

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

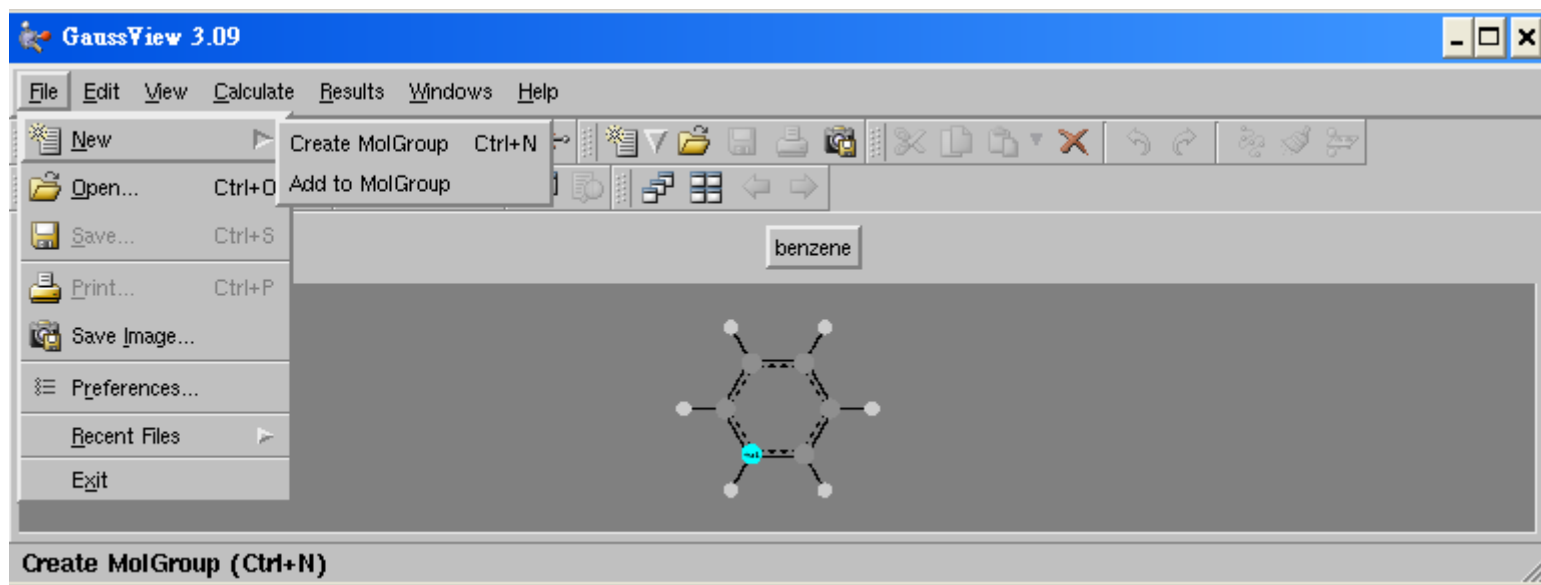
Some Useful Website

Technical Support Information

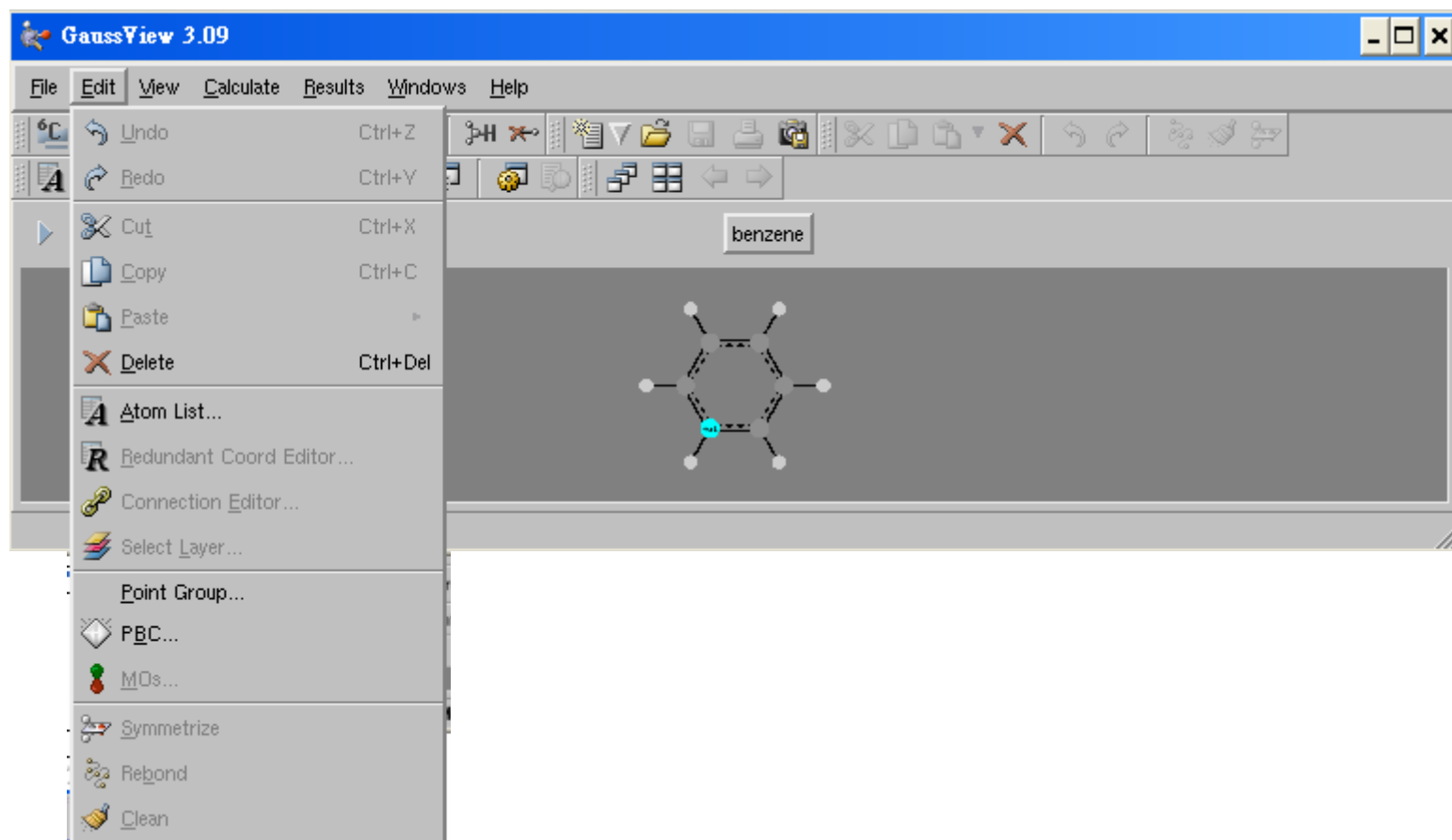
http://www.gaussian.com/tech_top_level.htm

Pull-down menu options:

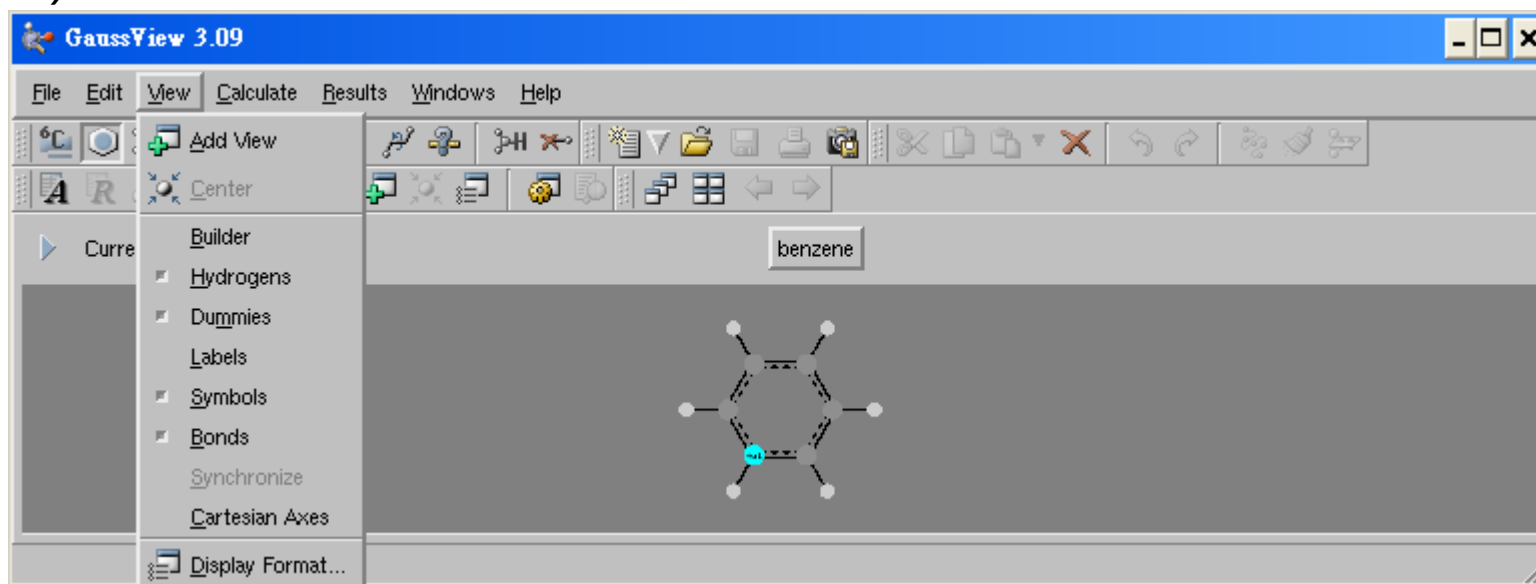
1) File:



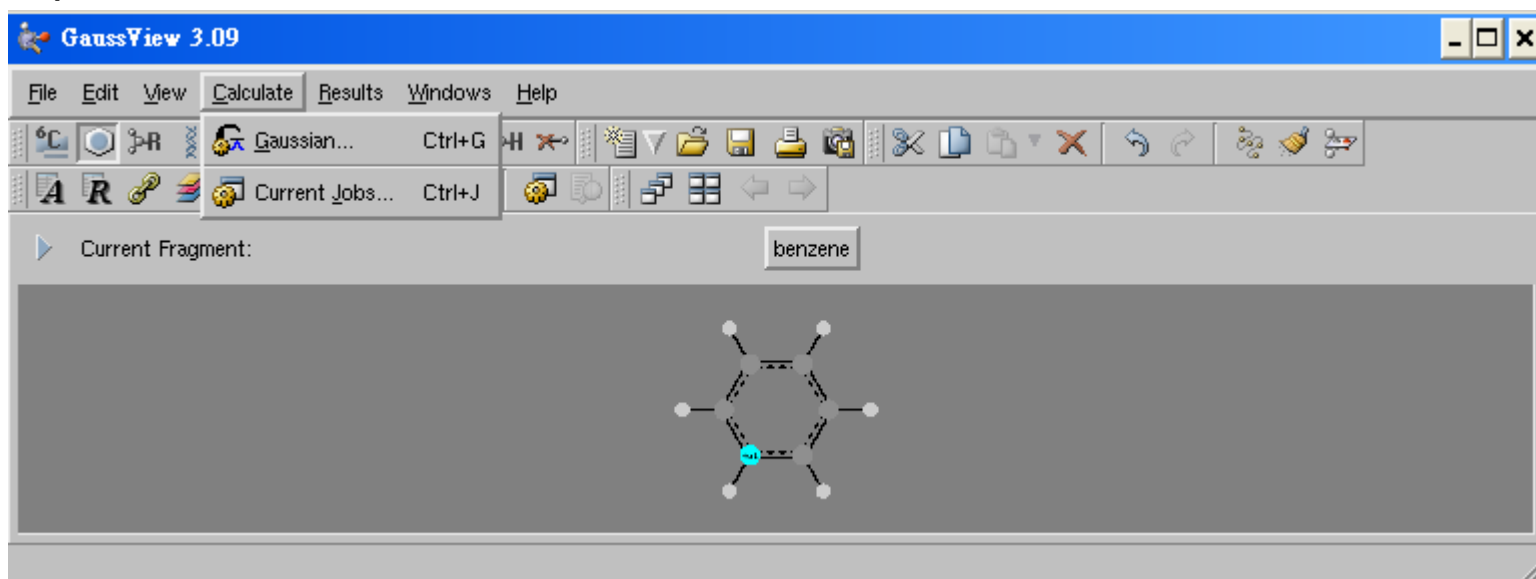
2) Edit:



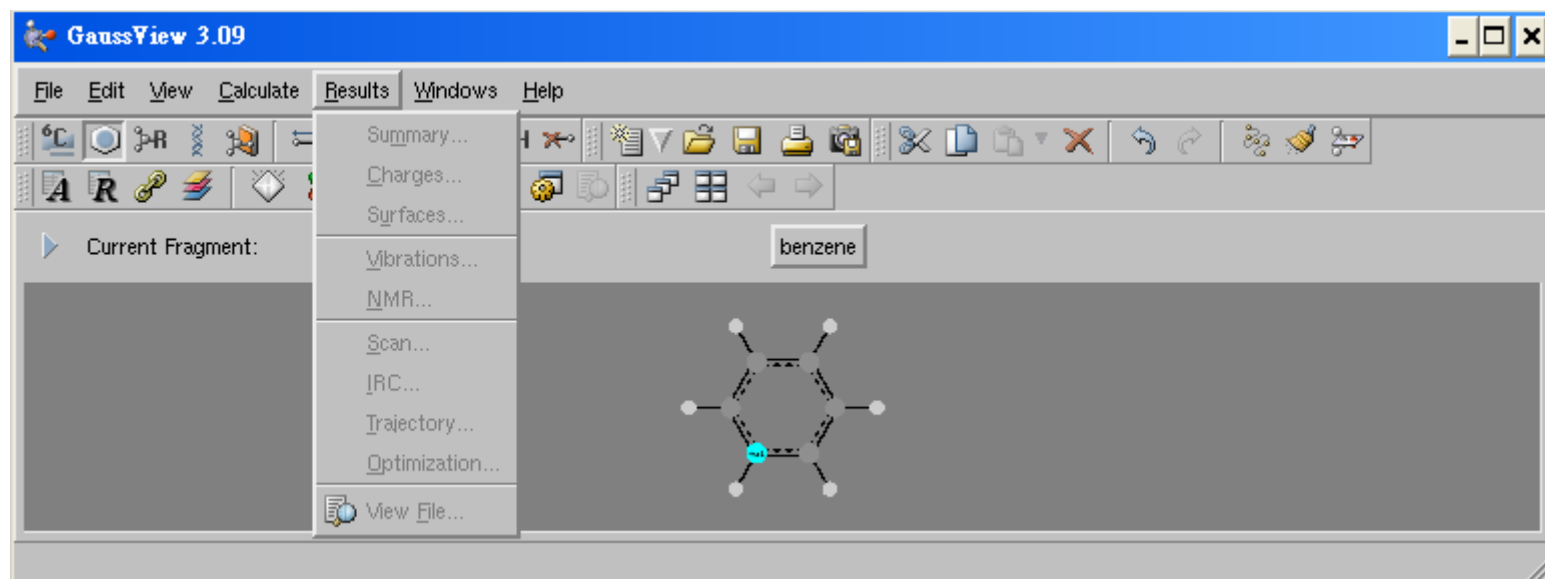
3) View:



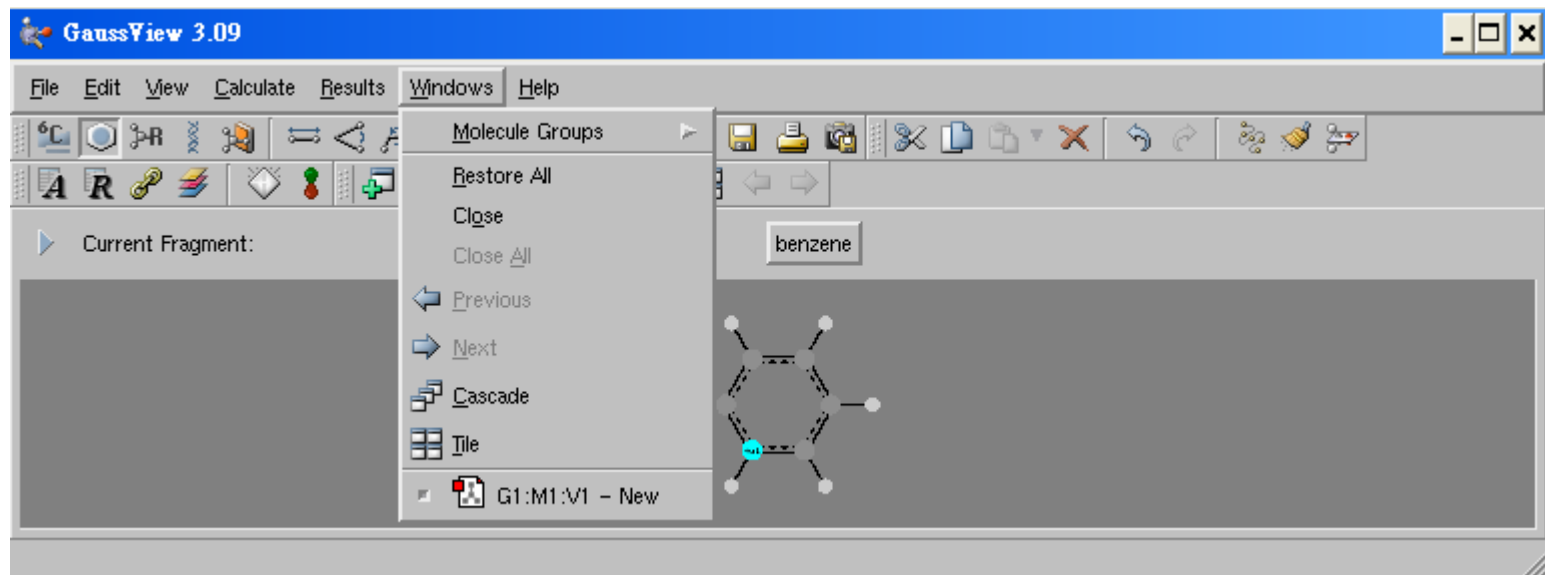
4) Calculate:



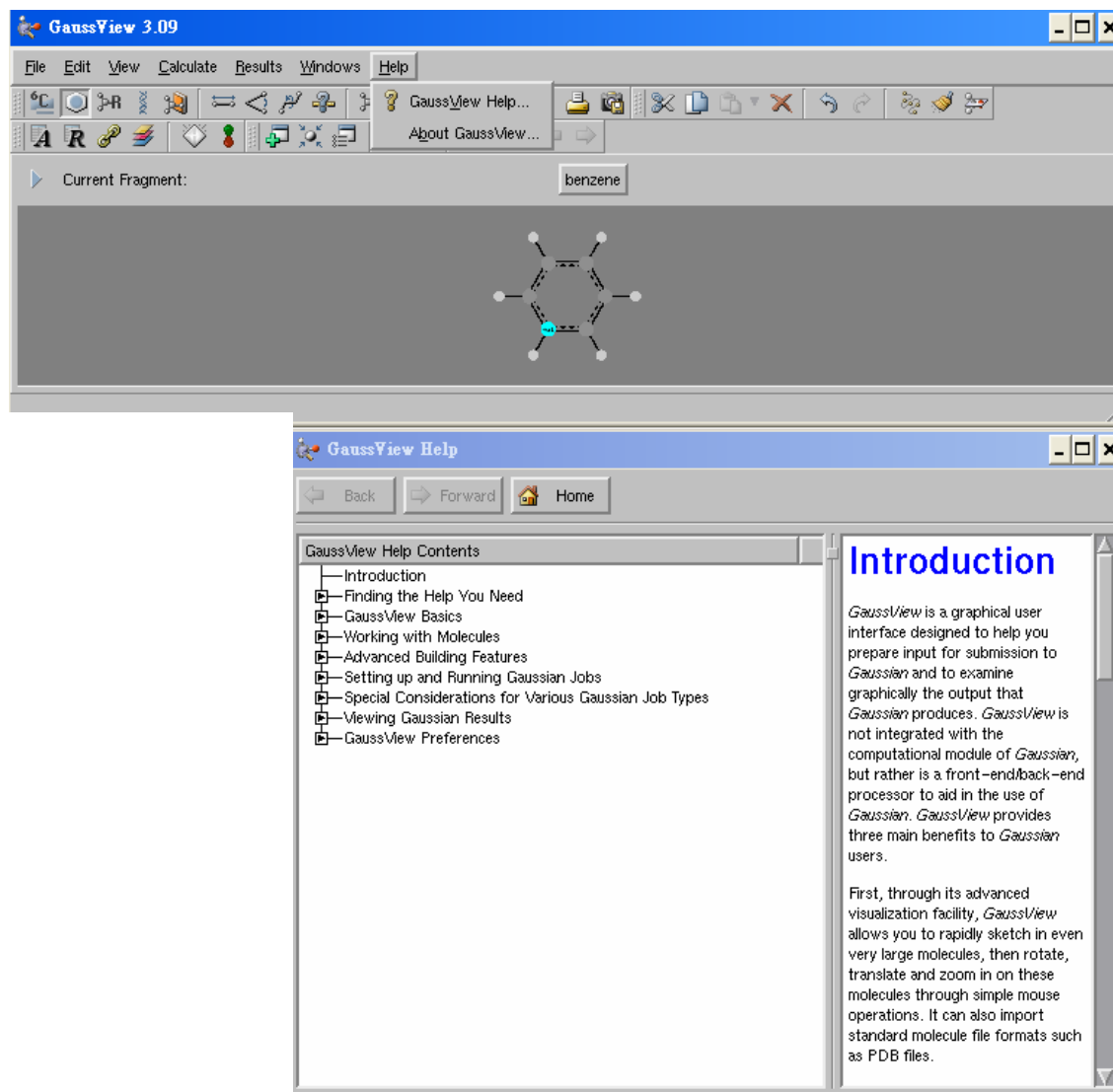
5) Results:



