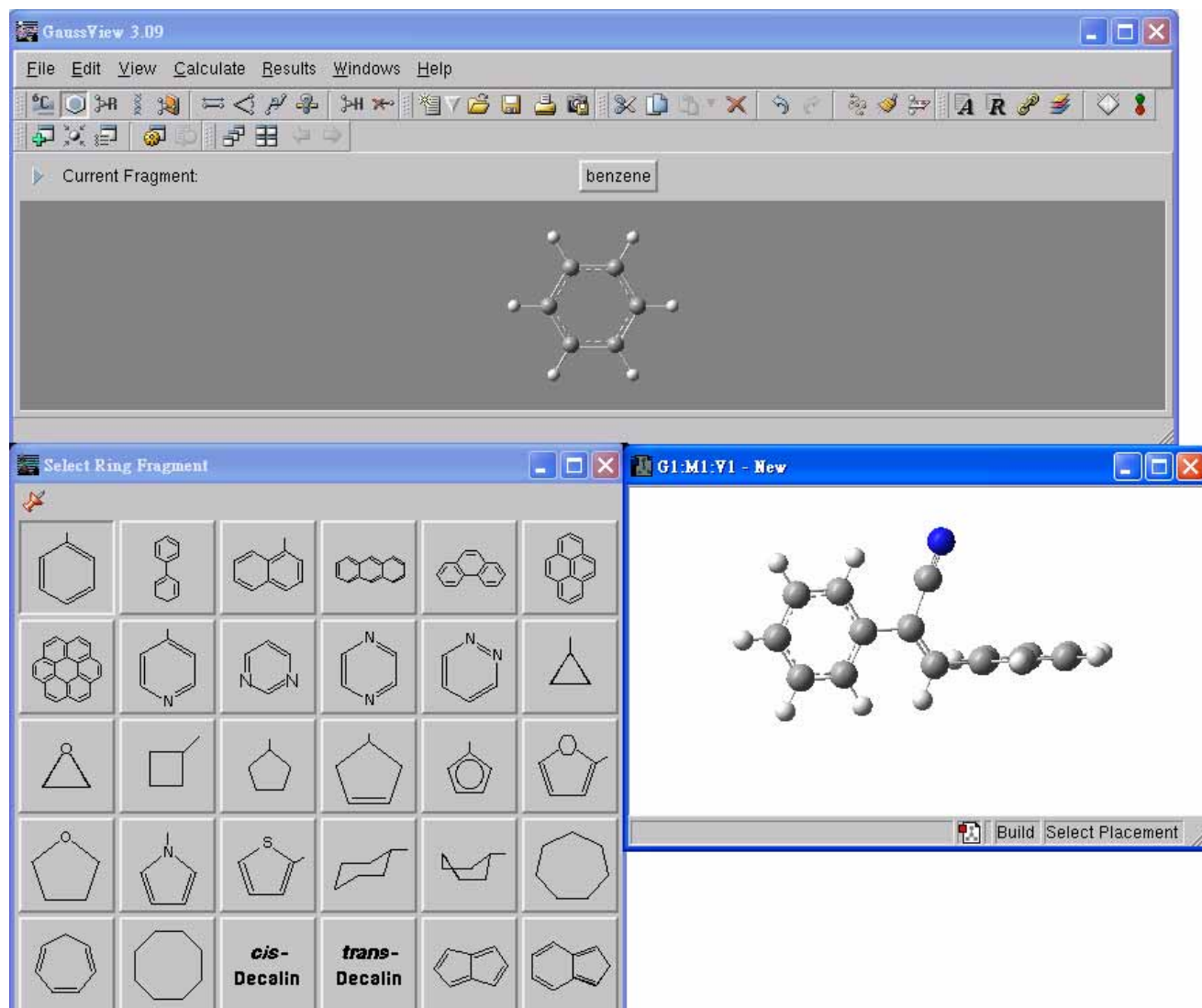
Key in the **angle** → Click **OK**



Add CN group

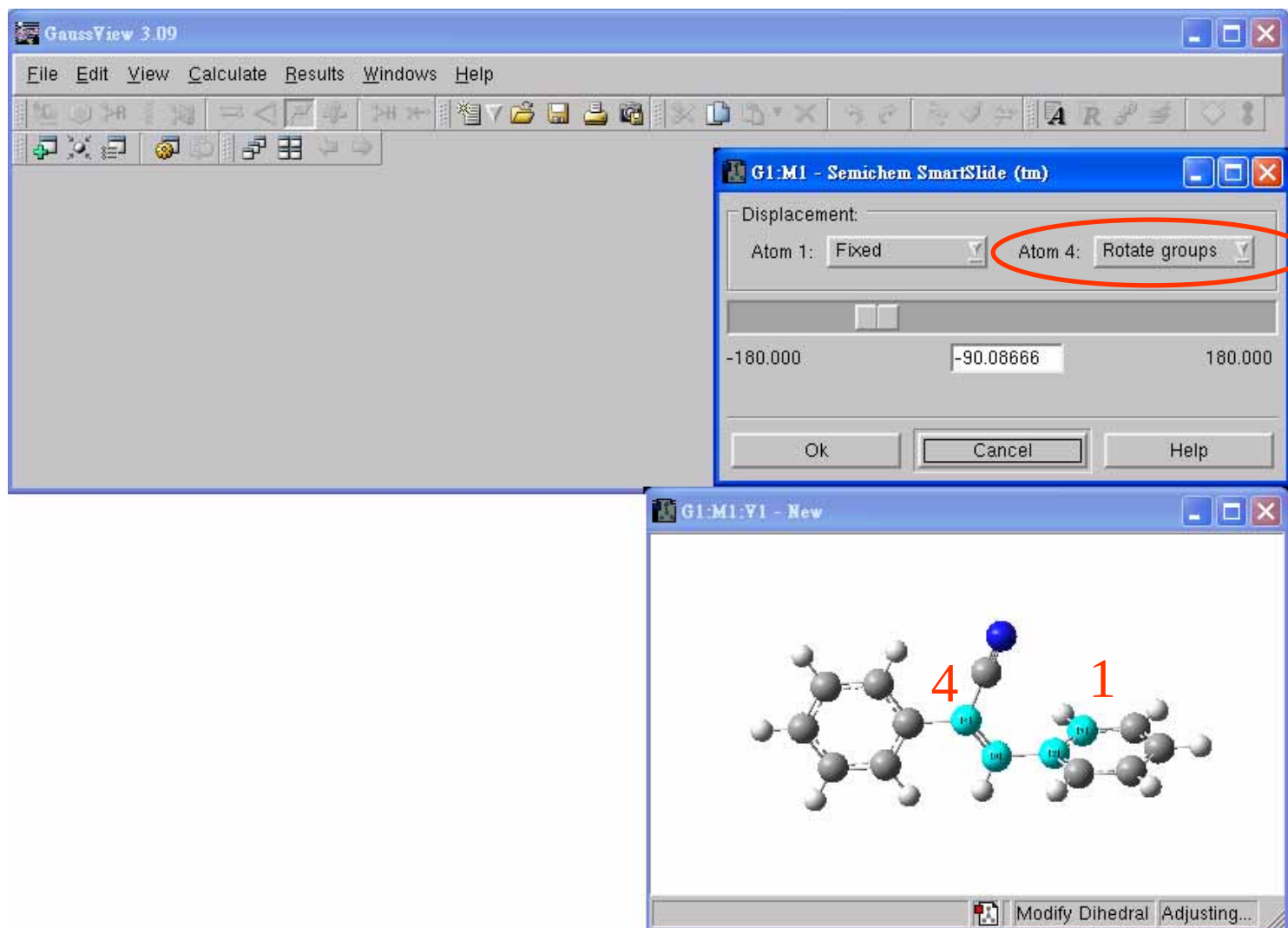


Add Benzene

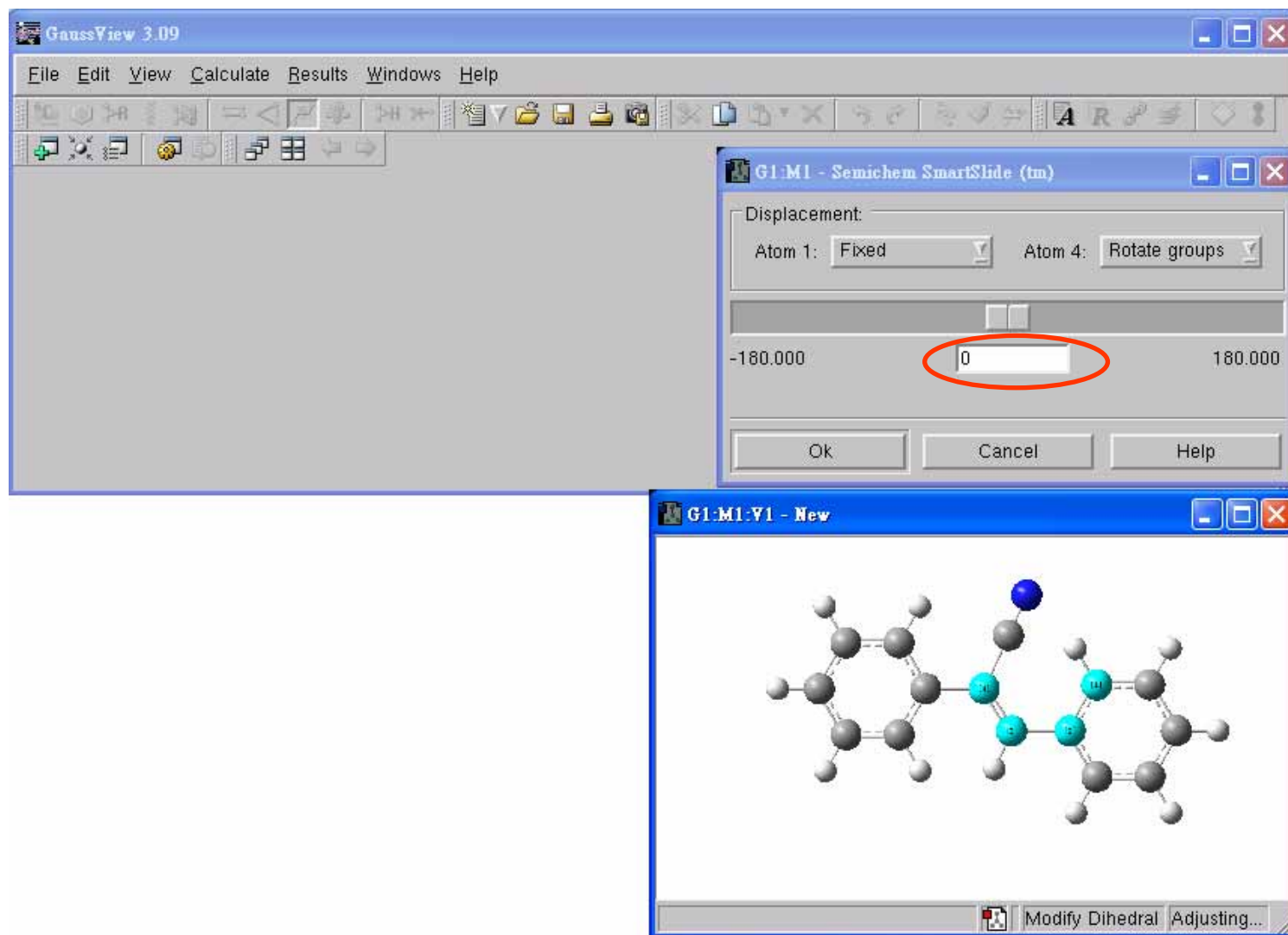


Rotate Benzene

Atom4 → Select Groups