6) Windows:

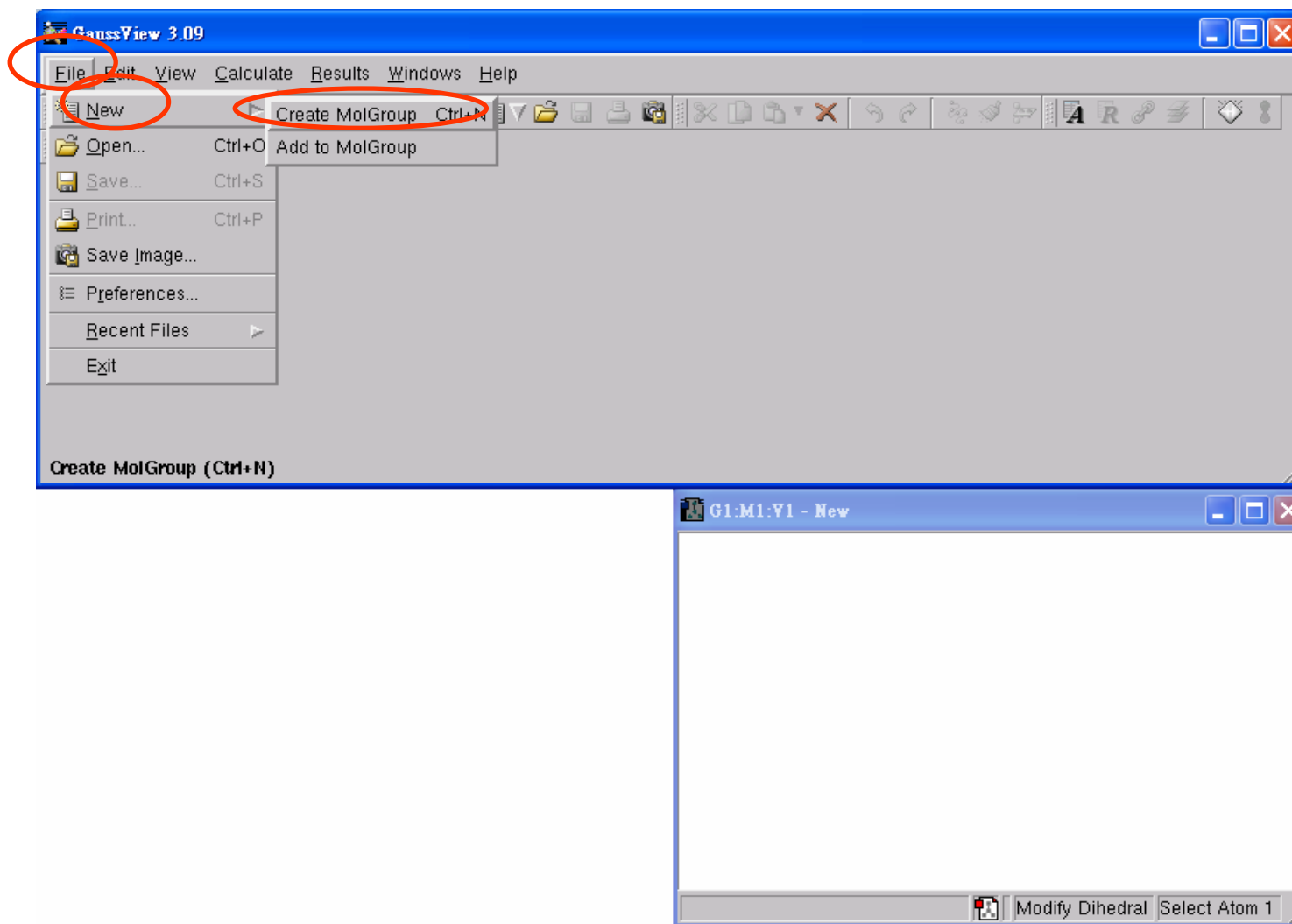


7) Help:



Step1 : Coarse Optimization

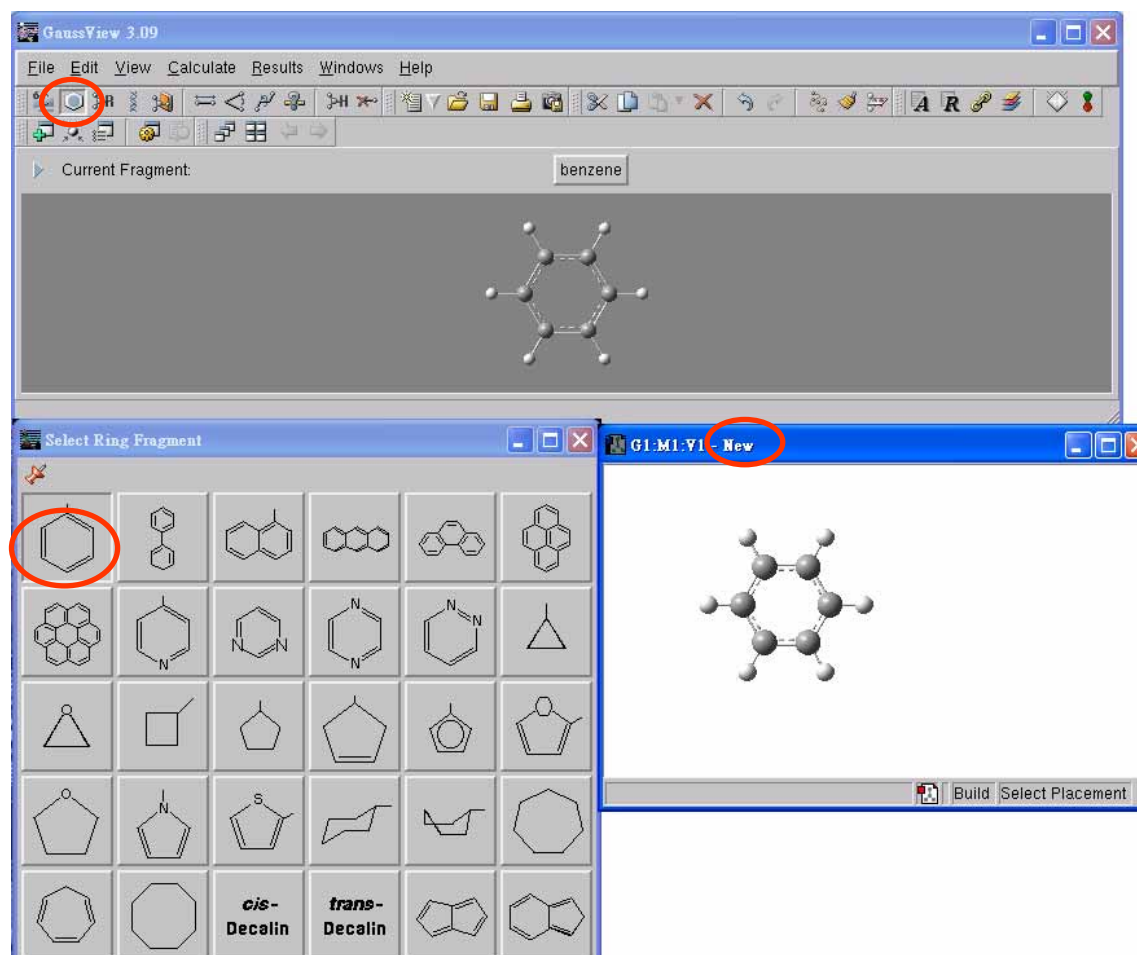
Open new file → File → New → Create MolGroup



Create Molecule : CN-PPV

Double Click at **Ring Fragment** →

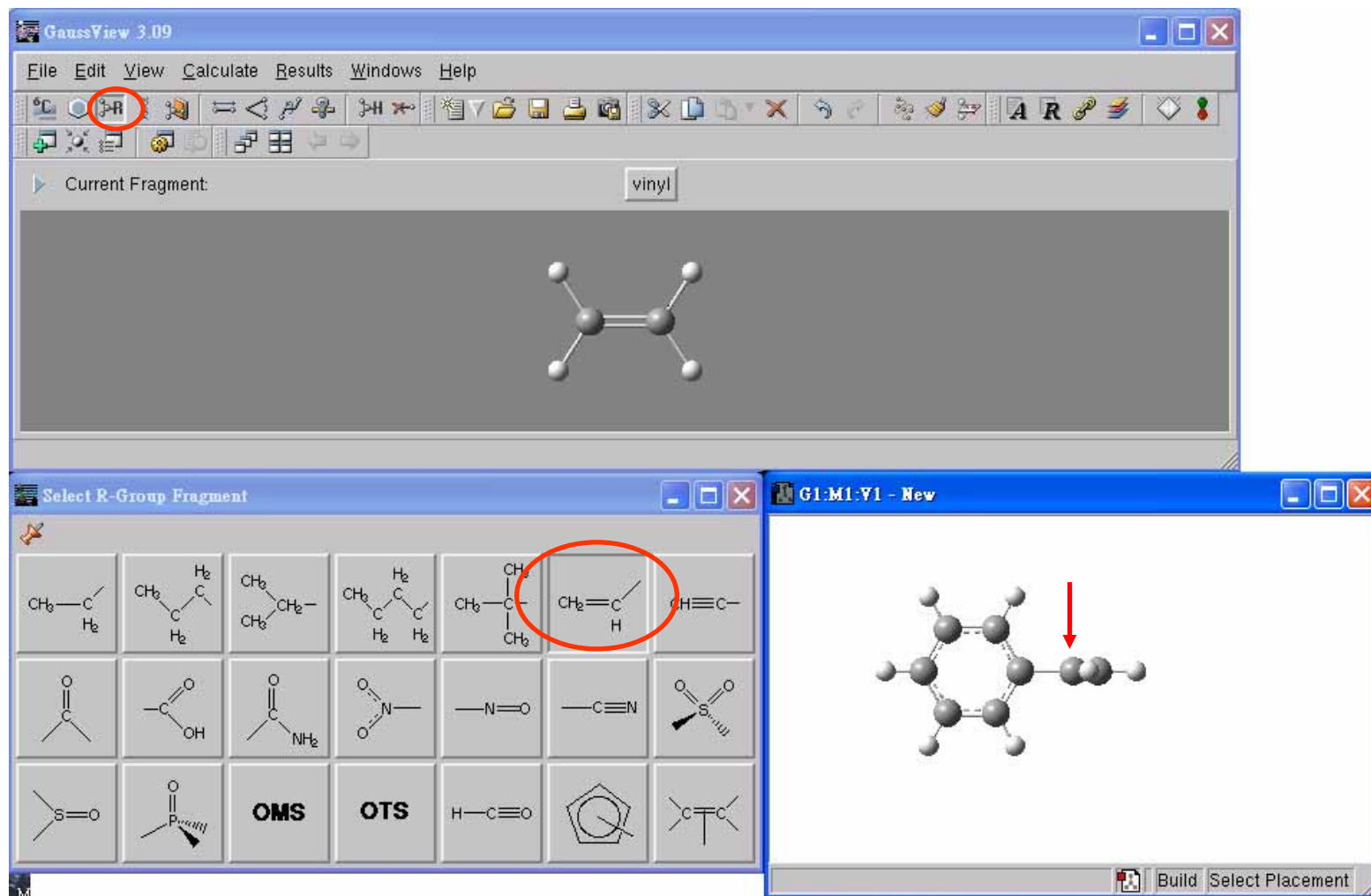
Select **Benzene** → Click at **new** window



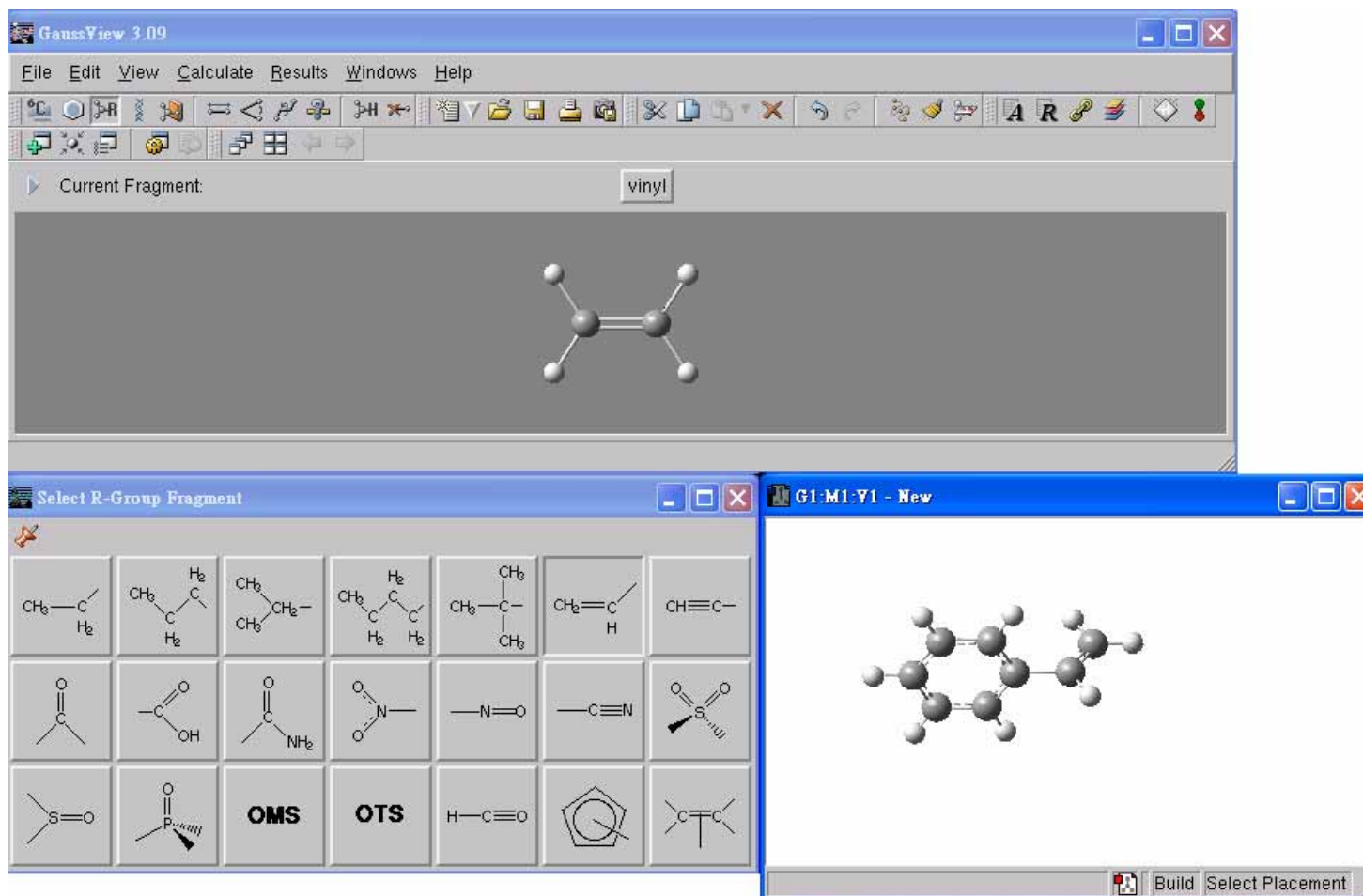
Create Molecule : CN-PPV

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

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

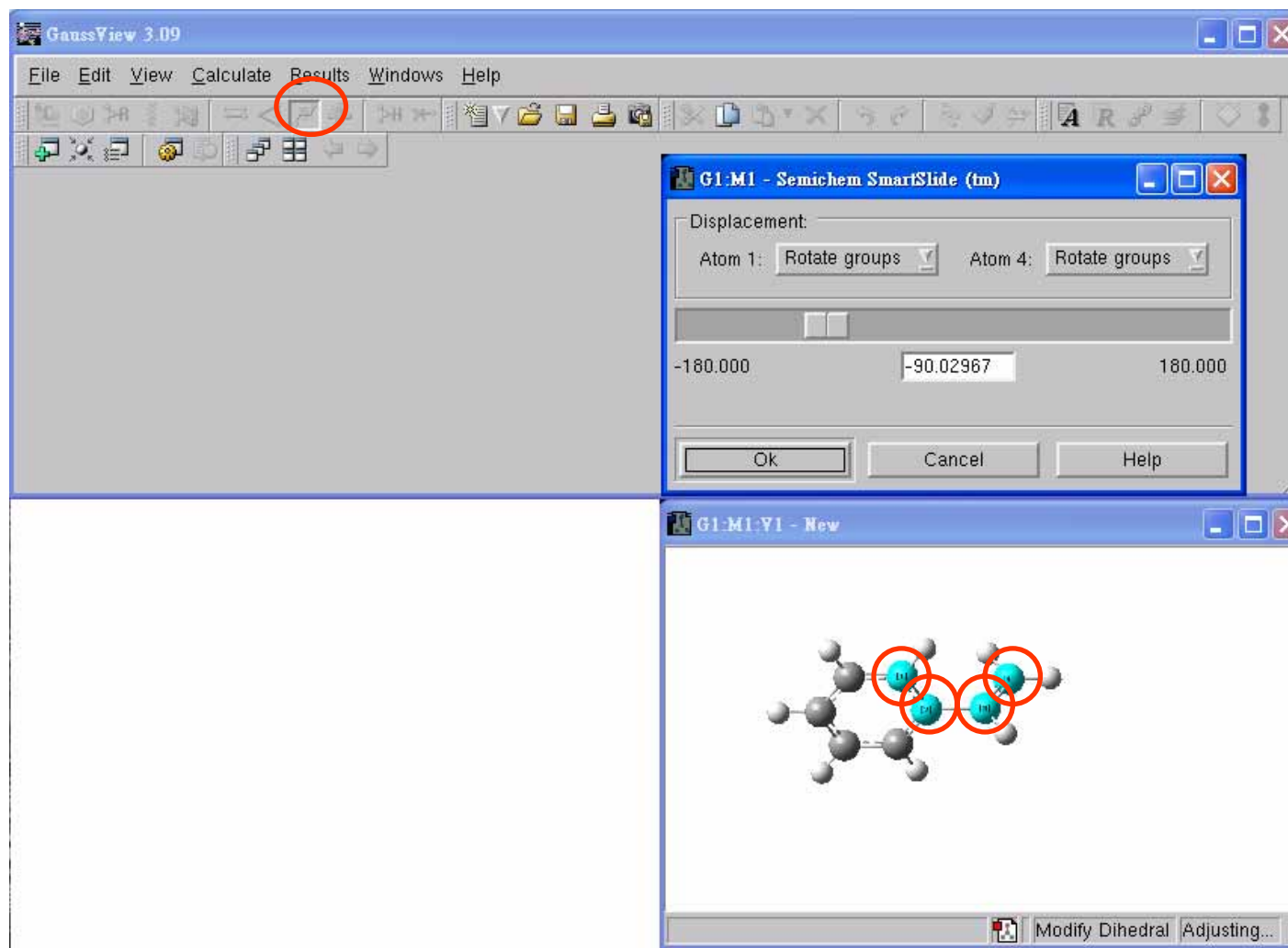


Rotate the molecule using left button



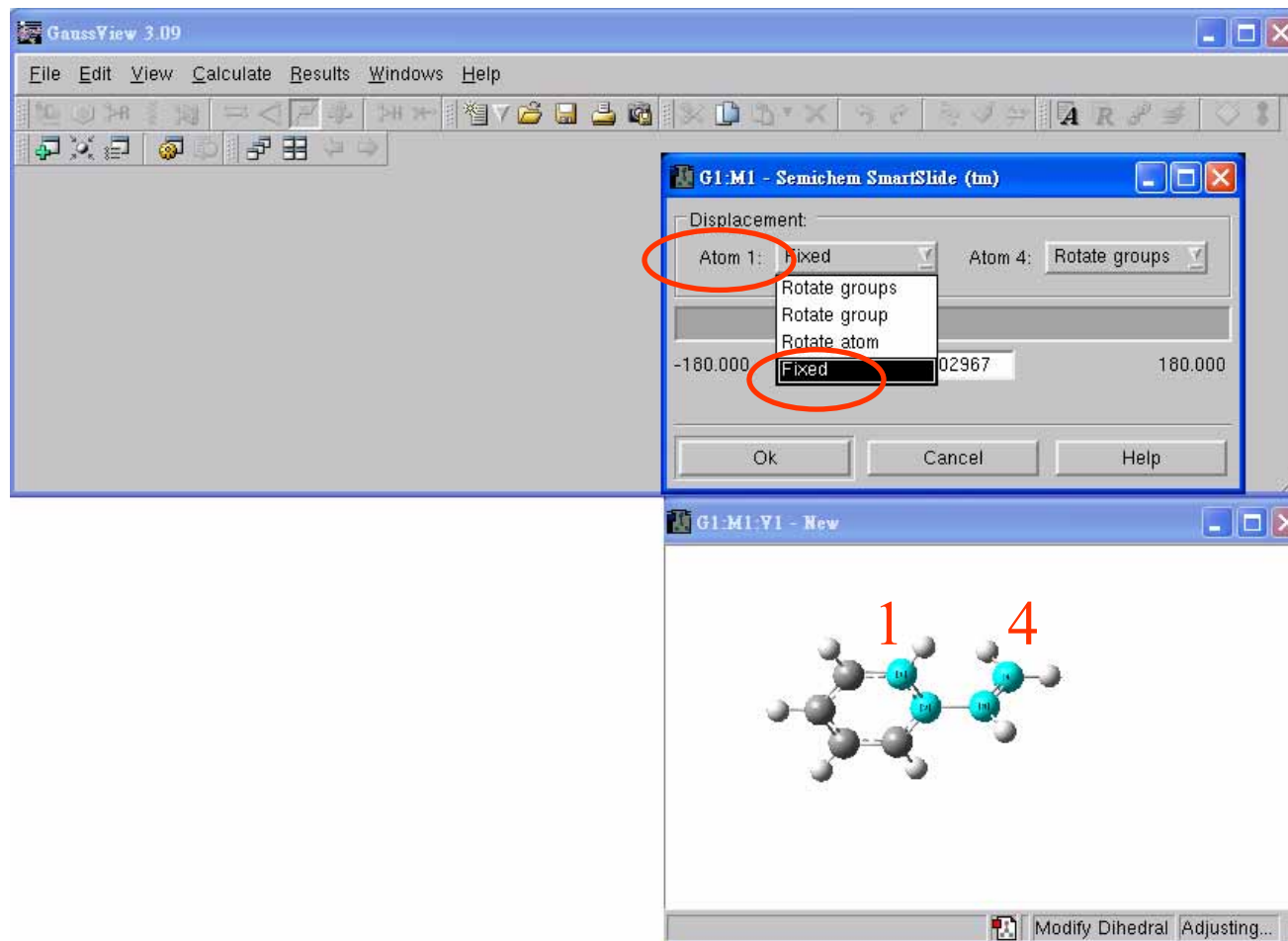
Modify Dihedral Angle

Click **Modify dihedral** → Select atoms



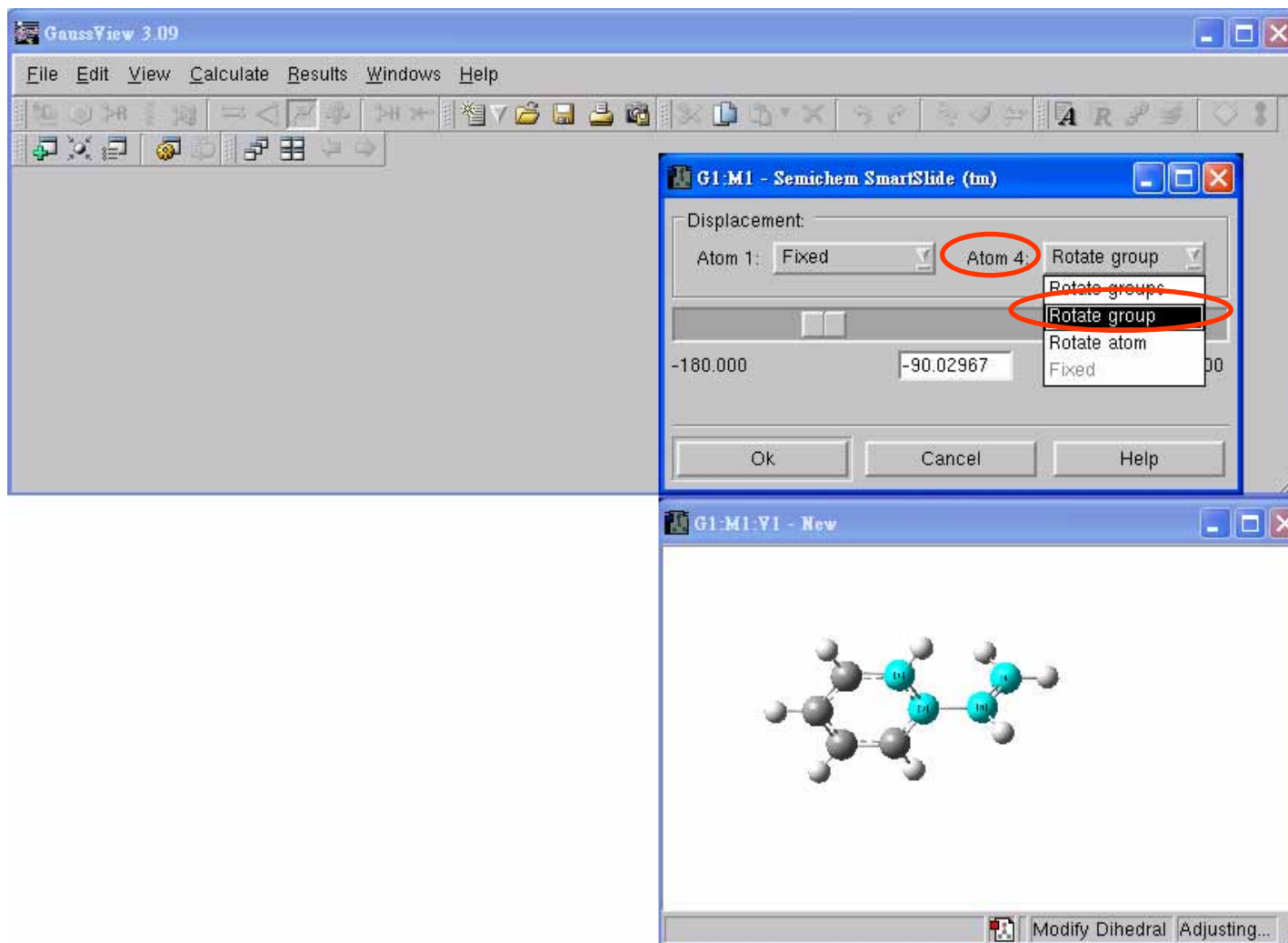
Coplanarity

Fixed atom1



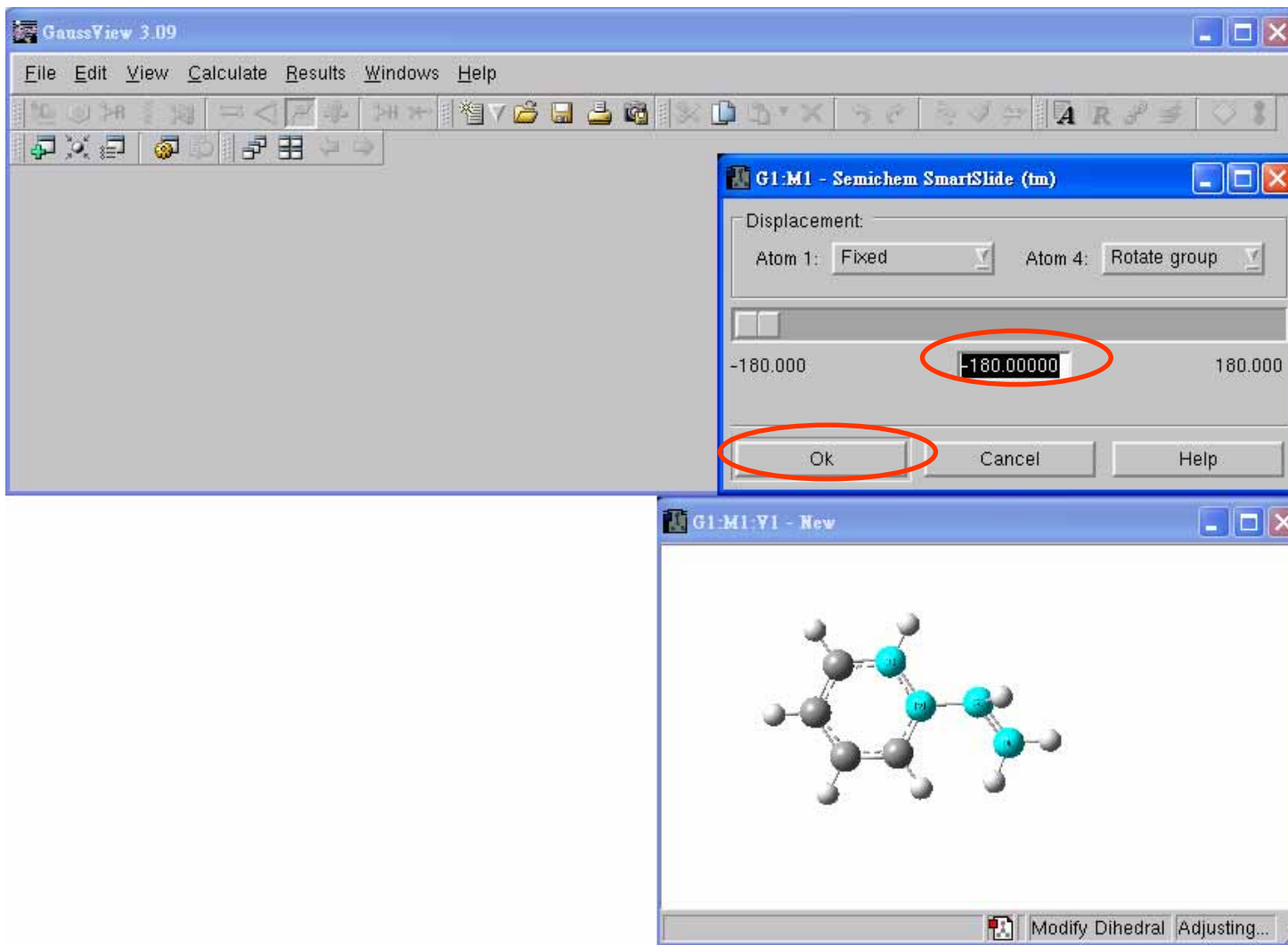
Coplanarity

Rotate atom4 → select **Rotate group**

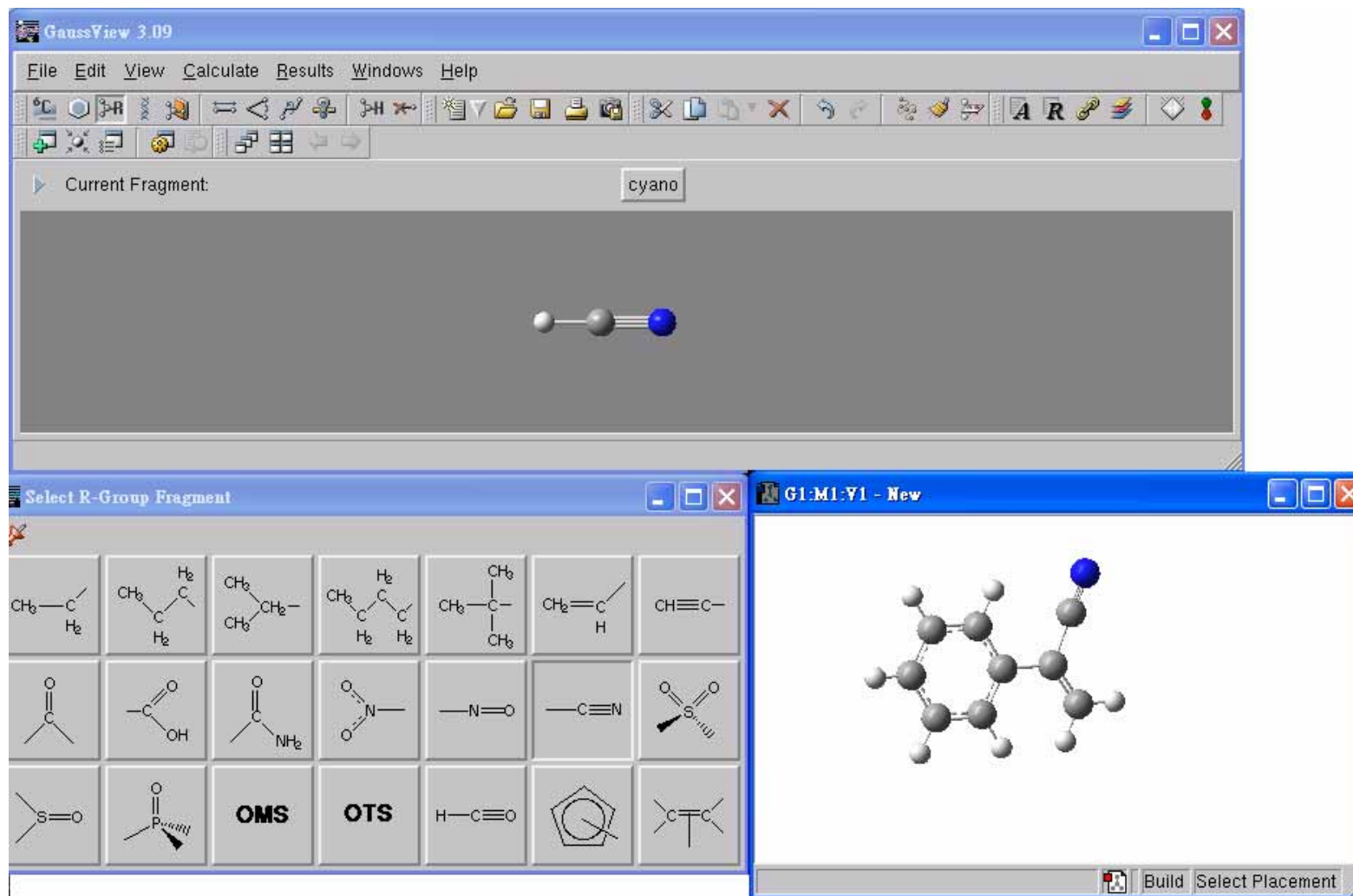


Coplanarity

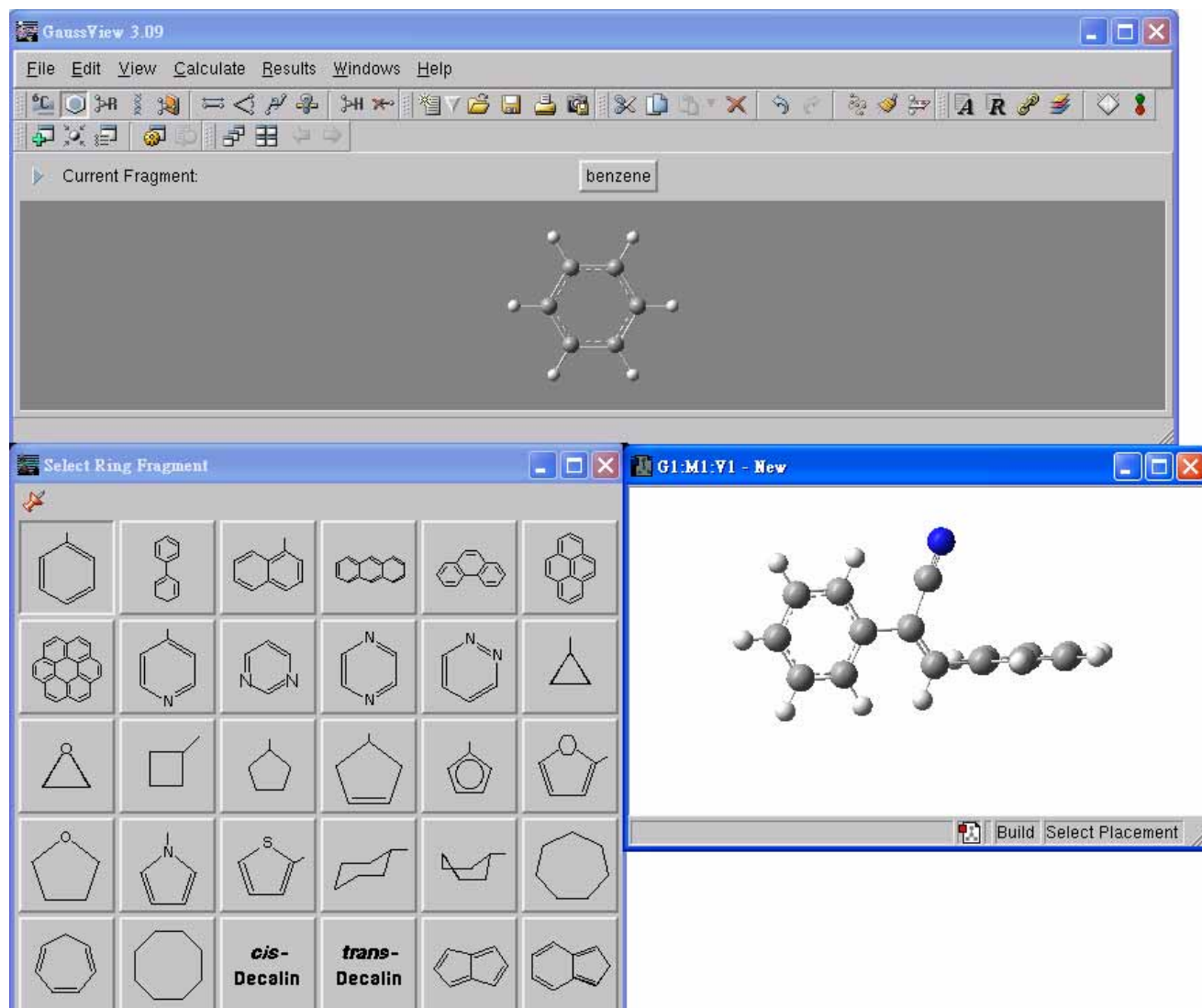
Key in the **angle** → Click **OK**



Add CN group

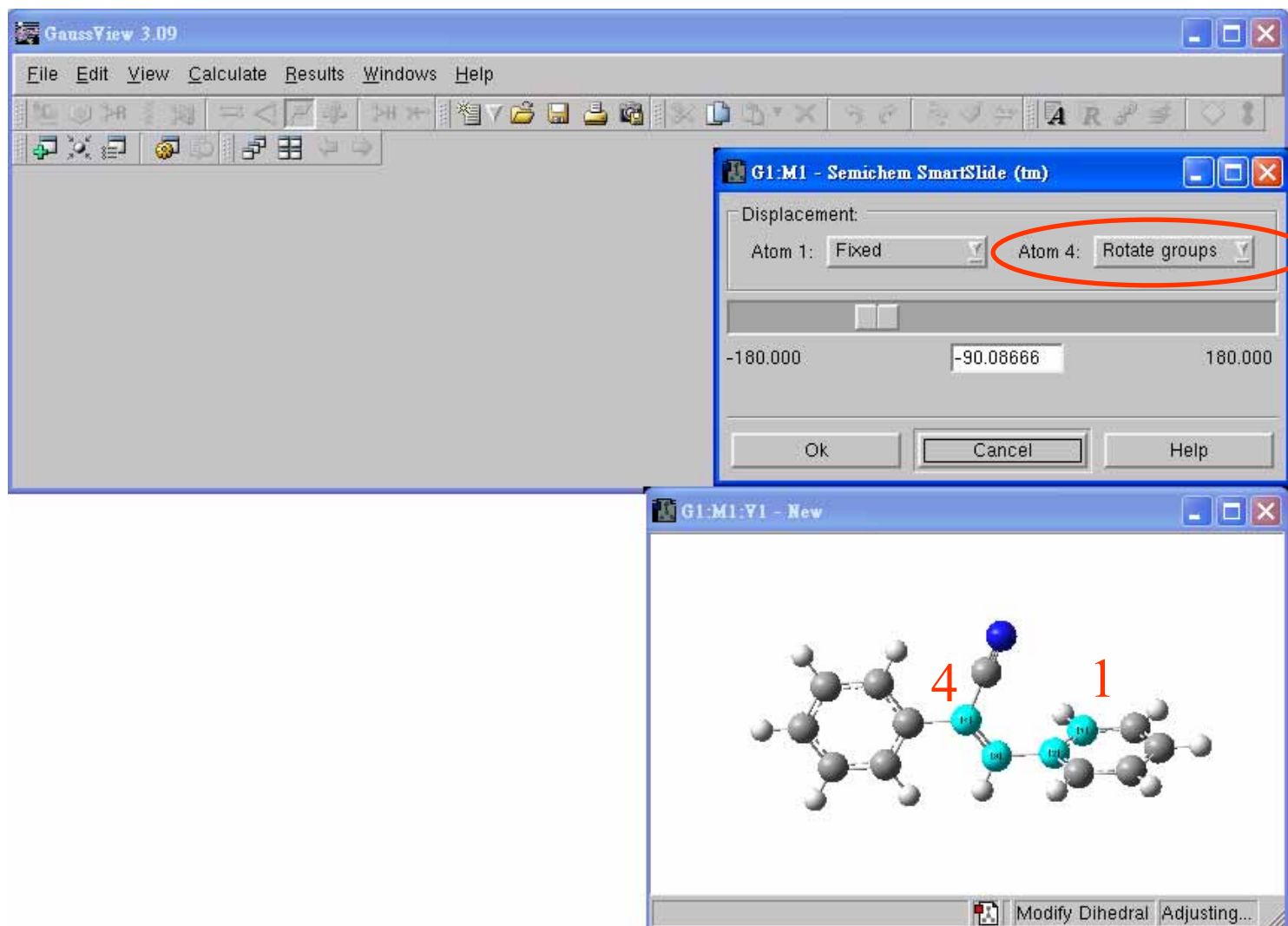


Add Benzene

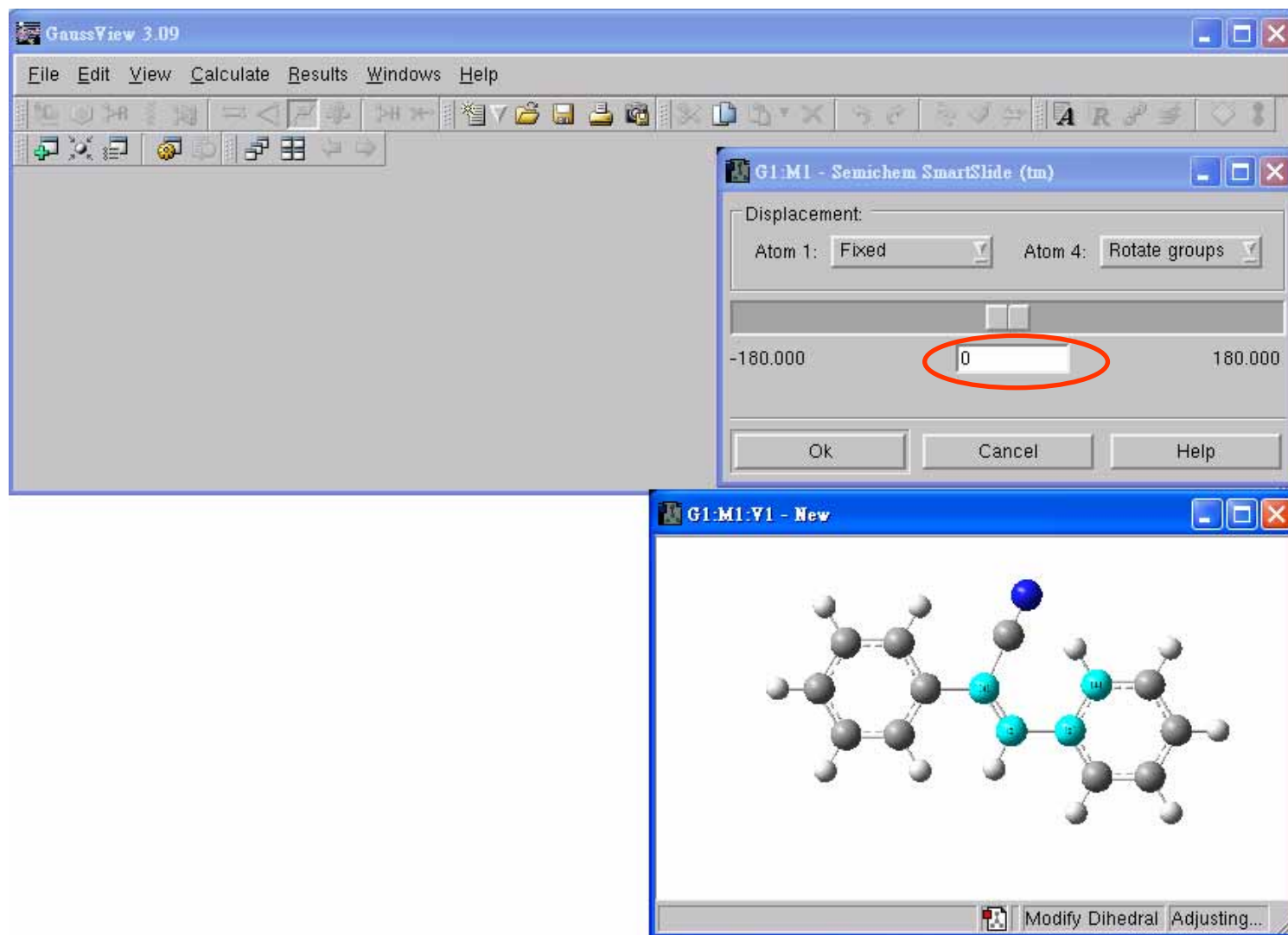


Rotate Benzene

Atom4 → Select Groups

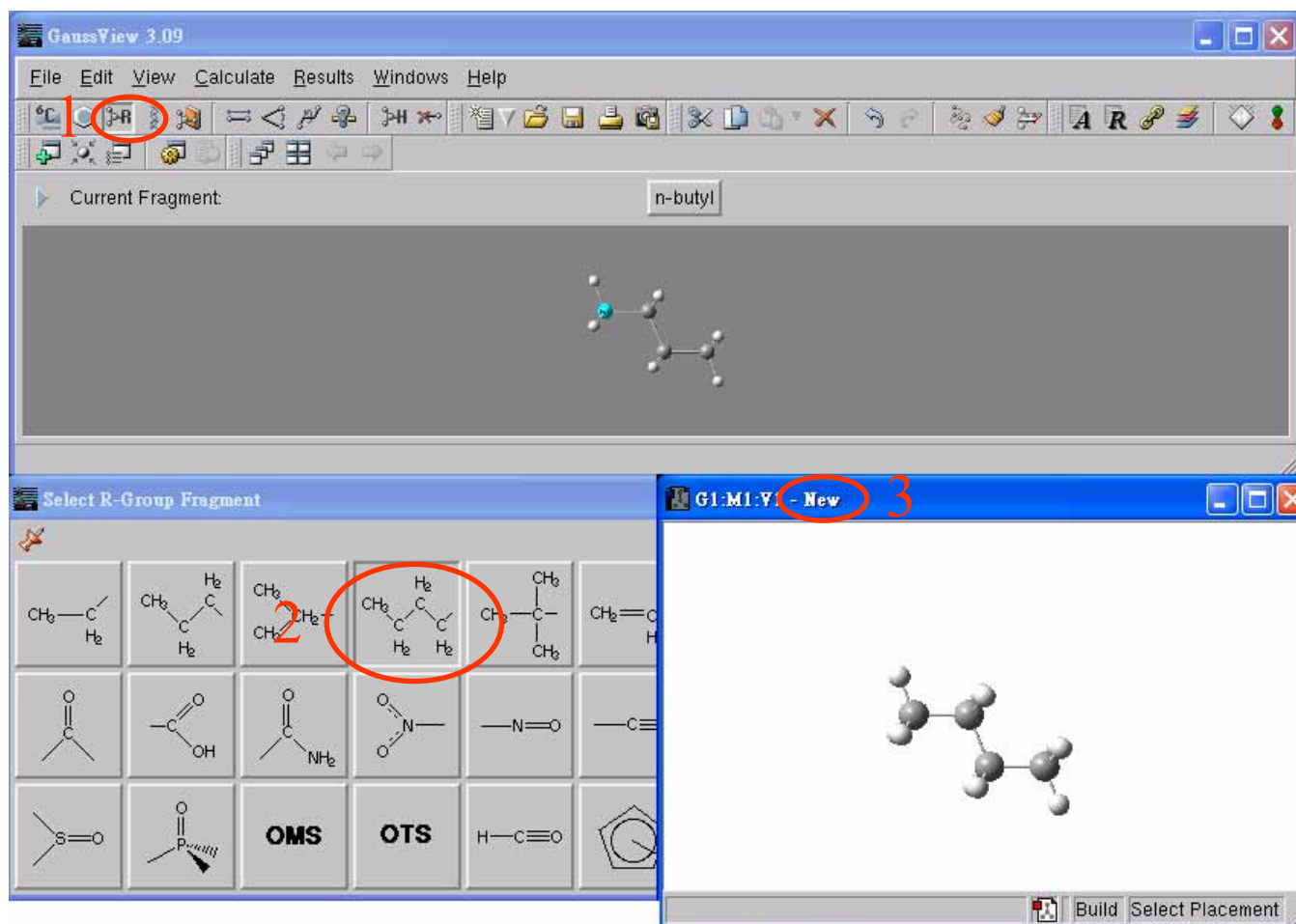


Key in the angle



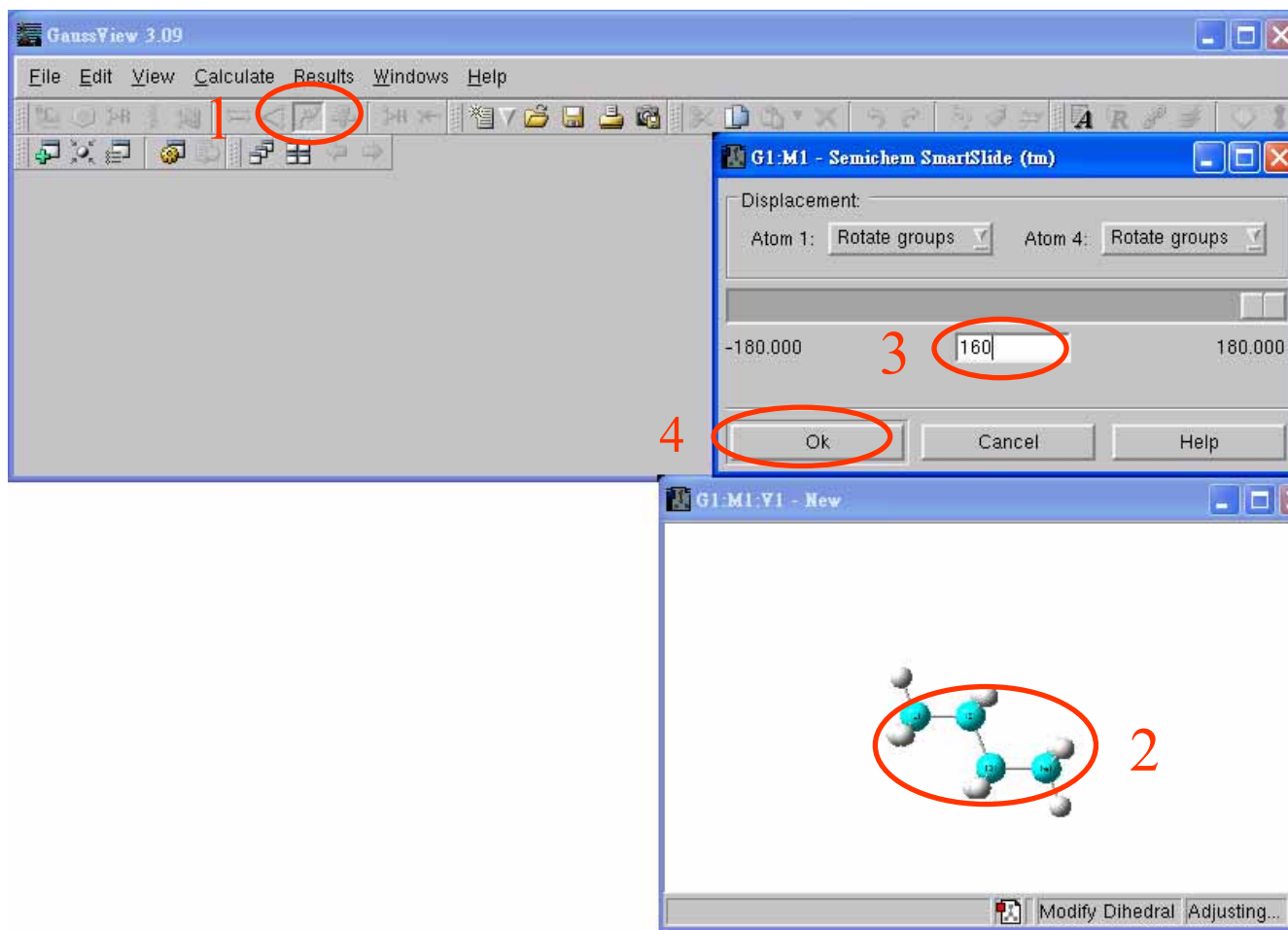