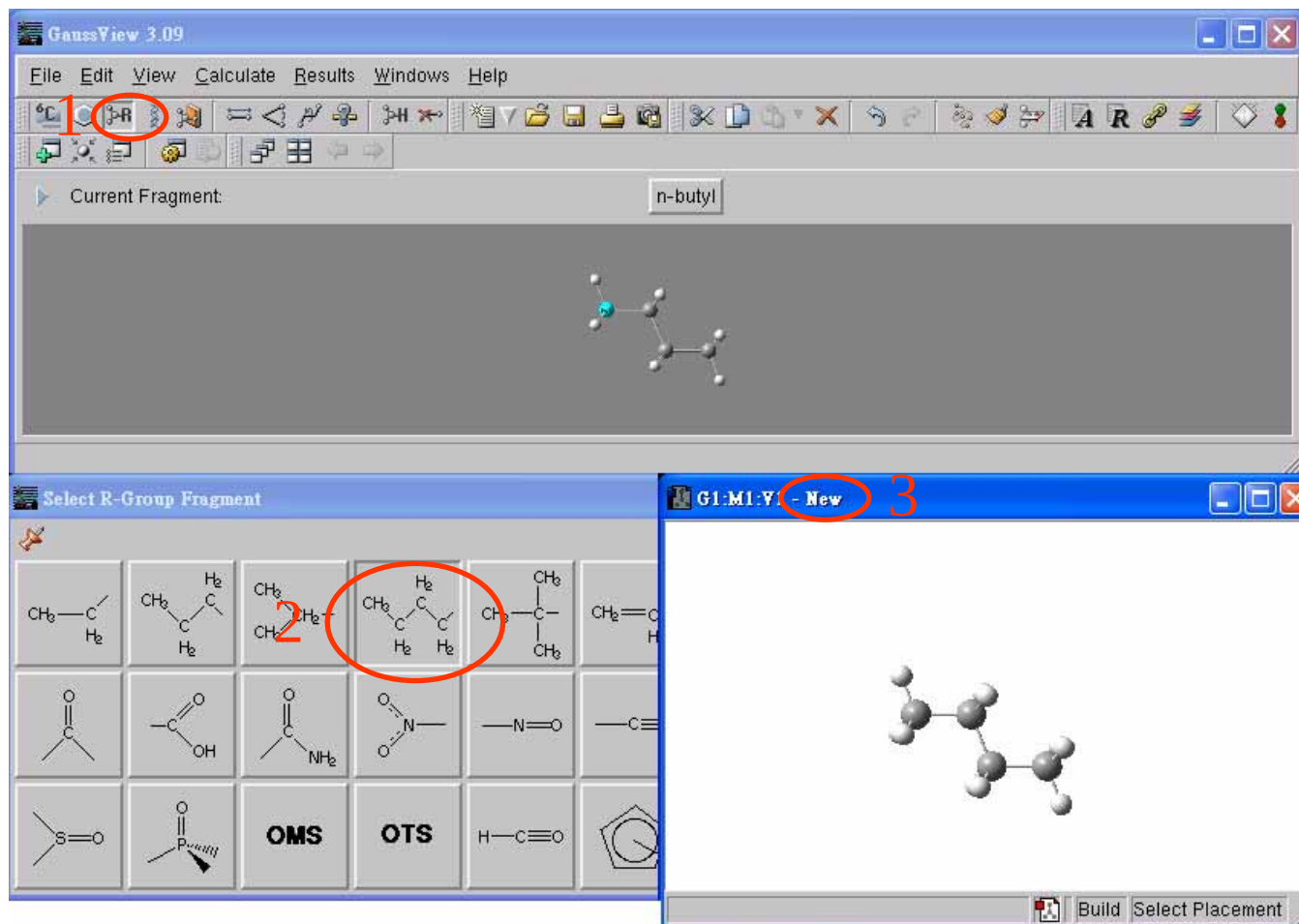


Key in the angle



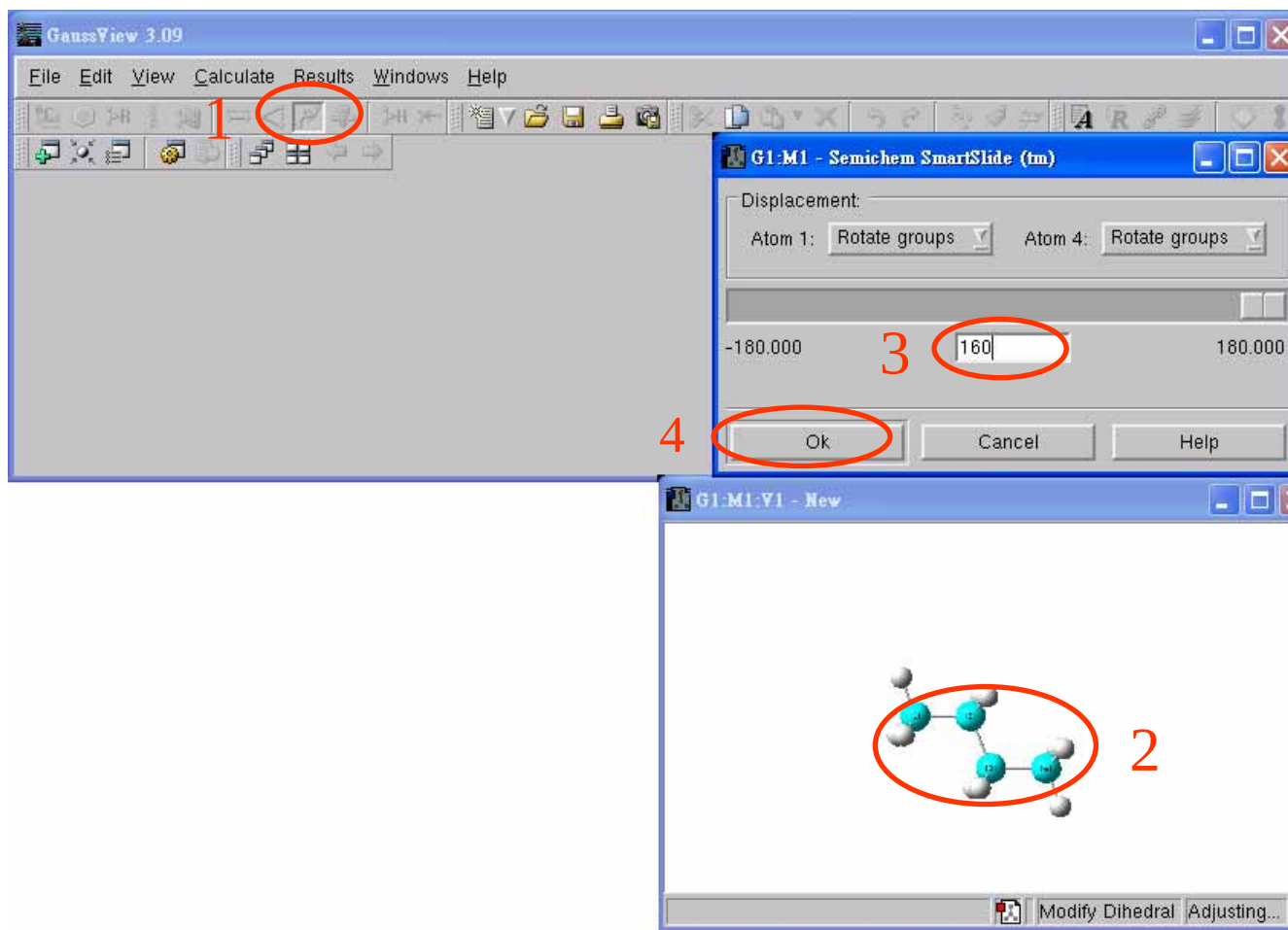
Mechanics Minimization

Double click **R-Group Fragment** → Select **n-butyl**
→ Click at new window



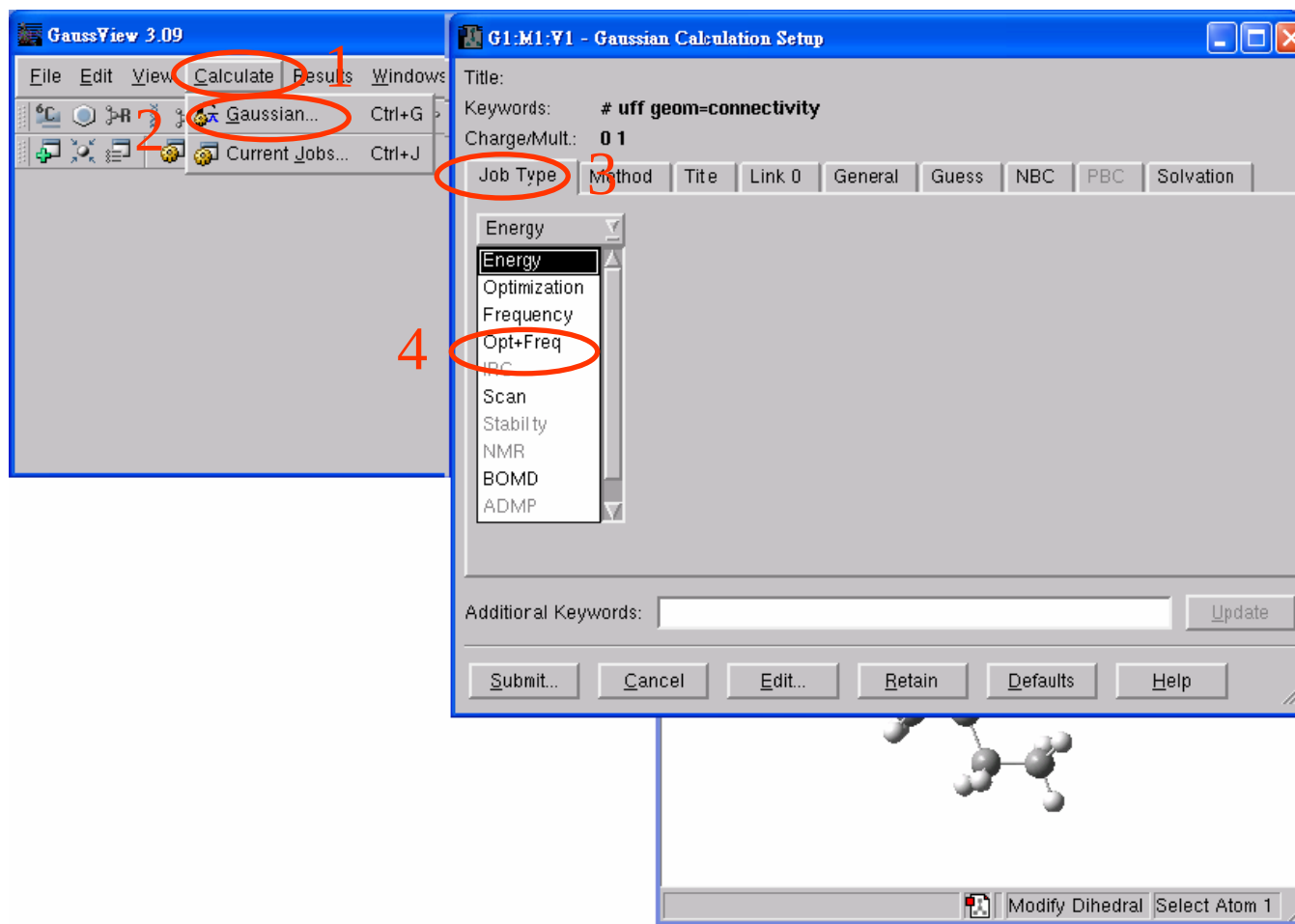
Modify dihedral angle

Click **modify dihedral angle** → **Select atoms** →
Key in the **angle** → Click **OK**



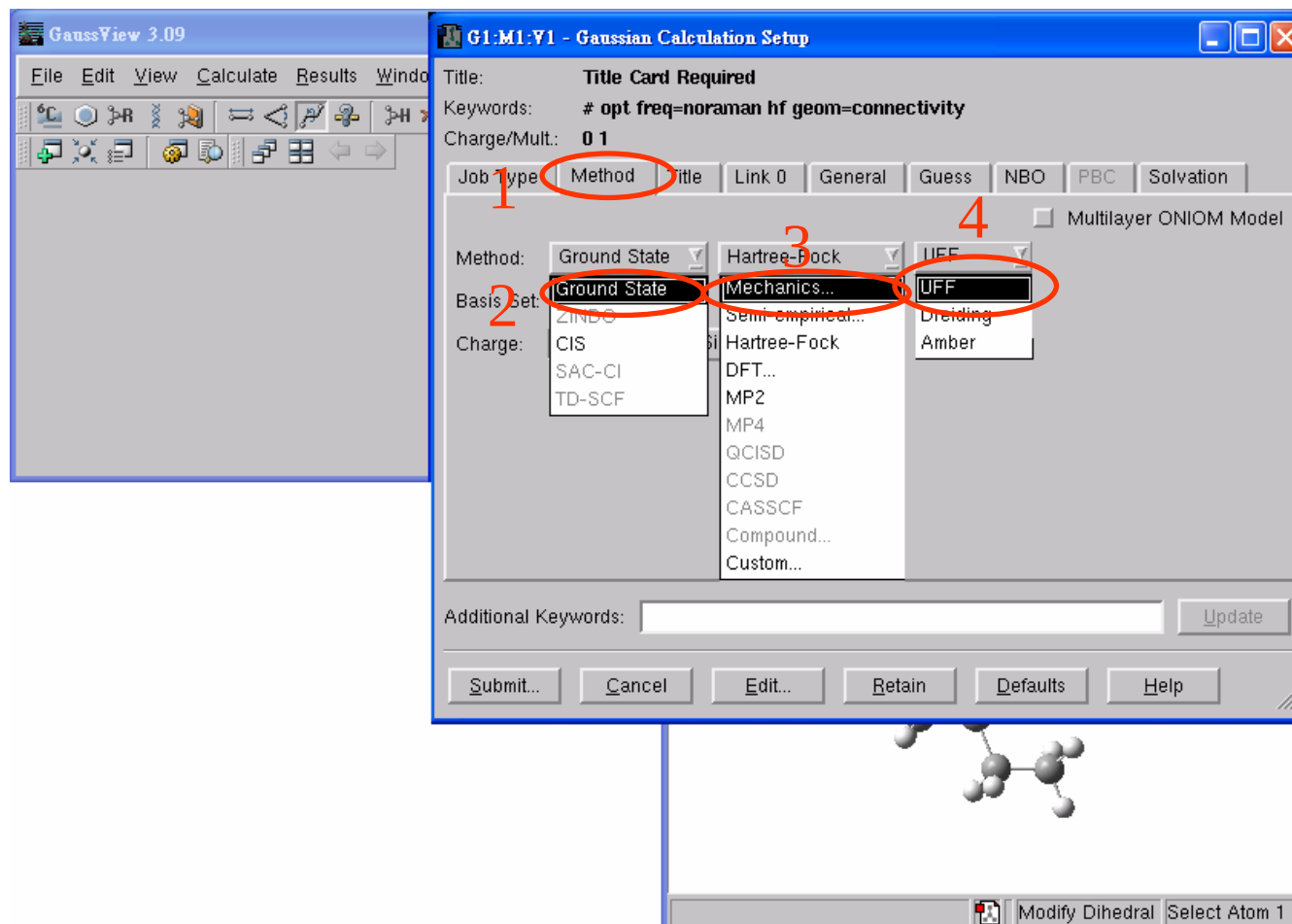
Minimization

Click **Calculate** → Select **Gaussian** →
Click **Job Type** → Select **Opt + Freq**