Mechanics Minimization

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



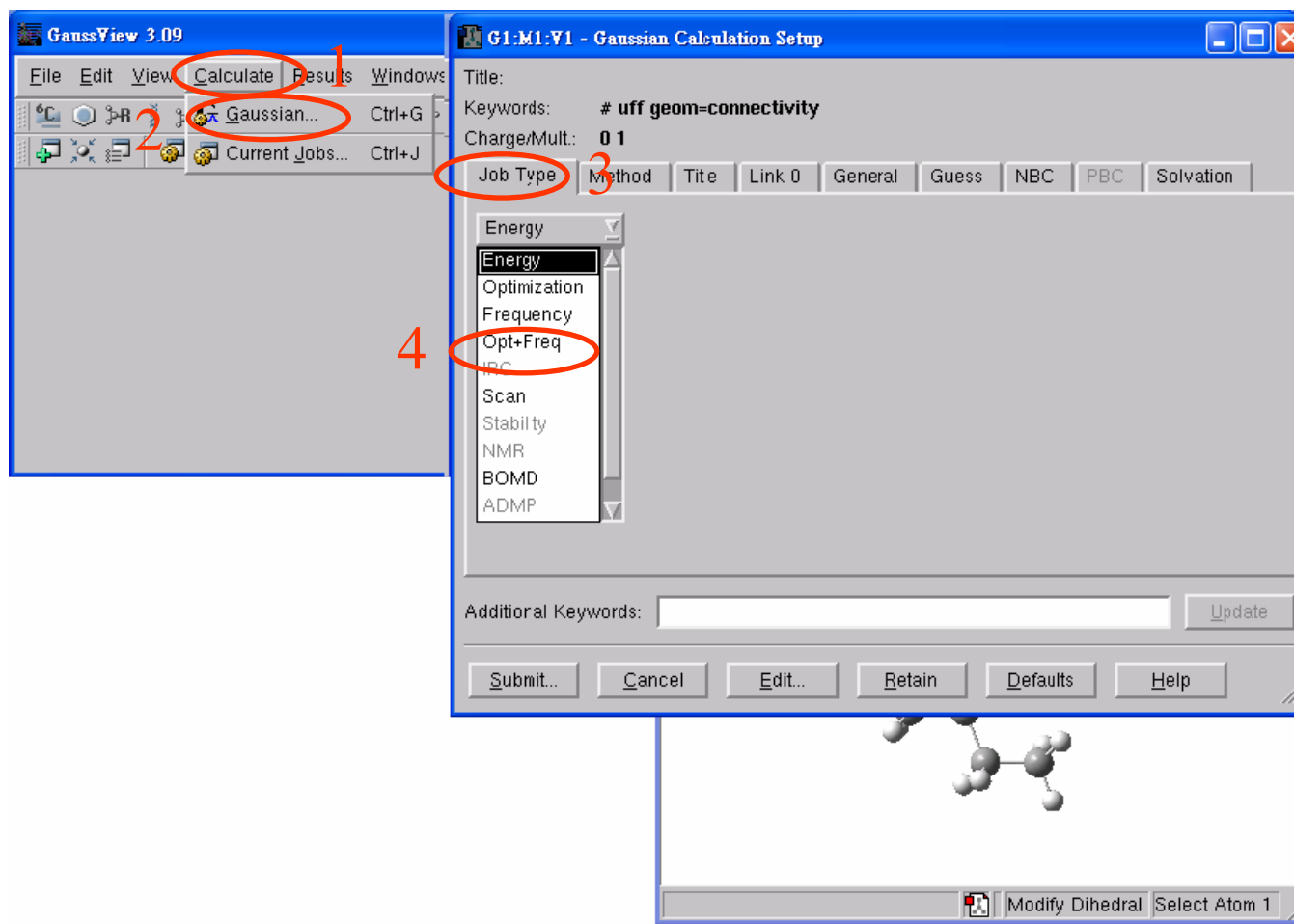
Modify dihedral angle

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



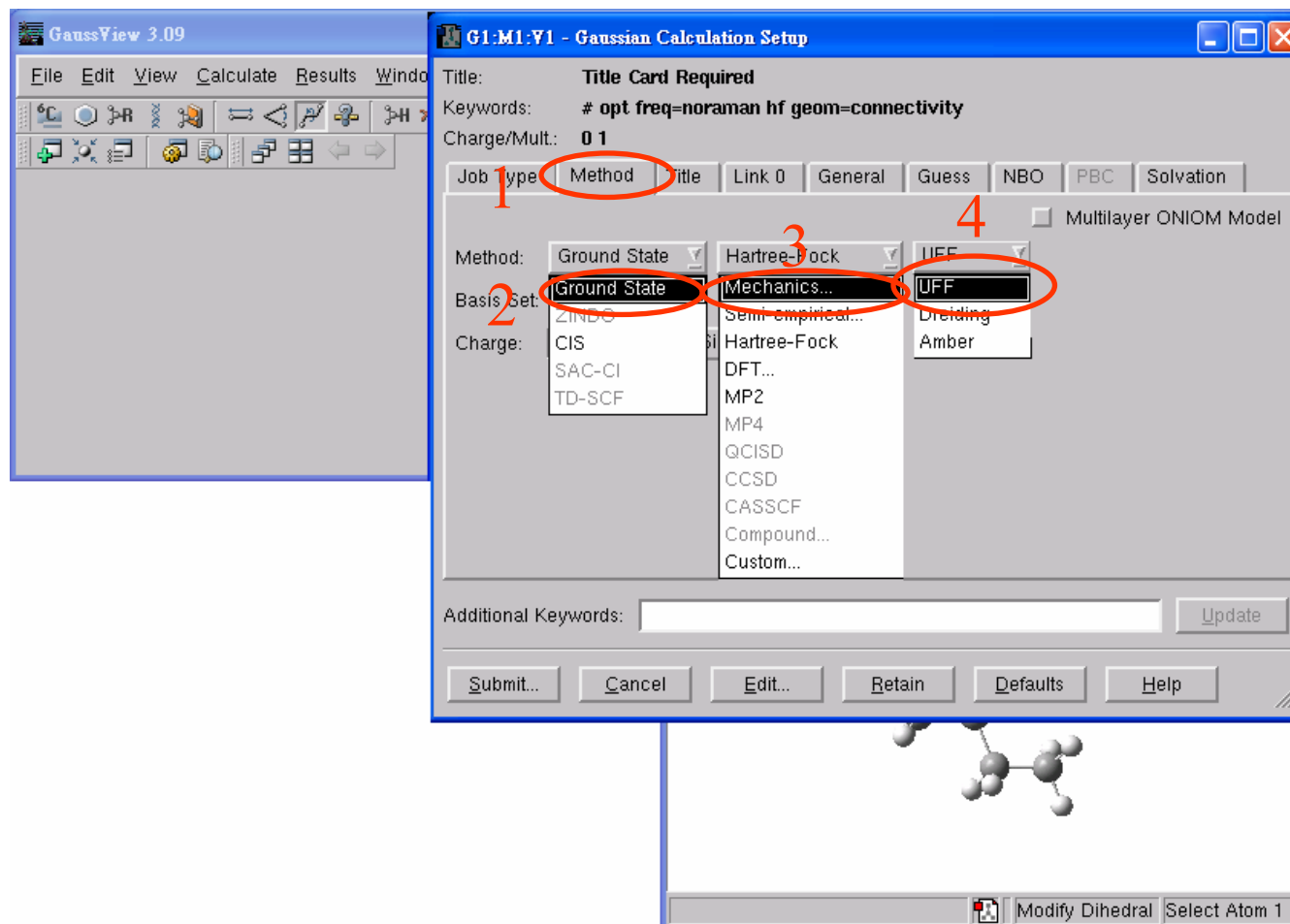
Minimization

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



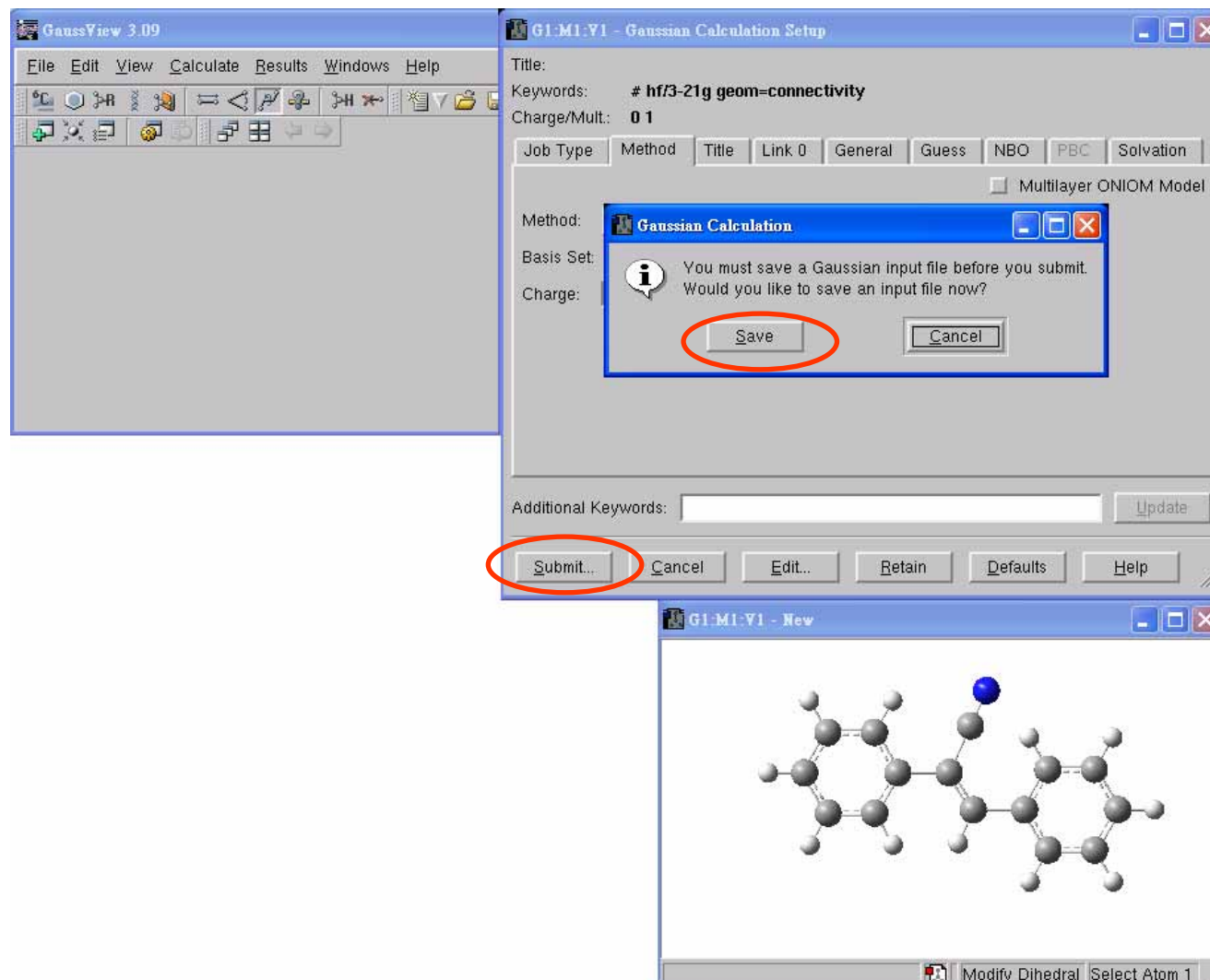
Method

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



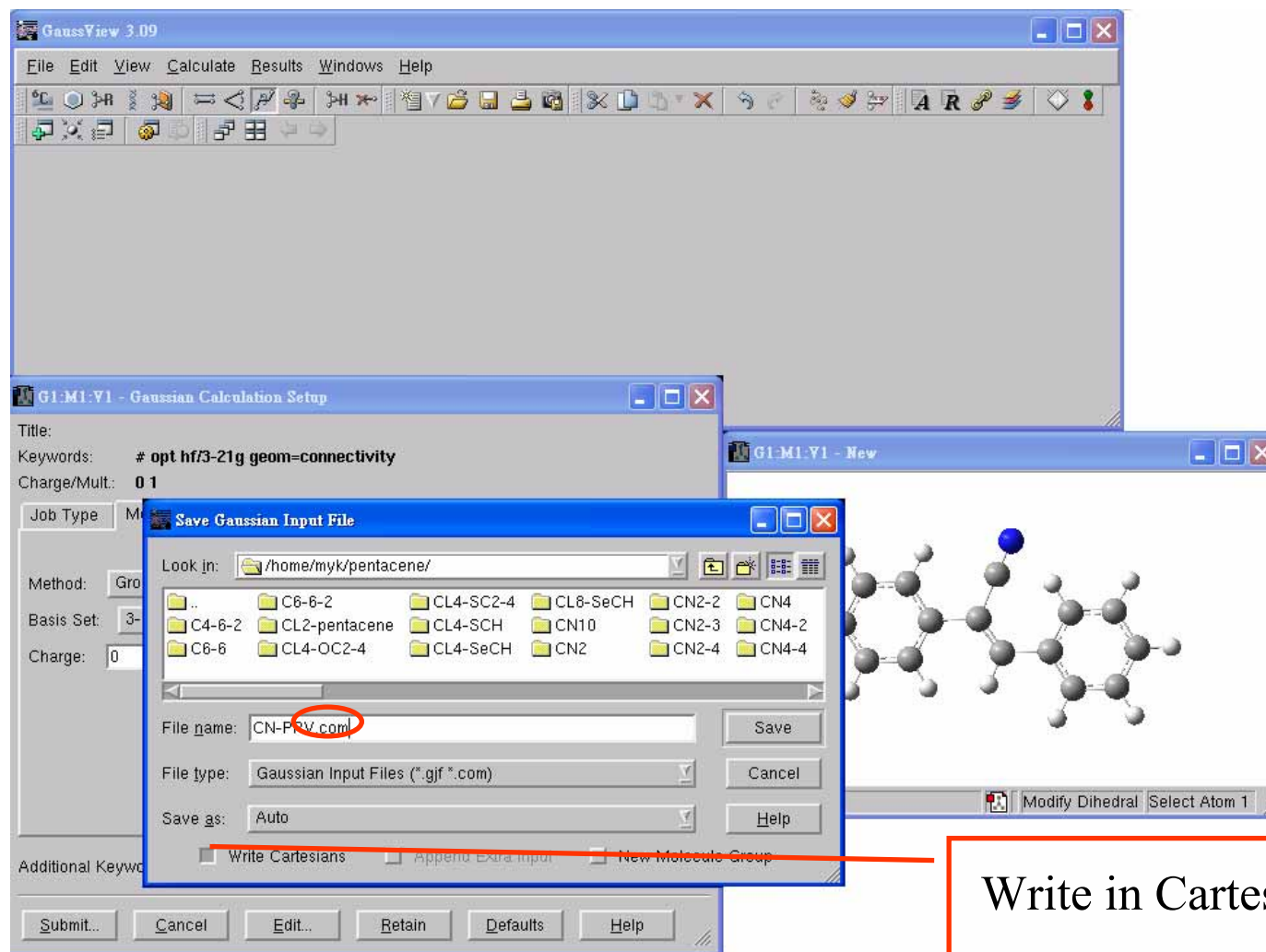
Submit the job

Click **Submit** → **Save** the job

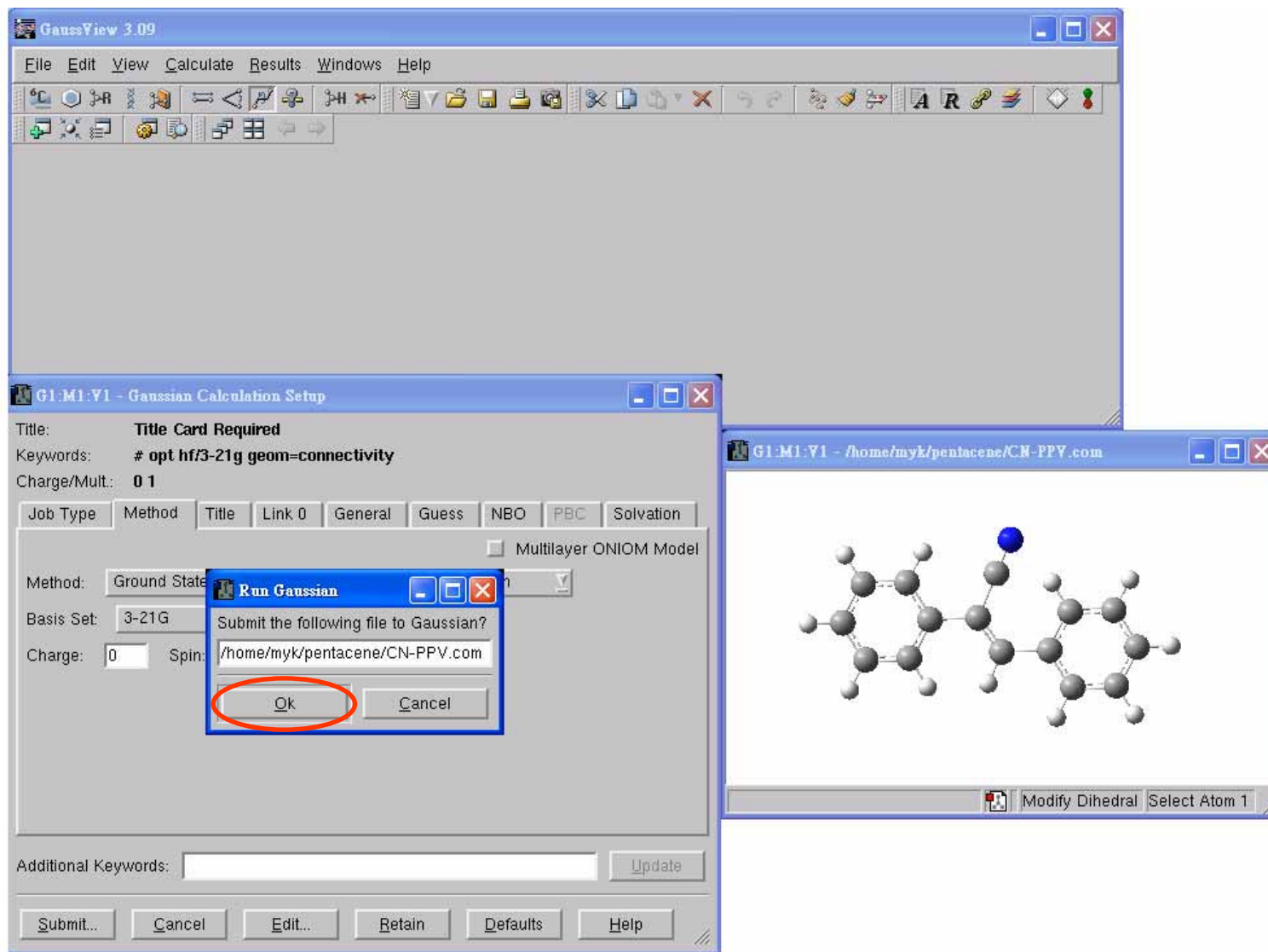


Save the job

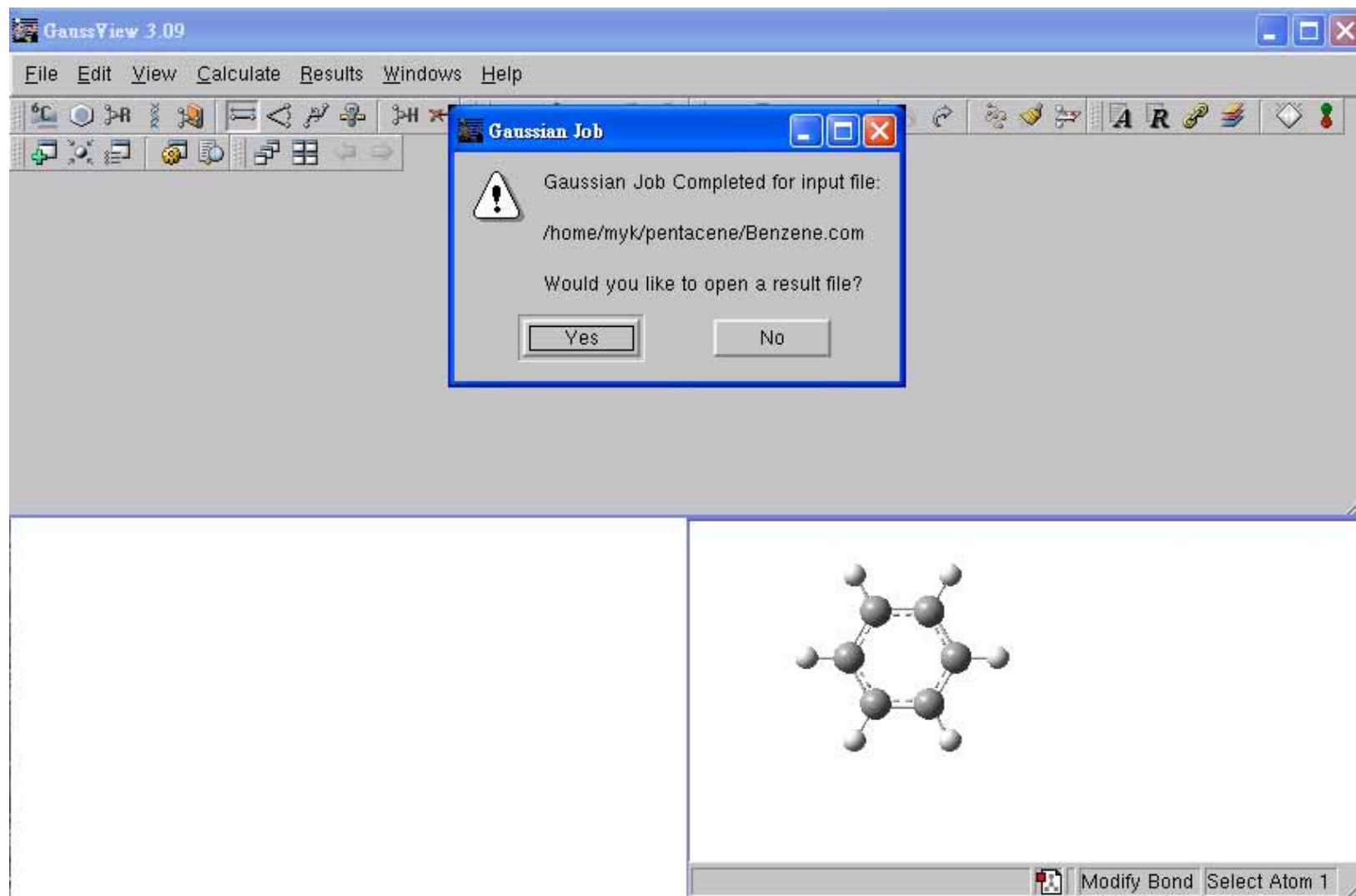
File type *.com



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

```

myk on jockol: /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.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

```

Input orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			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 -0.00005181 -0.000012977 0.000008326