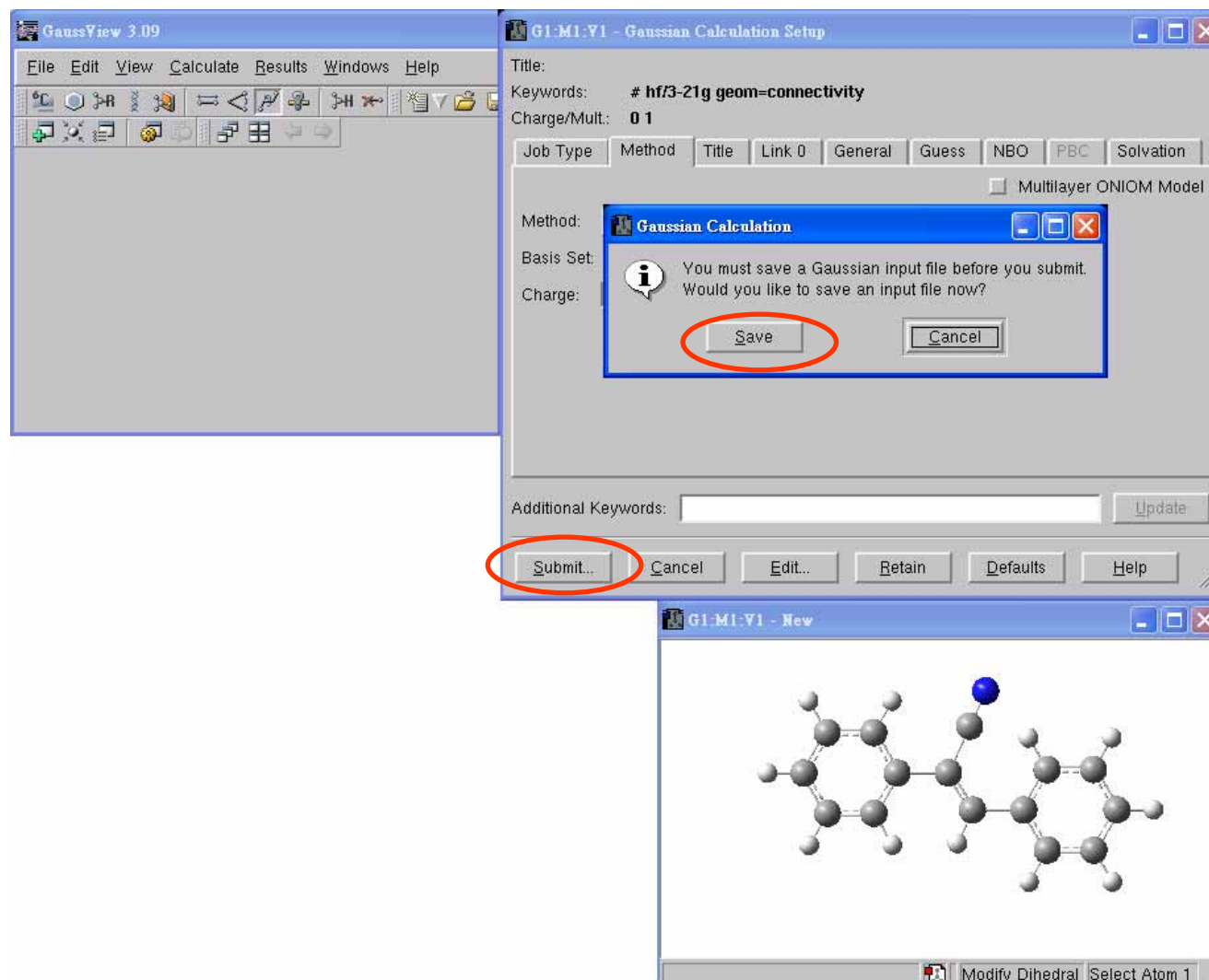
Method

Click **Method** → Select **Ground State** →
Select **Mechanics** → Select **Force Field**



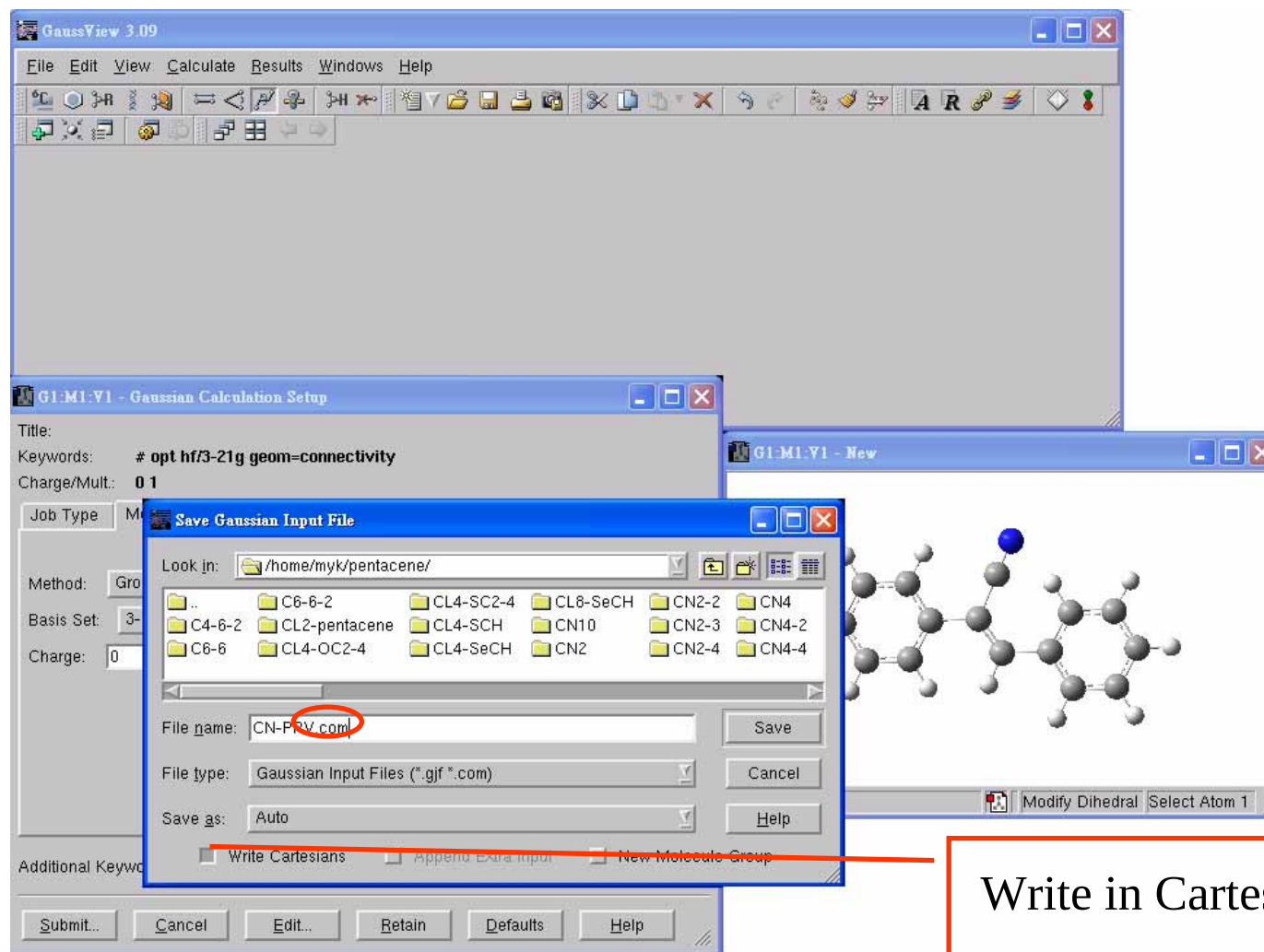
Submit the job

Click **Submit** → **Save** the job

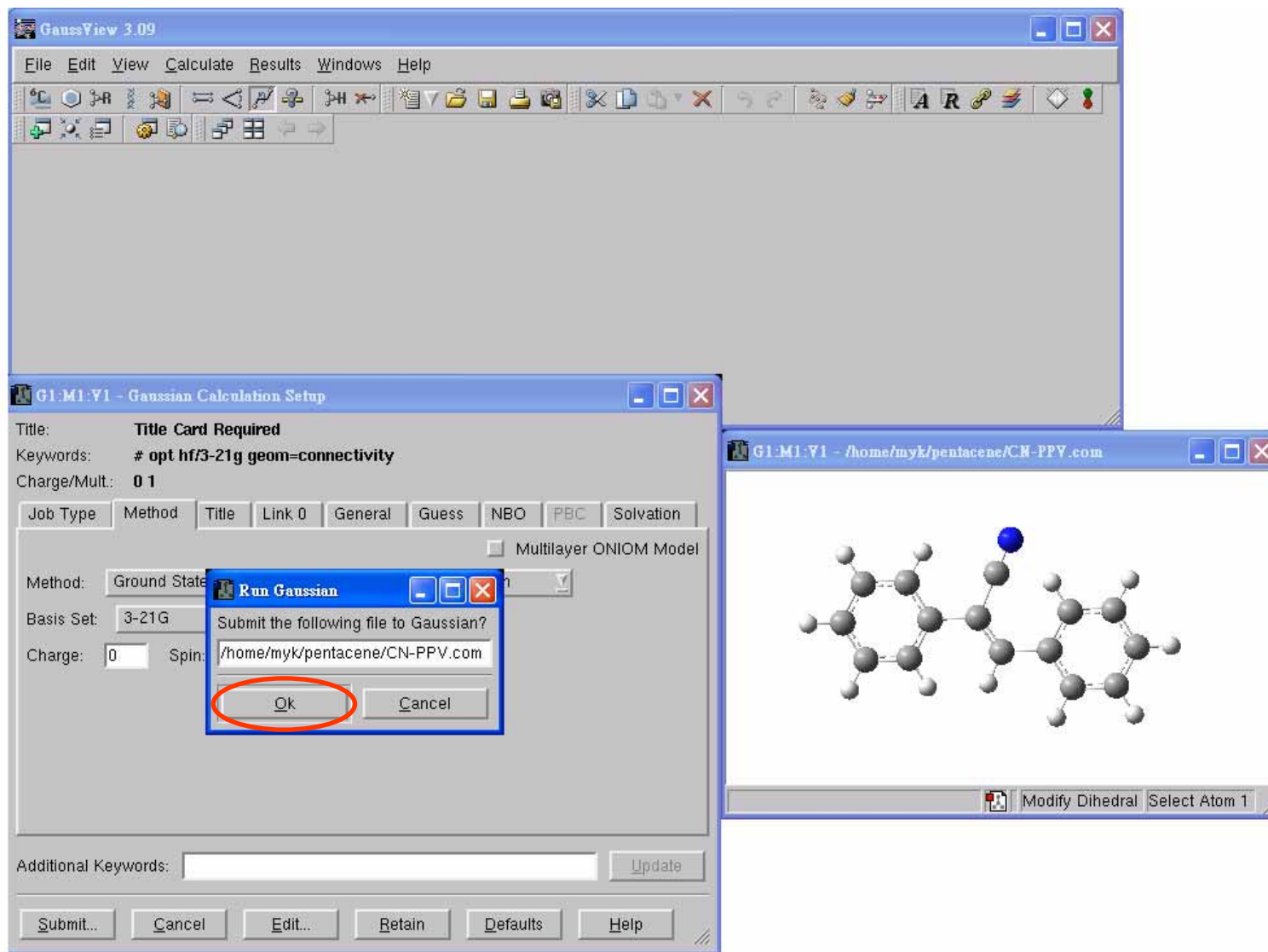


Save the job

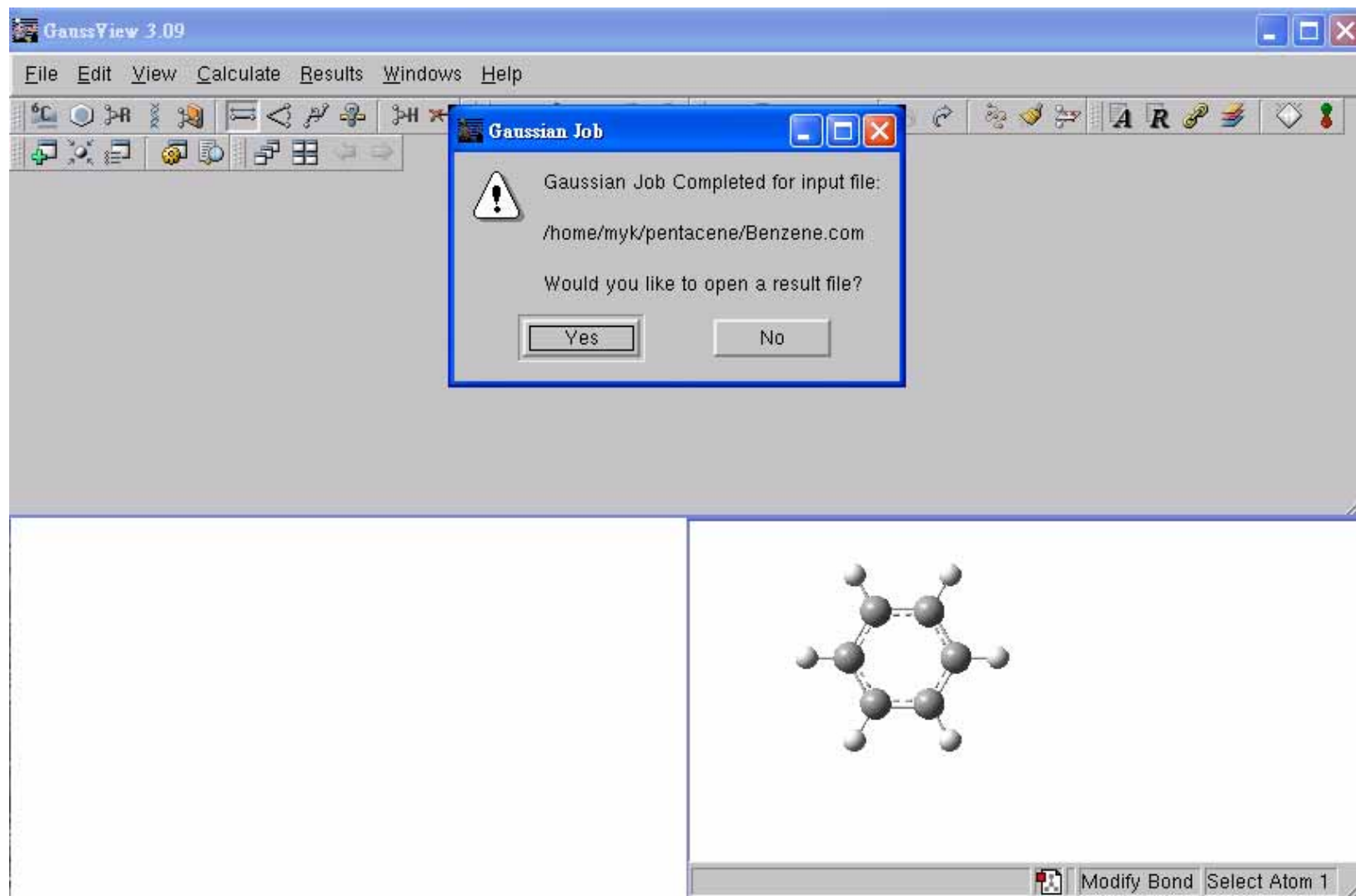
File type *.com



Run the Job



Finish Optimization



Check output *.log from startxwin

Type **vi *.log** → Enter

Check Optimization : Press **Esc** → type **:/Optimization** → Enter

Then press **Page Up** to find the final Geometry

```
myk on jockol: /home/myk/pentacene
X10      -3.59124  -0.00001  0.00000  -0.00001  -0.00001  -3.59125
Y10       1.55983  -0.00001  0.00000  -0.00001  -0.00001  1.55981
Z10       3.45861  0.00000  0.00000  0.00000  0.00000  3.45861
X11      -3.79561  0.00002  0.00000  0.00002  0.00002  -3.79560
Y11      -1.74505  0.00004  0.00000  0.00004  0.00004  -1.74501
Z11       2.92599  0.00001  0.00000  0.00001  0.00001  2.92600
X12      -4.67309  0.00002  0.00000  0.00002  0.00002  -4.67307
Y12      -0.70723  -0.00002  0.00000  -0.00002  -0.00002  -0.70725
Z12       7.38847  -0.00001  0.00000  -0.00001  -0.00001  7.38846
X13      -1.87592  -0.00003  0.00000  -0.00003  -0.00003  -1.87595
Y13      -2.54607  0.00003  0.00000  0.00003  0.00003  -2.54605
Z13       7.13284  0.00000  0.00000  0.00000  0.00000  7.13284
X14      -1.67168  -0.00001  0.00000  -0.00001  -0.00001  -1.67168
Y14       0.76963  -0.00001  0.00000  -0.00001  -0.00001  0.76961
Z14       7.66604  0.00001  0.00000  0.00001  0.00001  7.66605

Item      Value      Threshold  Converged?
Maximum Force      0.000049      0.000450      YES
RMS Force          0.000021      0.000300      YES
Maximum Displacement 0.000049      0.001800      YES
RMS Displacement   0.000021      0.001200      YES
Predicted change in Energy=-9.189714D-09
Optimization completed.
Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Final structure in terms of initial Z-matrix:
C
C, 1, B1
H, 1, B2, 2, A1
H, 1, B3, 2, A2, 3, D1, 0
H, 1, B4, 2, A3, 3, D2, 0
C, 2, B5, 1, A4, 3, D3, 0
H, 2, B6, 1, A5, 6, D4, 0
H, 2, B7, 1, A6, 6, D5, 0
C, 6, B8, 2, A7, 1, D6, 0
H, 6, B9, 2, A8, 1, D7, 0
H, 6, B10, 2, A9, 1, D8, 0
H, 9, B11, 6, A10, 2, D9, 0
H, 9, B12, 6, A11, 2, D10, 0
H, 9, B13, 6, A12, 2, D11, 0
Variables:
B1=1.53141363
B2=1.09034274
```

Final geometry

```

X myk on jocko: /home/myk/pentacene
Berny optimization.
Initialization pass.
No Z-matrix variables, so optimization will use Cartesian coordinates.