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

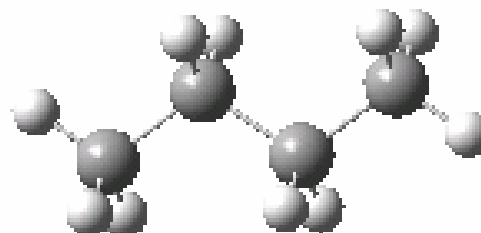
Energy

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

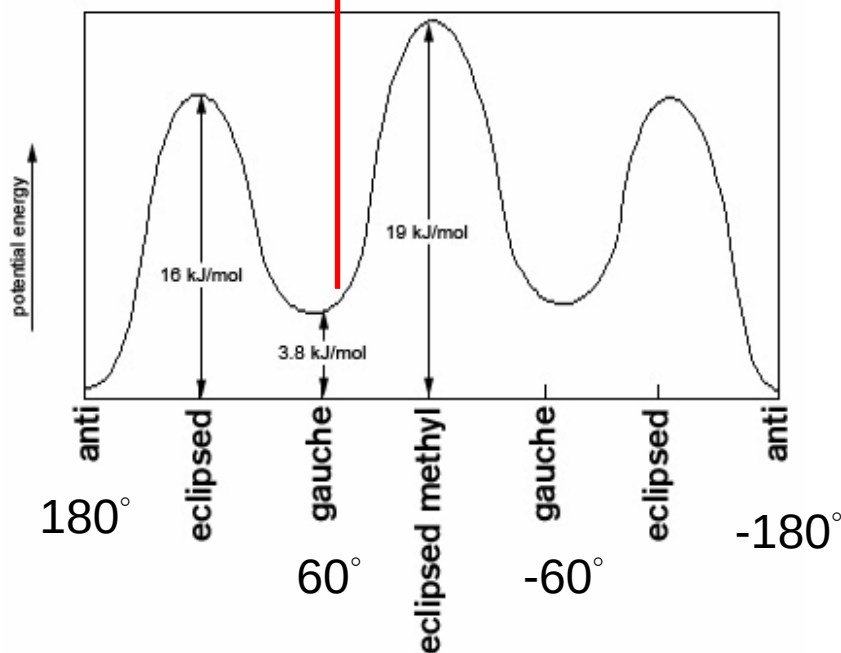
UFF 4.81
Dreiding 3.05
Amber 3.01



1 Hartree = 627.50956 kcal/mol

1 cal = 4.18 J

Torsion Angle

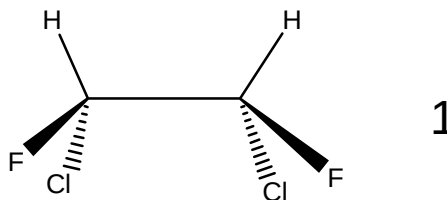


conformer potentials of butane about central C-C bond

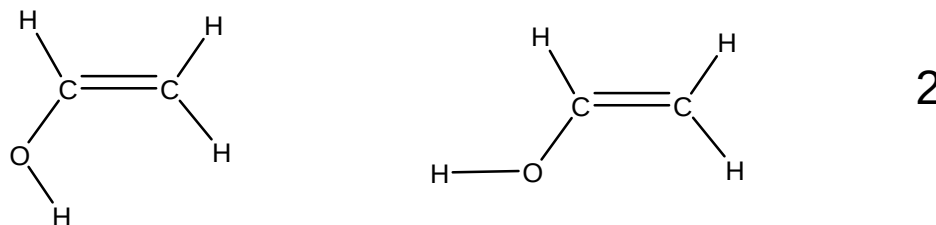
initial	Final
160°	UFF 179.45°
	Dreiding 179.89°
	Amber 179.75°
110°	UFF 70.98°
	Dreiding 67.86°
	Amber 67.84°

Exercises:

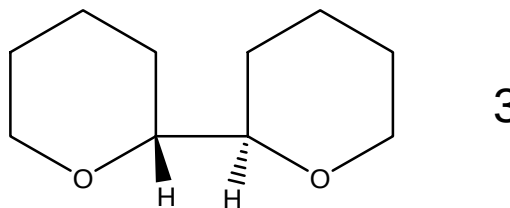
- 1) Build molecule 1 and manipulate to different stereoisomers.



- 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.



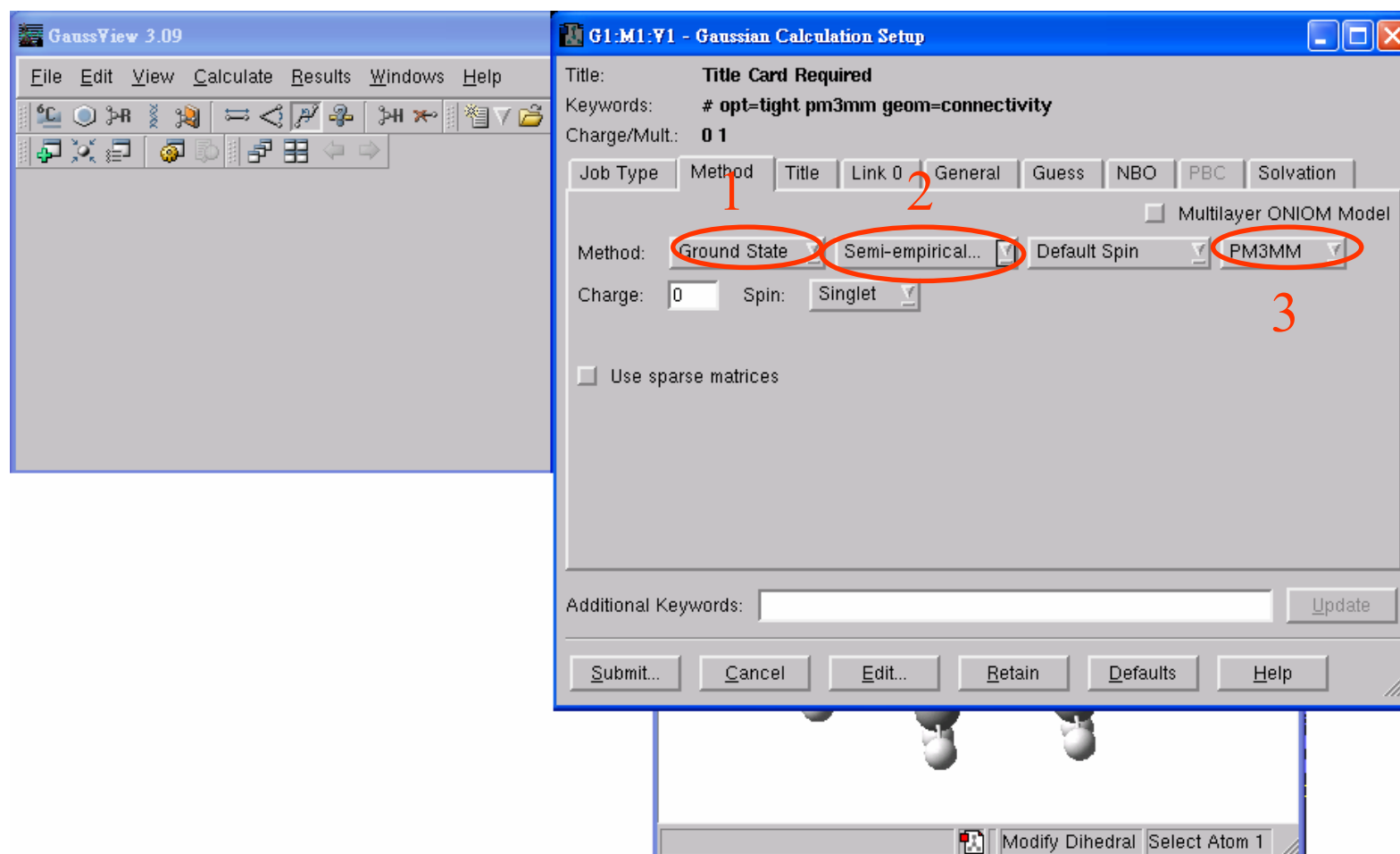
4) Conformational Search:

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.

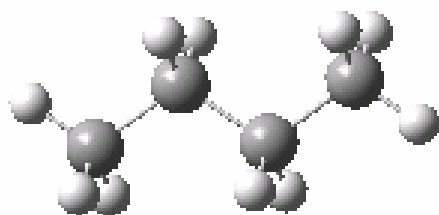
5) Build a water dimer, and try to manipulate them at different binding orientations.

Semi-empirical Optimization

Select **Group State** → Select **Semi-empirical** → Select **Method**



Different Method

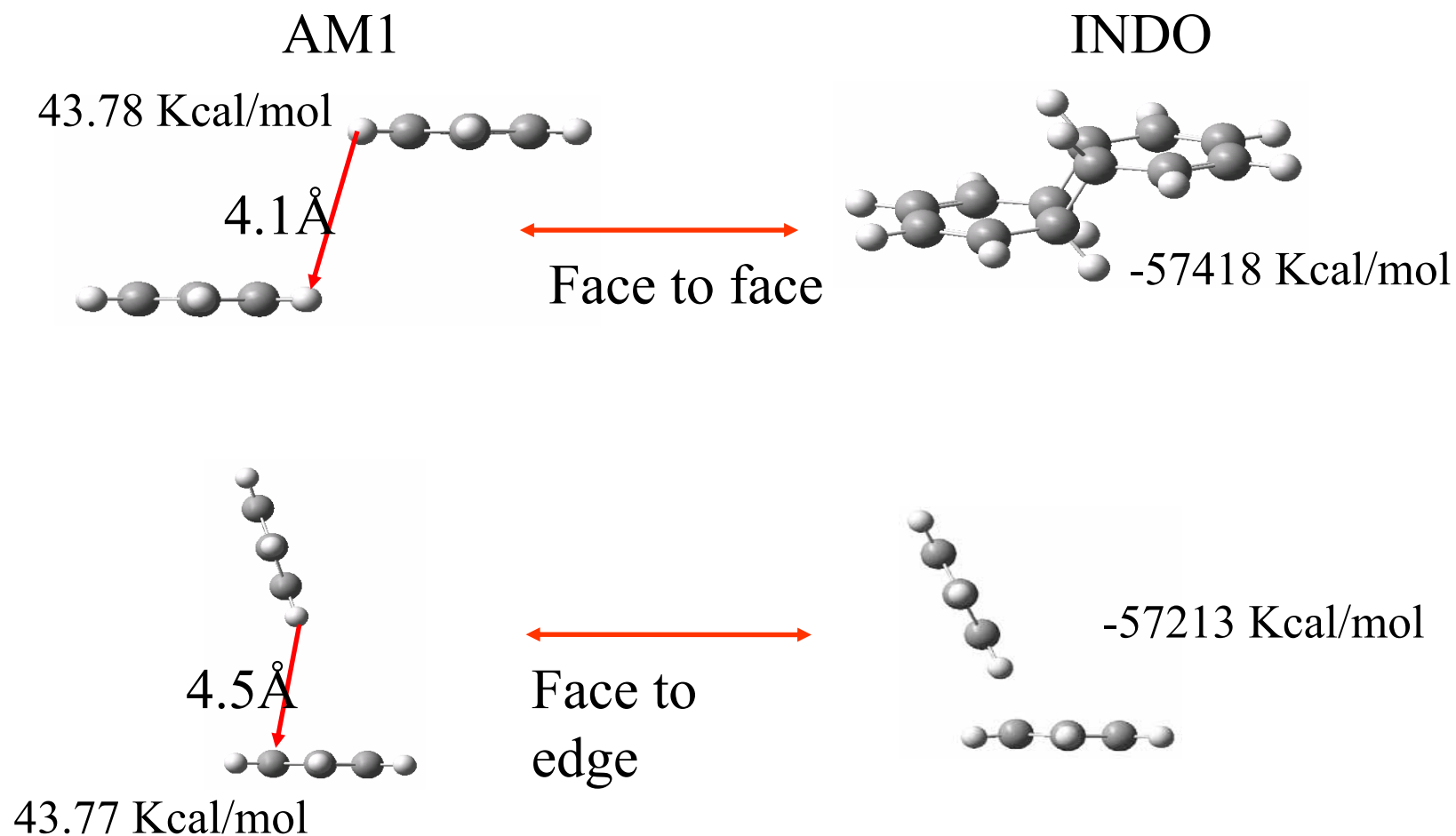


Torsion Angle

Final (initial 160°)	Final (initial 110° or 0°)	
AM1 180°	AM1 74.69°	→ 2.95 KJ/mol
PM3 180°	PM3 75°	→ 2.19 KJ/mol
PM3MM 180°	PM3MM 75°	→ 2.19 KJ/mol
MNDO 180°	MNDO 71.96°	→ -2.42 KJ/mol
MINDO/3 180°	MINDO/3 71.66°	→ 2.76 KJ/mol
INDO 180°	INDO 59.85°	→ -3.93 KJ/mol
CNDO 180°	CNDO 60.11°	→ -3.80 KJ/mol

► Starting from different geometries get different results

Benzene Dimer



► INDO optimization is poor; cannot calculate benzene dimer

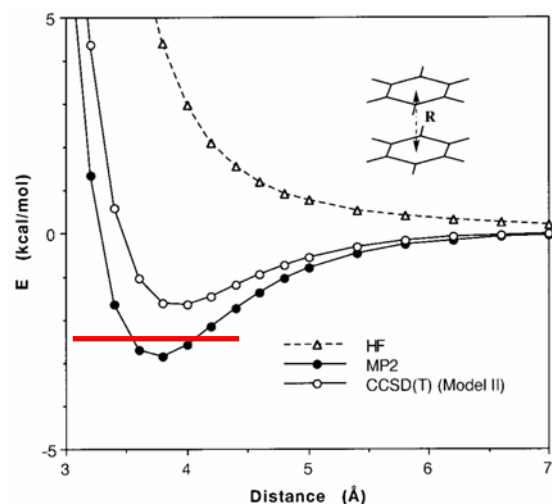


Figure 3. The HF, MP2, and CCSD(T) interaction energies of the benzene dimer A. The HF and MP2 interaction energies were calculated with the aug(d,p)-6-311G** basis set. The CCSD(T) interaction energy was calculated by the AIMI Model II. See text.

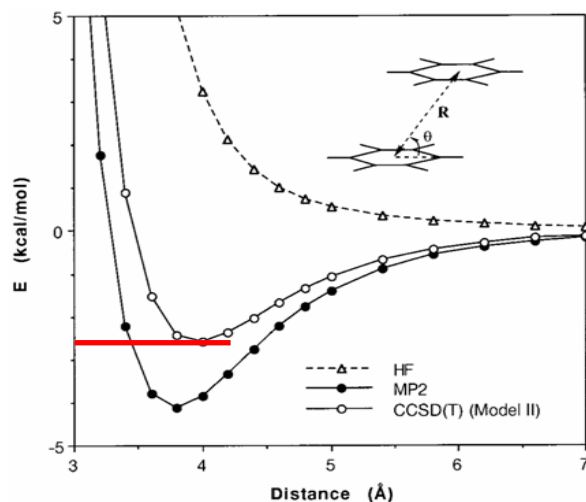


Figure 5. The HF, MP2, and CCSD(T) interaction energies of the benzene dimer C. The HF and MP2 interaction energies were calculated with the aug(d,p)-6-311G** basis set. The CCSD(T) interaction energy was calculated by the AIMI Model II. See text. The angle θ is 63° when $R_1 = 1.8$ Å and $R_2 = 3.5$ Å.

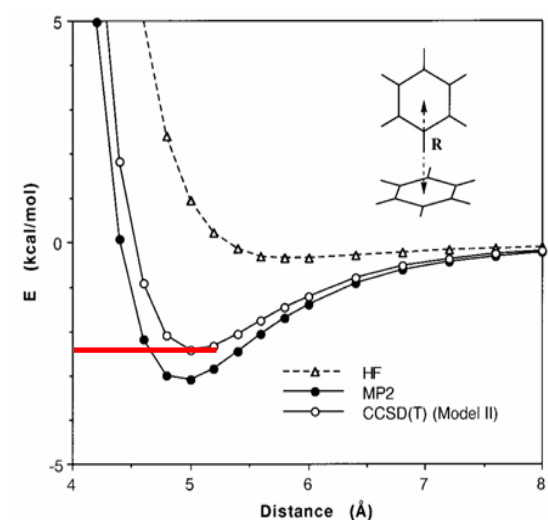
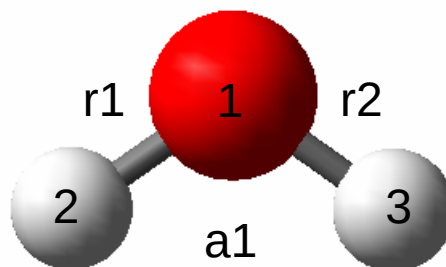


Figure 4. The HF, MP2, and CCSD(T) interaction energies of the benzene dimer B. The HF and MP2 interaction energies were calculated with the aug(d,p)-6-311G** basis set. The CCSD(T) interaction energy was calculated by the AIMI Model II. See text.

- ▶ Edge-to-face and shift-stack are better than parallel stack.
- ▶ HF cannot locate the minimum.
- ▶ For VDW complex, methods with the consideration of electron correlation are needed.

Coordinate: Cartesian vs Z-matrix



Cartesian

O	0.0000	0.0000	-0.1108
H	0.0000	-0.7840	0.4432
H	0.0000	0.7849	0.4432

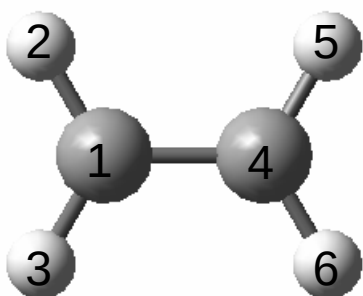
Z-matrix

O				
H	1	r1		
H	1	r2	2	a1

Variables:
r1=0.96
r2=0.96
a1=109.5

$$3N - 6 = 3$$

Z-matrix for more than 3 atoms



```
C
H  1  r1
H  1  r2  2  a1
C  1  r3  3  a2  2  d1
H  4  r4  1  a3  3  d2
H  4  r5  1  a4  3  d3
```

Variables:

r1=1.0698

r2=1.0698

r3=1.3552

.....

a1=119.5

a2=120.3

.....

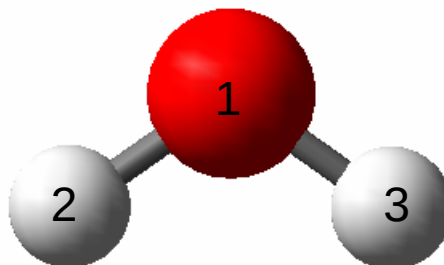
d1=180.0

d2=0.0

d3=180.0

$$3N - 6 = 12$$

Impose Symmetry on Molecule



C_1 no symmetry

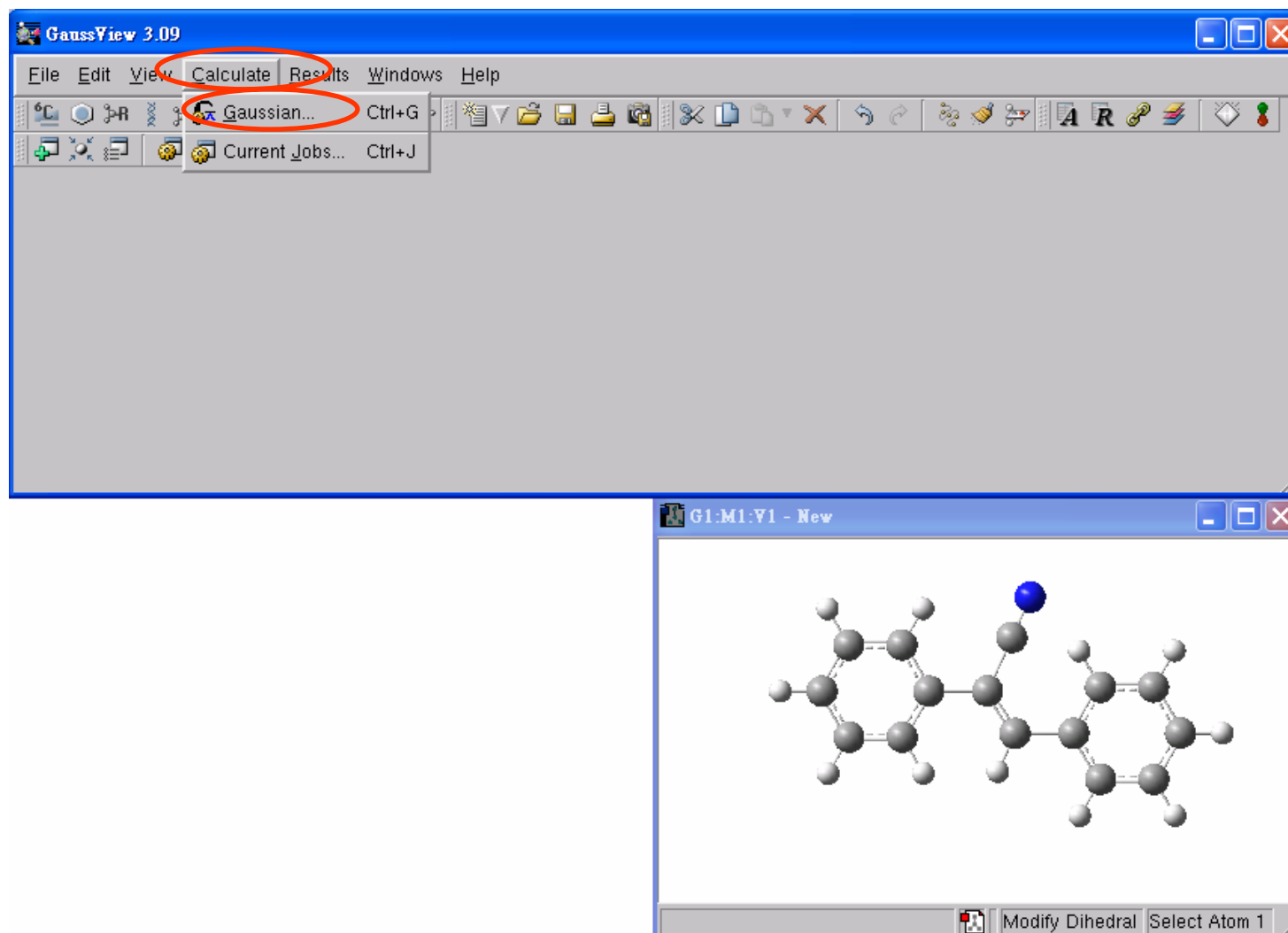
O
H 1 **r1**
H 1 **r2** 2 a1
Variables:
r1=0.960
r2=0.961
a1=109.5

C_{2v} symmetry

O
H 1 **r1**
H 1 **r1** 2 a1
Variables:
r1=0.960
a1=109.5

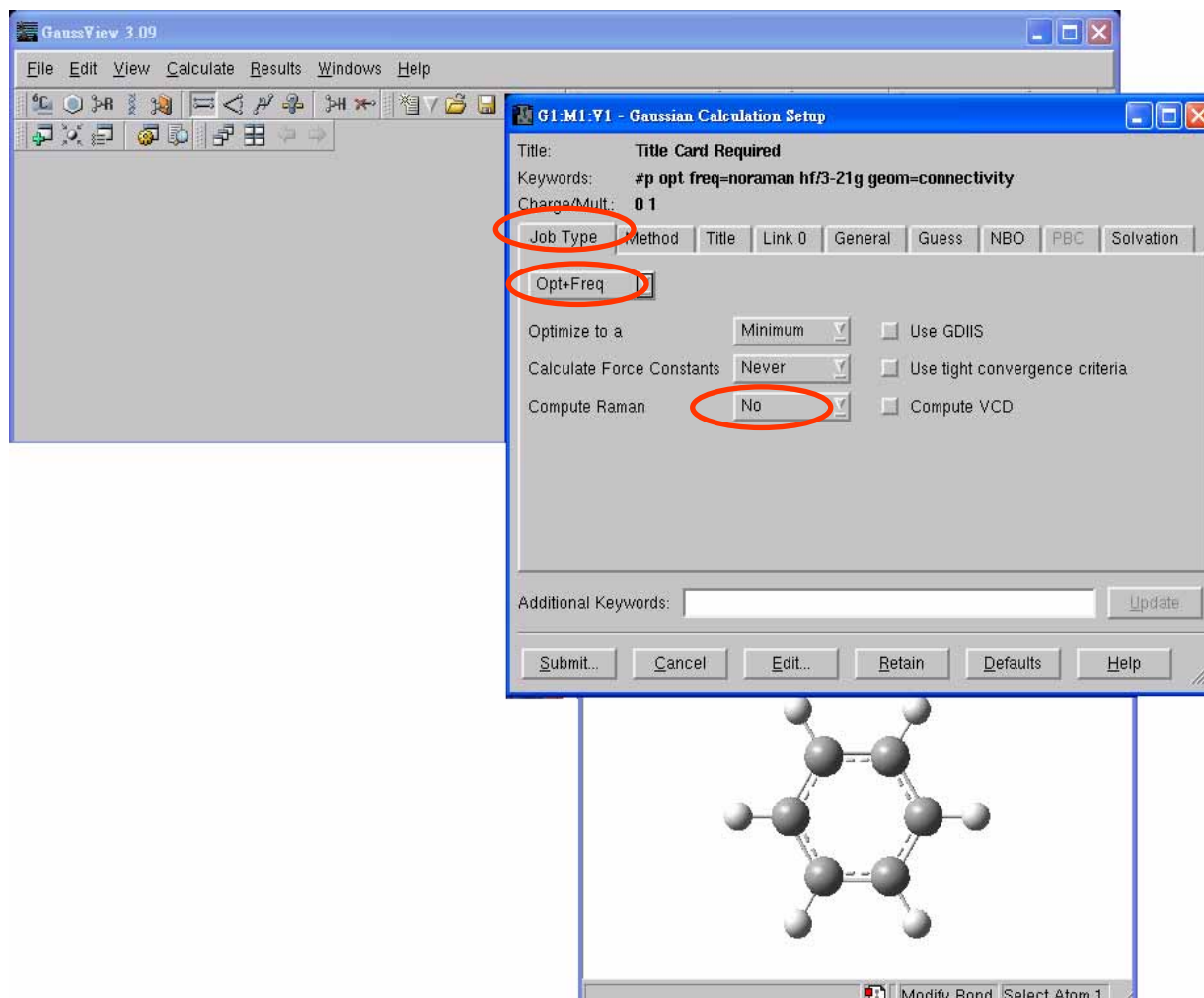
Optimization and Frequency

Click **Calculate** → Select **Gaussian**



Job Type

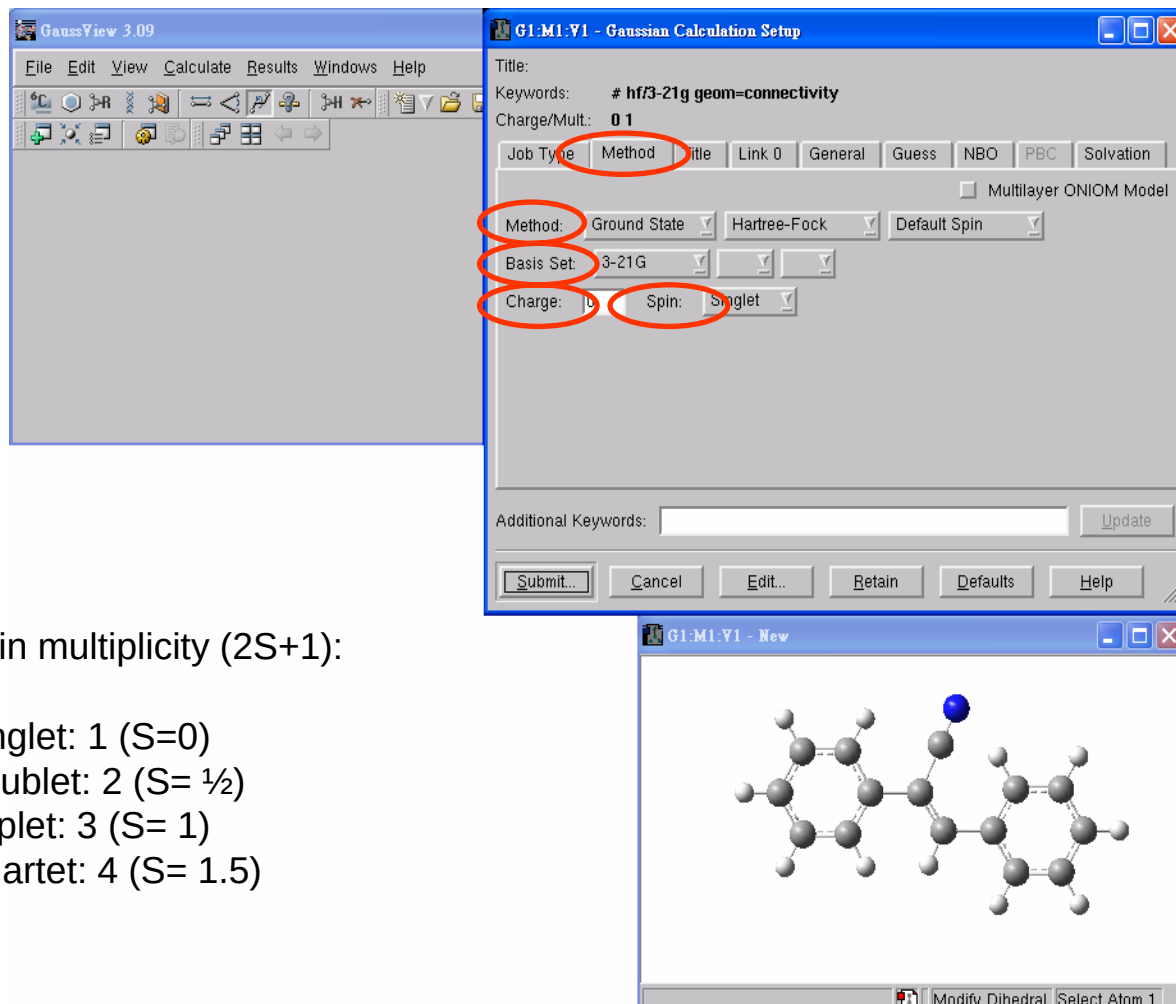
Job type $\rightarrow$ Opt + freq $\rightarrow$ Noraman