Trust Radius=1.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 2 maximum allowed number of steps= 2.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Input orientation:
-----
Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type          X           Y           Z
-----
  1          6      20001001      0.000000    0.000000    0.000000
  2          6      20001001      0.000000    0.000000    1.506718
  3          1      20001034      1.046893    0.000000   -0.388611
  4          1      20001034     -0.522633   -0.904842   -0.394513
  5          1      20001034     -0.522499    0.904976   -0.394435
  6          6      20001001     -1.407851    0.000178    2.064309
  7          1      20001034     0.550038   -0.902436    1.883912
  8          1      20001034     0.530585    0.915492    1.880311
  9          6      20001001     -1.438993   -0.478945    3.492496
 10          1      20001034     -1.831946    1.037375    2.005046
 11          1      20001034     -2.059390   -0.658465    1.431187
 12          1      20001034     -2.485255   -0.470612    3.882643
 13          1      20001034     -1.042745   -1.520525    3.567760
 14          1      20001034     -0.814581    0.180012    4.143227
-----
Distance matrix (angstroms):
      1          2          3          4          5
1  C      0.000000
2  C      1.506718    0.000000
3  H      1.116693    2.165238    0.000000
4  H      1.116927    2.169462    1.811680    0.000000
5  H      1.116945    2.169417    1.811631    1.809818    0.000000
6  C      2.498683    1.514250    3.470243    2.765588    2.765489
7  H      2.160106    1.122144    2.495119    2.518303    3.099668
8  H      2.157595    1.122149    2.500541    3.098017    2.506704
9  C      3.807574    2.498680    4.633790    4.016210    4.226515
10 H      2.907298    2.163447    3.885030    3.353266    2.736730
11 H      2.592867    2.163416    3.659813    2.399063    2.852942
12 H      4.633884    3.470301    5.562477    4.725939    4.902861
13 H      4.015996    2.765358    4.725617    4.043413    4.674687
14 H      4.226378    2.765344    4.902555    4.674743    4.604482

```

Dipole moment

Press **Esc** → type **:/Dipole** → Enter

```
myk on jocko1: /home/myk/pentacene
 65 0 0 F T 2.71D+00 0.00097480 0.00031298 0.00279892 0.00117717 0.0014877 ----