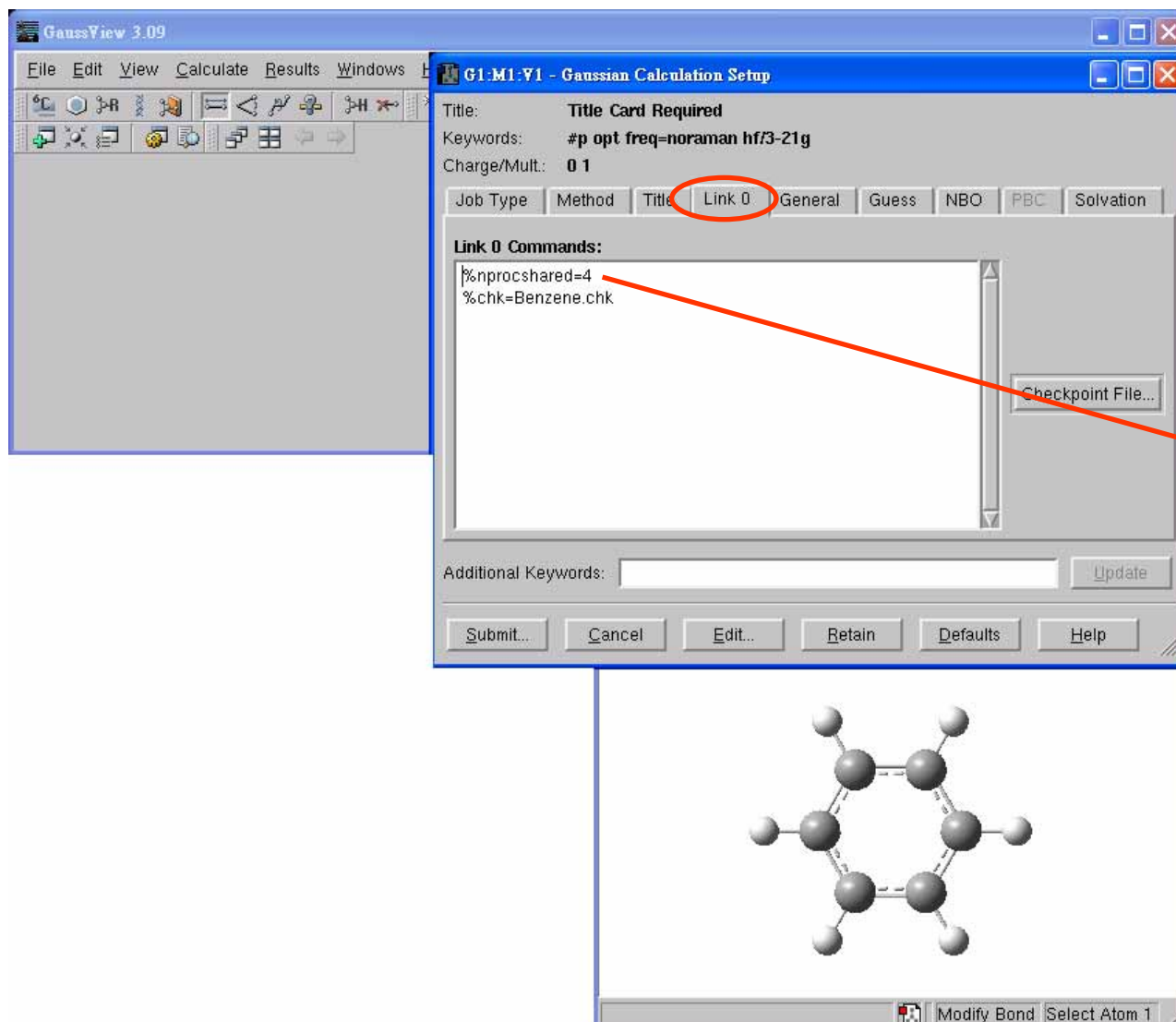
- Calculation of Raman spectrum is time-consuming: normally skip

Methods

Select **Method** → **Basis set** → **Charge** → **Spin**



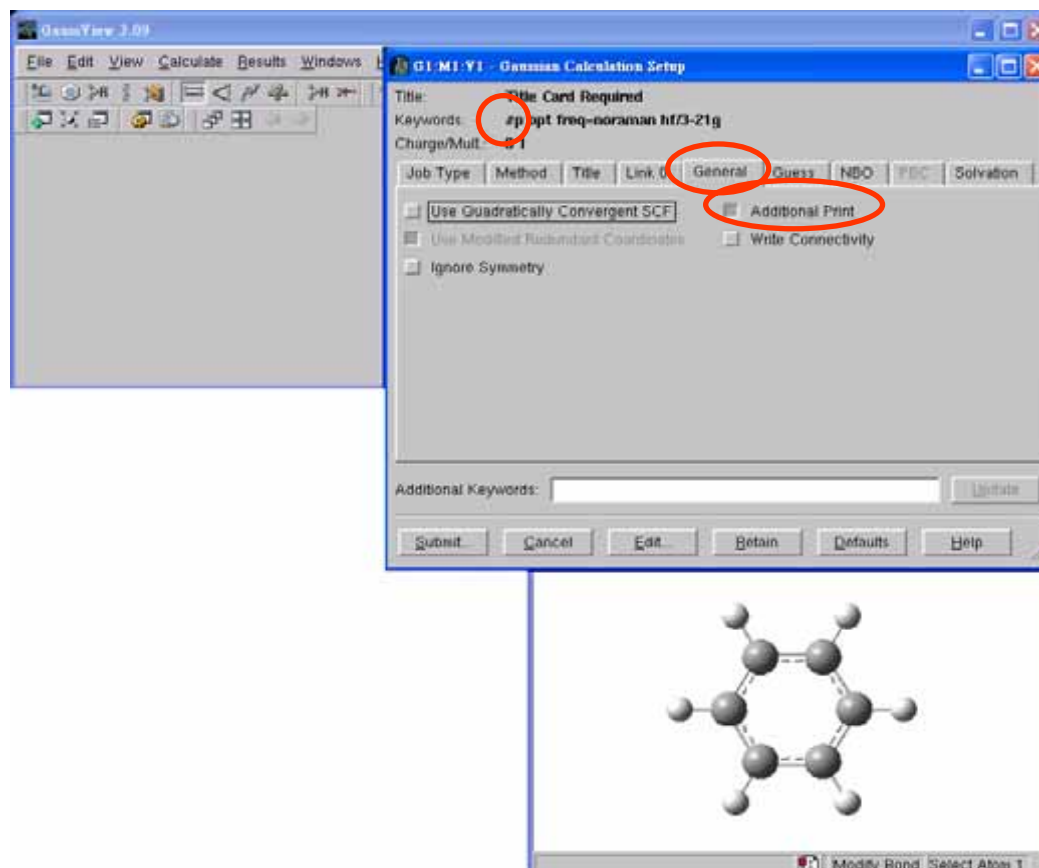
Link



of CPU

General

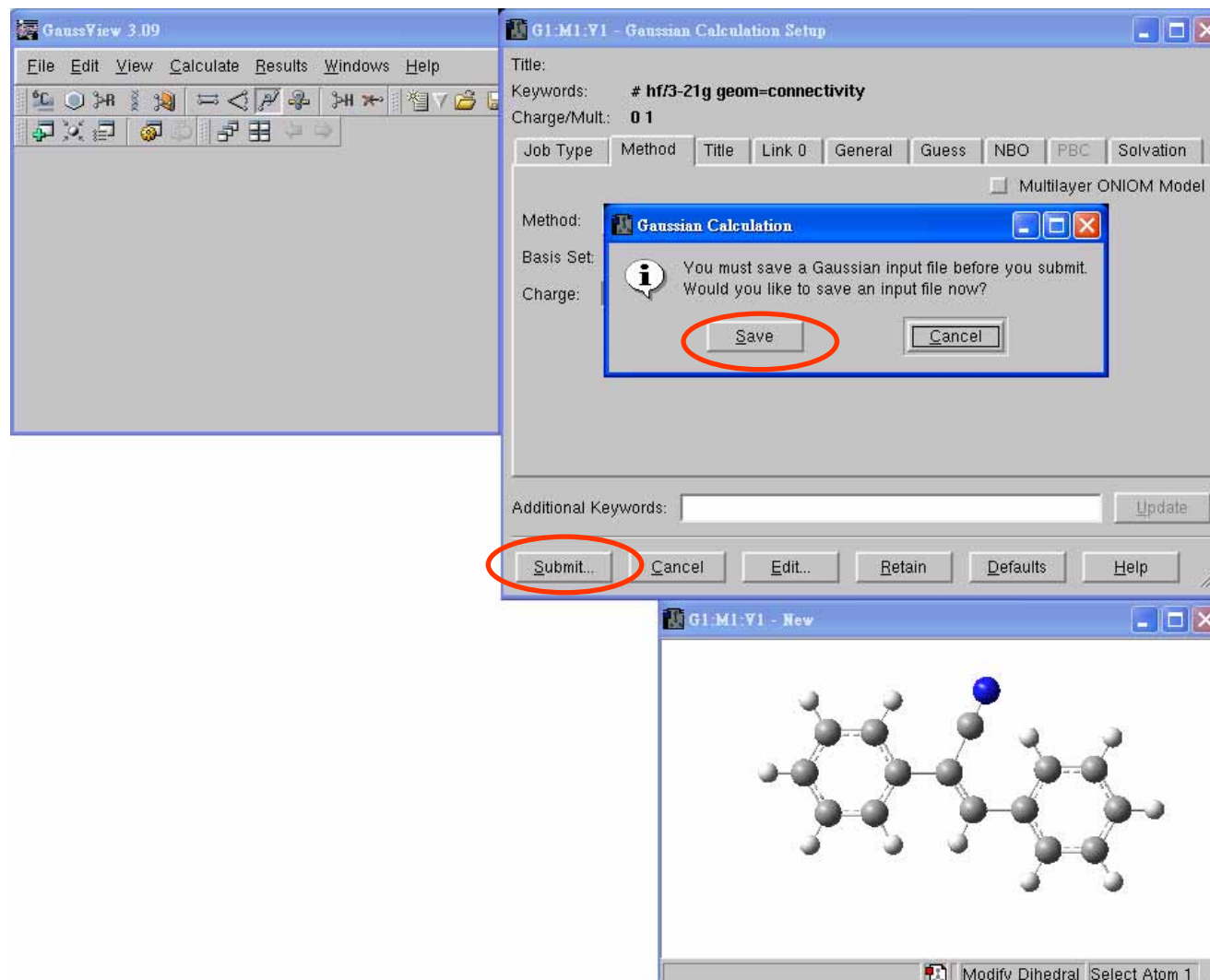
Click General → Select **Additional print**



► QC is used only when SCF convergence is difficult to achieve.