 66 0 0 F T 1.64D+01 0.00026226 0.00010872 0.00050011 0.00019420 0.0014821 ----+
 67 0 0 F T 2.06D-01 0.00026226 0.00010872 0.00821690 0.00319073 0.0014937 ----
 68 0 0 F T 2.60D+00 0.00042676 0.00011722 0.00056502 0.00025267 0.0014813 ----+
 69 0 0 F F 4.69D-01 0.00042676 0.00011722 0.00146878 0.00065681 0.0014803 ----
 70 0 0 F T 5.34D+00 0.00034646 0.00009143 0.00038324 0.00018055 0.0014802 ----+
 71 0 0 F F -3.62D-01 0.00034646 0.00009143 0.00204758 0.00096466 0.0014798 ----
 72 0 0 F T 5.94D+00 0.00015506 0.00006199 0.00024049 0.00010362 0.0014796 ----+
 73 0 0 F F -3.35D-01 0.00015506 0.00006199 0.00142797 0.00061528 0.0014794 ----+
 74 0 0 F T 2.66D+00 0.00020252 0.00007105 0.00045865 0.00015358 0.0014793 ----+
 75 0 0 F F 7.08D-01 0.00020252 0.00007105 0.00122166 0.00040907 0.0014789 ----+
 76 0 0 F T 6.05D+00 0.00014206 0.00005737 0.00038604 0.00011550 0.0014788 ----+
 77 0 0 F F -2.53D-01 0.00014206 0.00005737 0.00233534 0.00069870 0.0014785 ----+
 78 0 0 F T 5.51D+00 0.00014454 0.00004816 0.00031529 0.00009460 0.0014785 ----+
 79 0 0 F F -4.59D-01 0.00014454 0.00004816 0.00173872 0.00052170 0.0014784 ----+
 80 0 0 F T 3.05D+00 0.00014869 0.00004457 0.00029567 0.00009246 0.0014783 ----+
 81 0 0 F F 5.07D-01 0.00014869 0.00004457 0.00090305 0.00028240 0.0014782 ----+
 82 0 0 F T 7.74D+00 0.00012880 0.00003117 0.00016052 0.00005494 0.0014782 ----+
 83 0 0 F F 2.88D-01 0.00012880 0.00003117 0.00124322 0.00042547 0.0014784 ----+
 84 0 0 F T 3.78D+00 0.00005122 0.00002092 0.00008349 0.00003240 0.0014781 ----+
Energy= 0.0014781527 NIter= 0.
Dipole moment= 0.000000 0.000000 0.000000
**** Axes restored to original set ****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
-----
 1 6 0.000005495 -0.000011819 0.000011214
 2 6 0.000016321 -0.000048927 -0.000025443
 3 1 -0.000032356 0.000007279 -0.000010213
 4 1 -0.000006158 0.000002824 0.000016043
 5 1 -0.000005677 -0.000038845 0.000015036
 6 6 0.000034762 0.000010659 -0.000006714
 7 1 -0.000012370 0.000030763 -0.000010289
 8 1 0.000027545 0.000036676 0.000027666
 9 6 -0.000016058 -0.000005078 -0.000022878
10 1 -0.000009331 -0.000014587 0.000002421
11 1 0.000016103 0.000041234 0.000009767
12 1 0.000018665 -0.000022267 -0.000011644
13 1 -0.000031762 0.000025063 -0.000003294
14 1 -0.000005181 -0.000012977 0.000008326

Cartesian Forces: Max 0.000048927 RMS 0.000020919
search hit BOTTOM, continuing at TOP
```

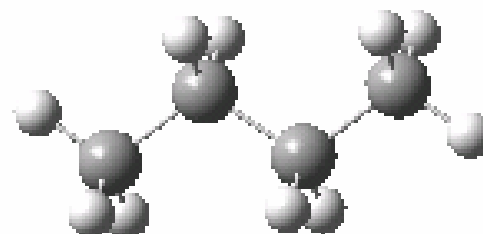
Energy

Press **Esc** → type **:/HF=** → Enter

```
myk on jocko1: /home/myk/pentacene
A2=109.92140693
A3=109.91767052
A4=111.27918903
A5=108.92867122
A6=108.89888735
A7=111.1984849
A8=109.43872707
A9=109.44629082
A10=109.42797514
A11=109.91340336
A12=109.90243008
D1=119.74602817
D2=-119.74059929
D3=-179.91400646
D4=120.72711217
D5=-120.71715619
D6=-179.74419854
D7=-59.36588935
D8=59.84654399
D9=179.98395283
D10=-60.2380844
D11=60.24562197
I\1\GINC-JOCKO1\FOpt\AMBER\ZDO\C4H10\MYK\11-May-2006\0\#\ OPT AMBER GE
OM=CONNECTIVITY\Title Card Required\0,1\C,-0.094518871,-0.0070329665
,-0.0654139693\C,0.2221549285,1.446434761,0.298422483\H,0.3389134061,-
0.2396148211,-1.0384964038\H,0.3288060637,-0.678084545,0.6828141464\H,
-1.1745197952,-0.1513523012,-0.1127305882\C,-0.3679159454,1.8197601392
,1.6655061326\H,1.3049780045,1.5773582289,0.3225446085\H,-0.1946382329
,2.1013421345,-0.4679210858\C,-0.0555668404,3.2753517712,2.0246466684\
H,-1.4503096557,1.6854716211,1.6426629349\H,0.0521531611,1.1677172076,
2.4327290262\H,-0.4871155205,3.509307949,2.9982238882\H,1.0240439518,3
.4238014822,2.0680352109\H,-0.4835653306,3.9425932084,1.2756597714\Ve
rsion=AM64L-G03RevC.02\HF=0.0014781\RMSD=0.000e+00\RMSF=2.092e-05\Dipo
le=0.,0.,0.\PG=C01 [X(C4H10)]\ve
ALL MY ATTEMPTS TO ADAPT THE THEORETICAL FOUNDATIONS OF PHYSICS
TO THESE NEW NOTIONS FAILED COMPLETELY. IT WAS AS IF THE GROUND HAD
BEEN PULLED OUT FROM UNDER ONE WITH NO FIRM FOUNDATION TO BE SEEN ANYWHERE,
UPON WHICH ONE COULD HAVE BUILT. -- A. EINSTEIN
Job cpu time: 0 days 0 hours 0 minutes 2.0 seconds.
File lengths (MBytes): RWF= 18 Int= 0 D2E= 0 Chk= 10 Scr= 1
Normal termination of Gaussian 03 at Thu May 11 16:02:34 2006.
```

Different Force Field

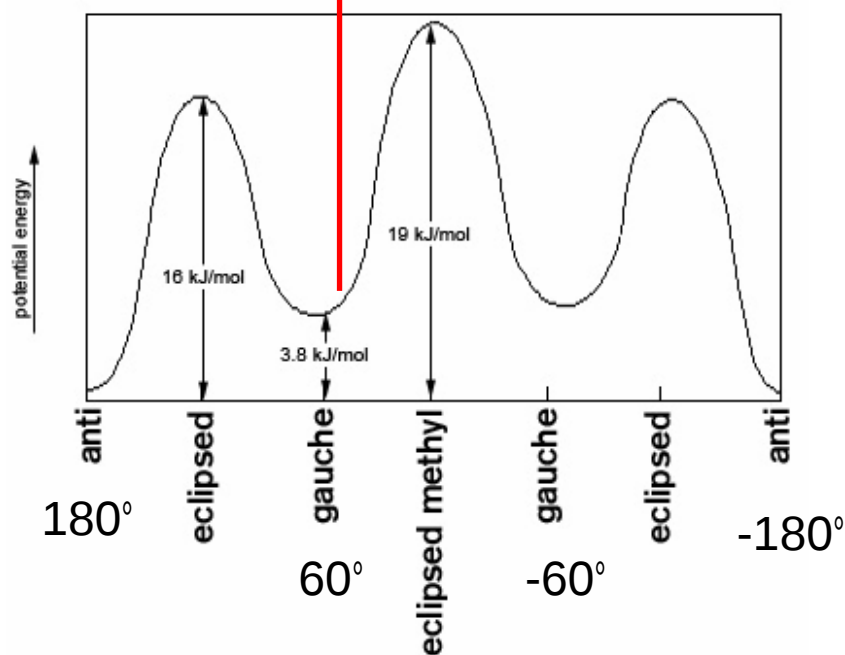
UFF 4.81
Dreiding 3.05
Amber 3.01



1 Hartree = 627.50956 kcal/mol

1 cal = 4.18 J

Torsion Angle

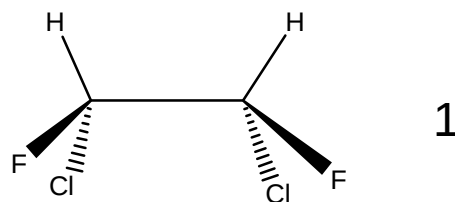


conformer potentials of butane about central C-C bond

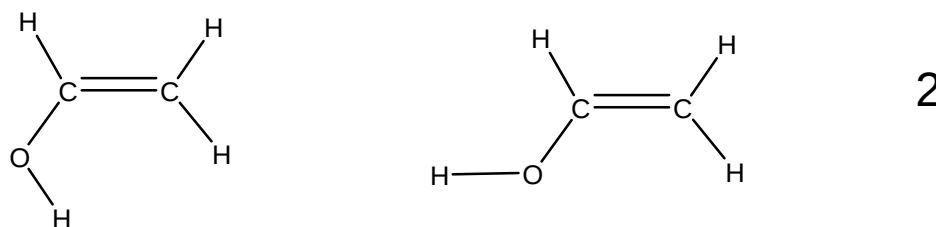
initial	Final
160°	UFF 179.45°
	Dreiding 179.89°
	Amber 179.75°
110°	UFF 70.98°
	Dreiding 67.86°
	Amber 67.84°

Exercises:

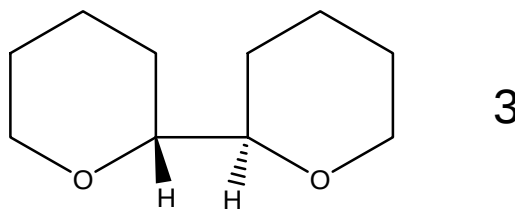
- 1) Build molecule 1 and manipulate to different stereoisomers.



- 2) Build molecule 2 and calculate the energy for the two geometries.



- 3) Build molecule 3 and optimize with molecular mechanics using UFF, amber and Dreiding force-fields.



4) Conformational Search:

Build a butane molecule ($\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-CH}_3$), use the **Redundant Coordinator editor** to specify the dihedral angle C1-C2-C3-C4, do **Relaxed Redundant coord Scan** using **am1**, run job, and determine which is the most stable geometry.

5) Build a water dimer, and try to manipulate them at different binding orientations.