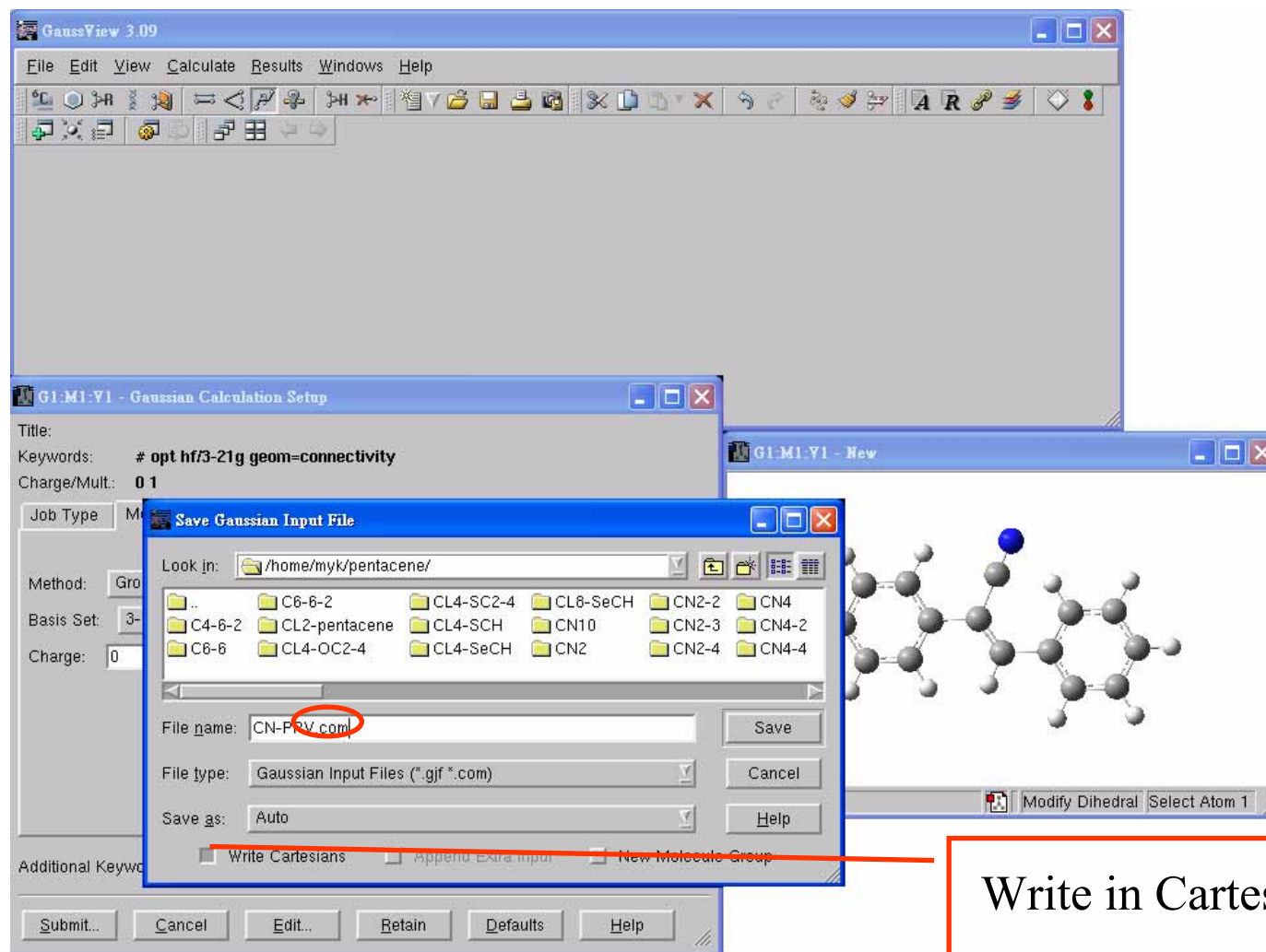
Submit the job

Click **Submit** → **Save** the job

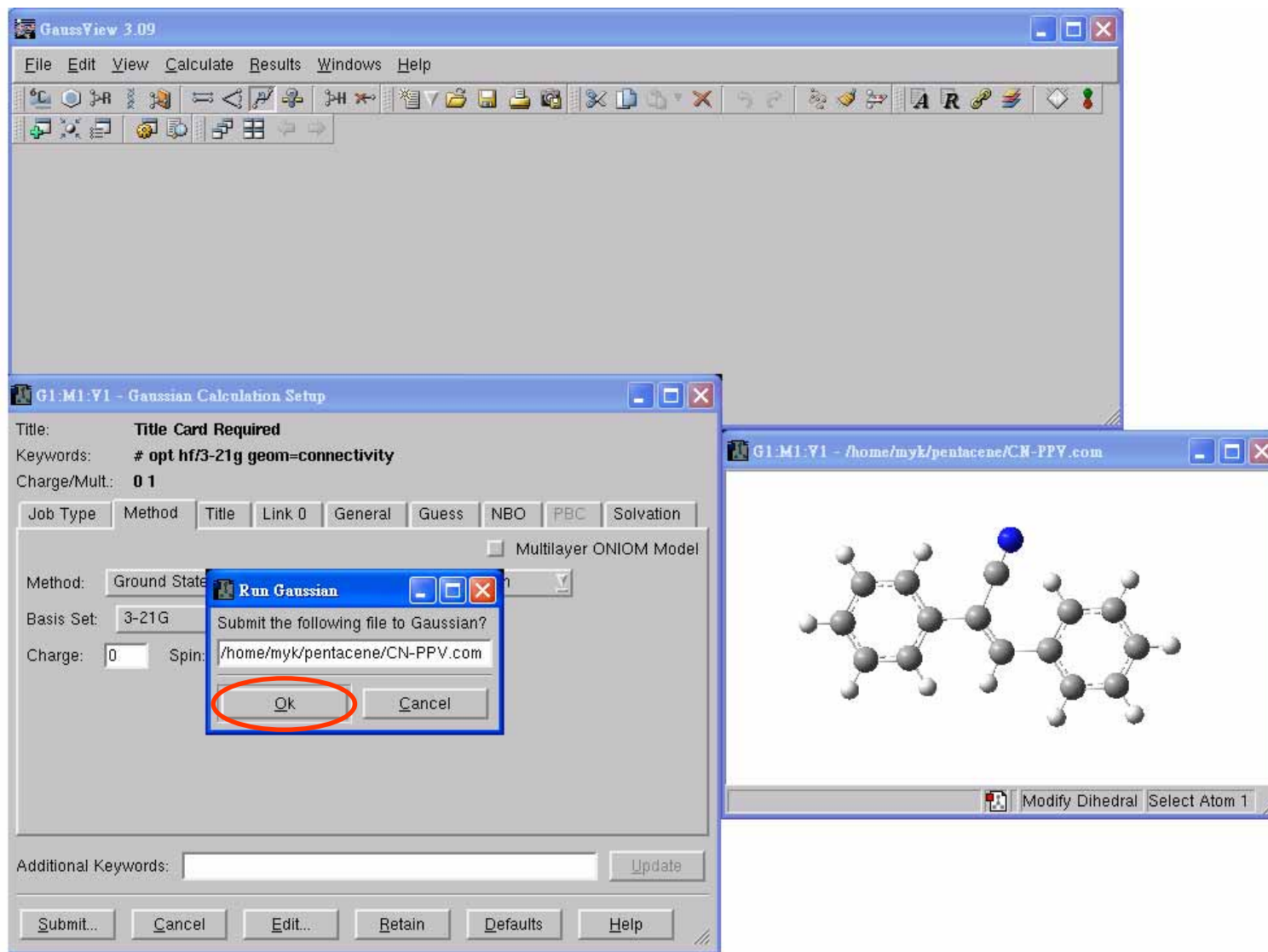


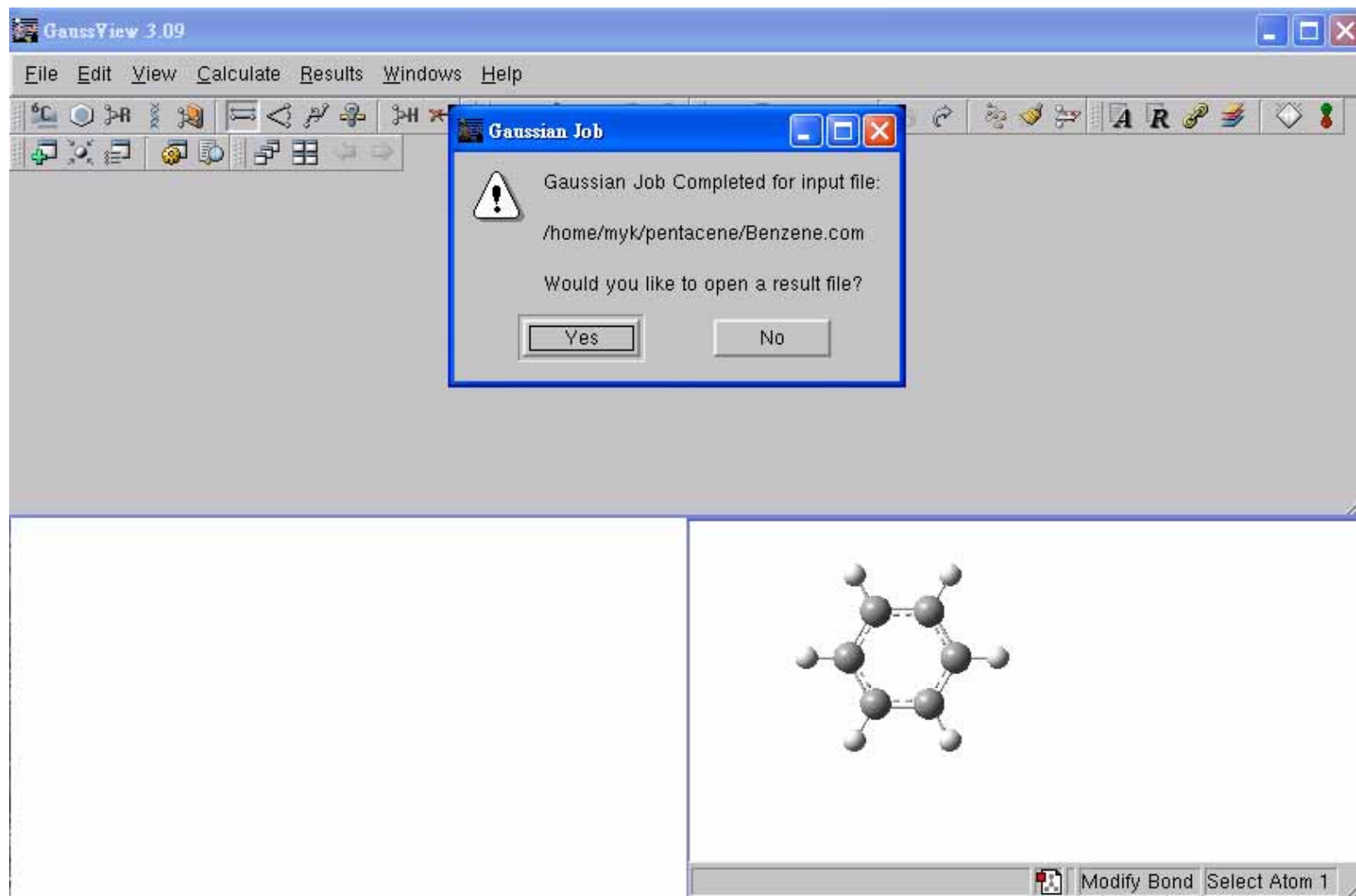
Save the job

File type *.com

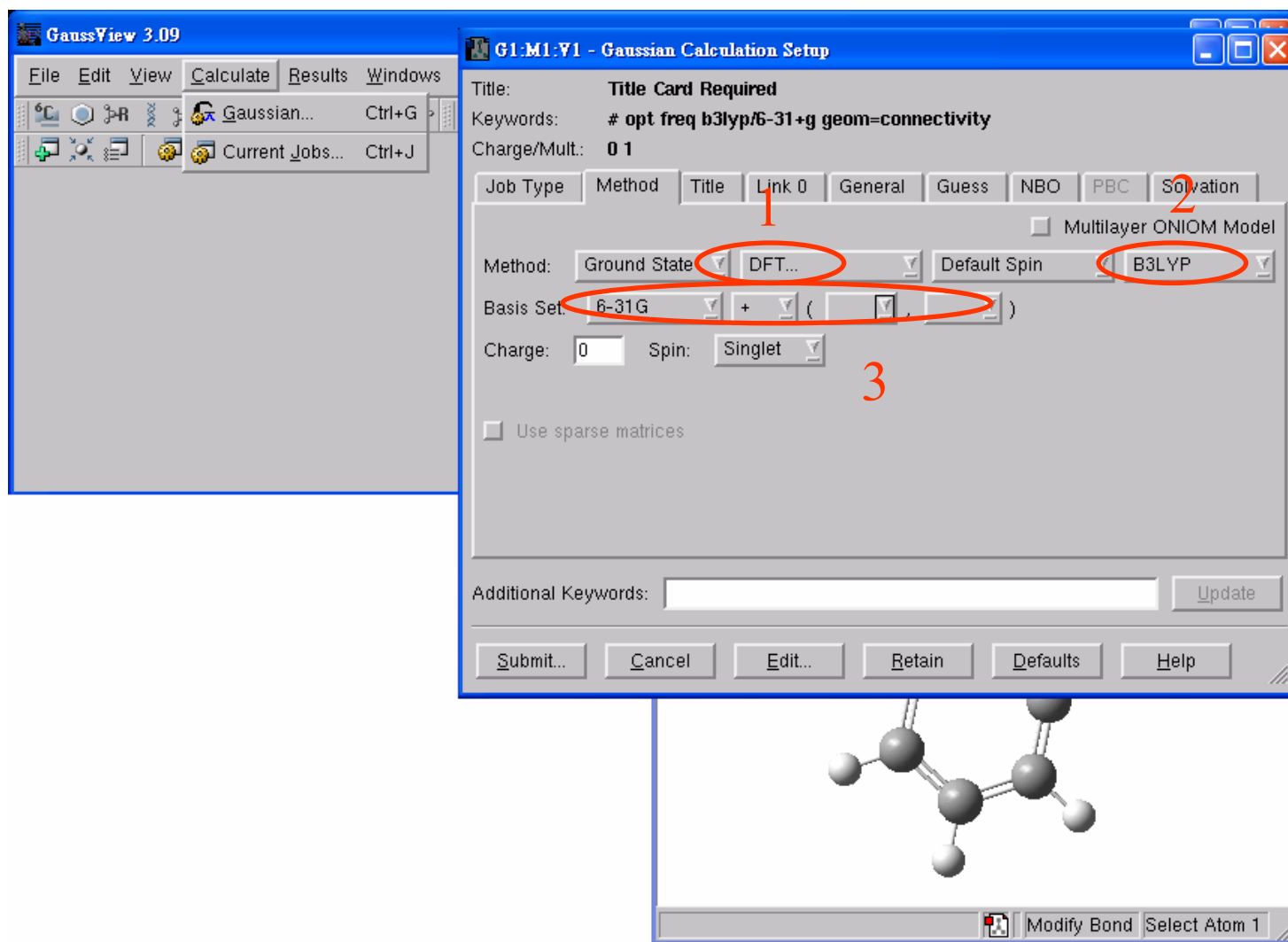


Run the Job





Again : Job type → Method → Link → General
Method (**DFT**) → Exchange-Correlation (**B3LYP**) → Basis set



Input File XXX.com of Gaussian

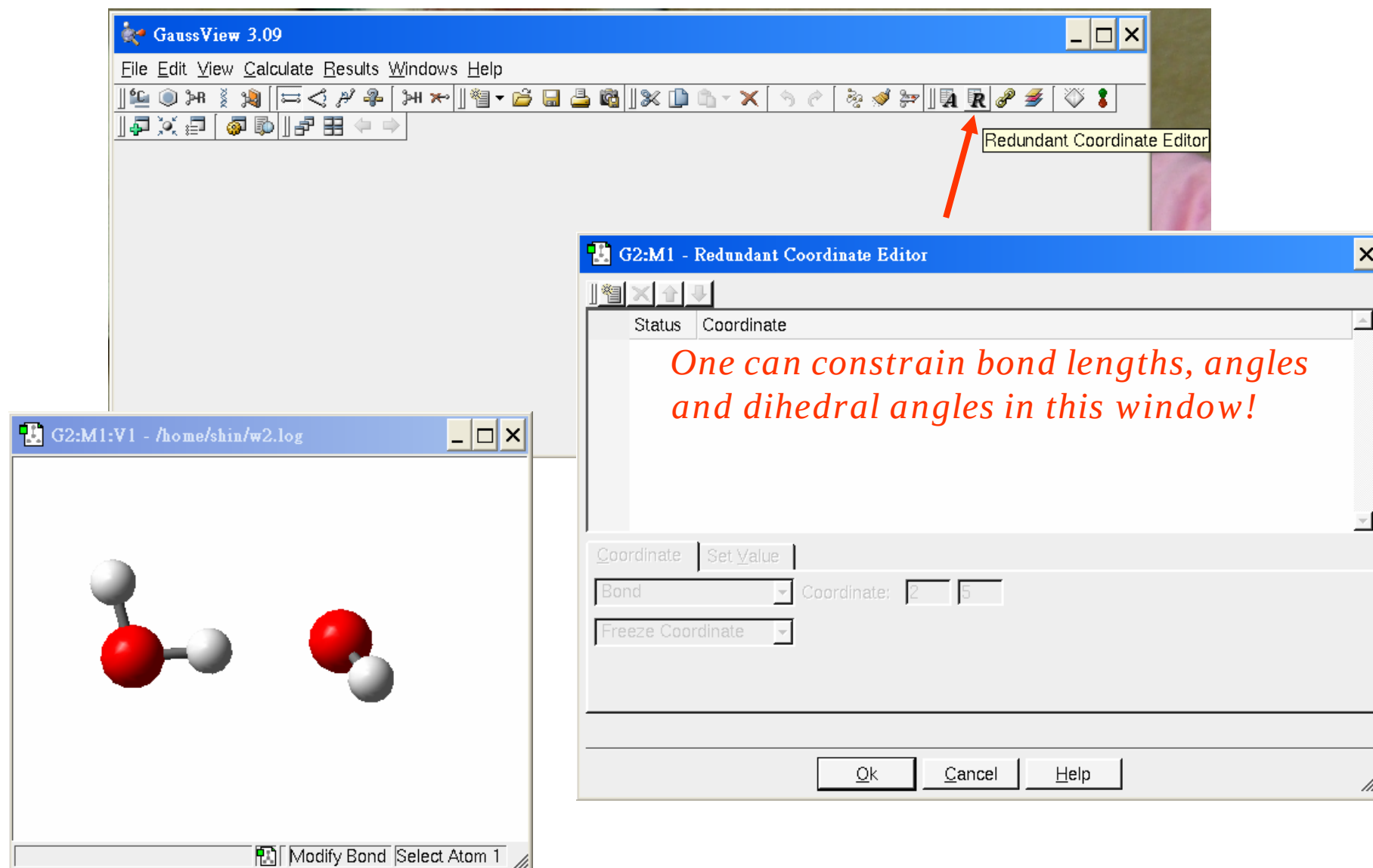
```
shin on jockol: /home/shin
%mpprocshared=4
%chk=benzene.chk
#p opt freq=noraman hf/3-21g

Title Card Required

0 1
C      1.13914292   -0.82278480   -0.01491222
C      2.53430292   -0.82278480   -0.01491222
C      3.23184092    0.38496620   -0.01491222
C      2.53418692    1.59347520   -0.01611122
C      1.13936192    1.59339720   -0.01659022
C      0.44176092    0.38519120   -0.01559422
H      0.58938392   -1.77510180   -0.01446222
H      3.08381092   -1.77529780   -0.01359722
H      4.33152092    0.38504620   -0.01427822
H      3.08438692    2.54561820   -0.01617022
H      0.58923992    2.54567820   -0.01754322
H     -0.65784308    0.38537420   -0.01577422

~
~
~
"benzene.com" 20L, 796C                               1,1           All
```

Partial Optimization: How to Constrain Coordinates

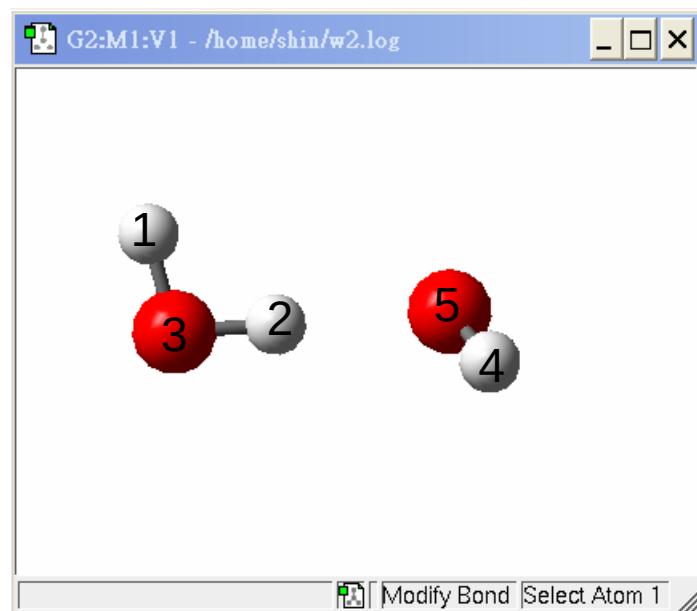


The image displays the GaussView 3.09 software interface. The main window shows a 3D ball-and-stick model of a water molecule (H2O) and a separate molecule consisting of two red spheres and one white sphere. The title bar of the main window reads "GaussView 3.09". The menu bar includes "File", "Edit", "View", "Calculate", "Results", "Windows", and "Help". The toolbar contains various icons for file operations, editing, and calculations. A red arrow points to the "Redundant Coordinate Editor" icon in the toolbar.

The "Redundant Coordinate Editor" window is open, titled "G2:M1 - Redundant Coordinate Editor". It contains a table with two columns: "Status" and "Coordinate". The text "One can constrain bond lengths, angles and dihedral angles in this window!" is overlaid on the table. Below the table, there are input fields for "Bond" (a dropdown menu), "Coordinate" (two input boxes with values "2" and "5"), and "Freeze Coordinate" (a dropdown menu). At the bottom of the window are buttons for "Ok", "Cancel", and "Help".

The window also shows a status bar at the bottom with the text "Modify Bond Select Atom 1".

Constrain Bond Length



G2:M1 - Redundant Coordinate Editor

Status	Coordinate
	Add Bond (2, 5)

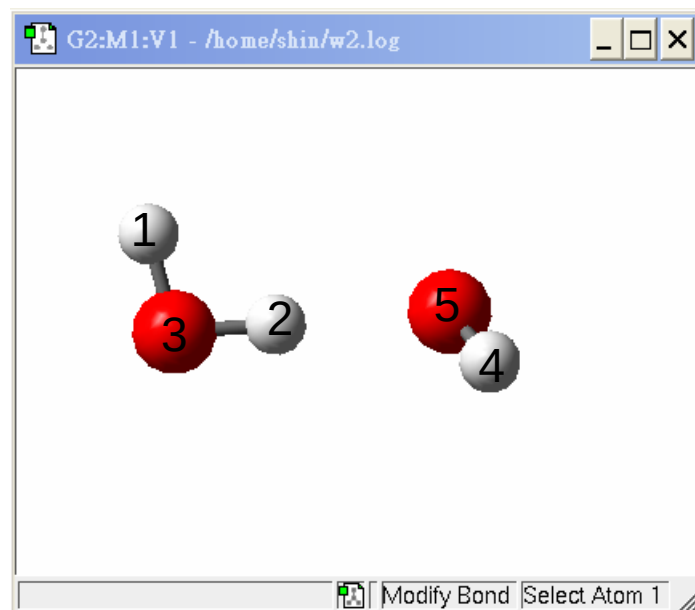
Coordinate Set Value

Bond Coordinate: 2 5

- Cartesian Coordinate
- Bond
- Angle
- Dihedral
- Linear Bend
- Out-of-Plane Bend
- Unidentified

Ok Cancel Help

Freeze Atom Positions



G1:M1 - Redundant Coordinate Editor

Status	Coordinate
	Freeze Cartesian (1)
	Freeze Cartesian (2)
	Add Cartesian (3)

Coordinate Set Value

Cartesian Coordinate Coordinate: 3

Add

- Add
- Activate
- Freeze Coordinate
- Build Coordinate
- Kill Coordinate
- Remove Coordinate
- Derivative
- Hessian
- Scan Coordinate

Ok Cancel Help

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/CN2
D100      -0.00001  0.00000  0.00000  0.00001  0.00001  0.00000
D101       0.00002  0.00000  0.00000 -0.00002 -0.00002  0.00001
D102      -3.14158  0.00000  0.00000 -0.00001 -0.00001 -3.14159
D103      -3.14156  0.00000  0.00001 -0.00003 -0.00002 -3.14158
D104       0.00002  0.00000  0.00001 -0.00002 -0.00001  0.00001
Item      Value      Threshold  Converged?
Maximum Force      0.000136    0.000450      YES
RMS Force          0.000035    0.000300      YES
Maximum Displacement 0.001070    0.001800      YES
RMS Displacement   0.000318    0.001200      YES
Predicted change in Energy=-4.394364D-07
Optimization completed.
-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name Definition      Value      Derivative Info.
!
@
4608, 2 43%
```


Final geometry

Remember to search upward from the string "Optimization completed"

```

X myk on jocko1: /home/myk/pentacene
Berny optimization.
Initialization pass.
No Z-matrix variables, so optimization will use Cartesian coordinates.
Trust Radius=1.000-07 FncErr=1.000-07 GrdErr=1.000-07
Number of steps in this run= 2 maximum allowed number of steps= 2.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
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

```

Check Frequency and Polarizability

All positive

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

```
myk on jocko1: /home/myk/pentacene/CN2
Compute integral second derivatives, UseDBF=F.
Integral derivatives from FoFDir, PRISM(SPDF).
Symmetry not used in FoFDir.
MinBra= 0 MaxBra= 2 Meth= 1.
IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 JSym2E=0.
Leave Link 703 at Wed Mar 22 13:17:23 2006, MaxMem= 67108864 cpu: 3493.7
(Enter /package/chem/g03/l716.exe)
Dipole = 5.10154987D-04 -3.04874027D-05 -4.99998320D-04
Polarizability= 6.01902746D+02 -5.42921182D-05 3.25324597D+02
-5.49065709D-04 1.07912039D-03 7.74548747D+01
Full mass-weighted force constant matrix:
Low frequencies --- -0.0006 0.0007 0.0008 3.8847 6.5396 7.7111
Low frequencies --- 33.5371 69.2399 75.2820
Diagonal vibrational polarizability:
20.2967023 8.7223537 84.7250693
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:
1 2 3
A A A
Frequencies -- 33.5371 69.2399 75.2820
Red. masses -- 7.0581 3.9420 9.7123
7032, 2 66%
```

Dipole moment and total charge

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

```
myk on jocko1: /home/myk/pentacene/CN4-2
23 C 0.006825
24 C -0.003821
25 C -0.003806
26 C 0.186571
27 H -0.004078
28 H -0.004075
29 H -0.004071
30 H -0.004071
31 H -0.008109
32 H -0.008103
33 N 0.011653
34 N 0.011619
35 N 0.011613
36 N 0.011619
37 H -0.006995
38 H -0.006995
39 H -0.006994
40 H -0.006992
Sum of Mulliken spin densities= 1.00000
Electronic spatial extent (au): <R**2>= 20960.9368
Charge= -1.0000 electrons
Dipole moment (field-independent basis, Debye):
X= -0.0013 Y= -0.0007 Z= -0.1688 Tot= 0.1688
Quadrupole moment (field-independent basis, Debye-Ang):
XX= -494.9548 YY= -178.7876 ZZ= -173.1553
XY= 0.0103 XZ= -0.0552 YZ= 0.0189
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= -212.6556 YY= 103.5117 ZZ= 109.1439
XY= 0.0103 XZ= -0.0552 YZ= 0.0189
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= 0.6031 YYY= -0.0166 ZZZ= 0.5555 XYY= -0.3906
XXY= -0.0549 XXZ= -16.4606 XZZ= -0.0355 YZZ= 0.0008
YYZ= -1.3343 XYZ= -1.1433
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -53791.5351 YYYY= -2082.2300 ZZZZ= -175.8584 XXXY= 0.7483
XXXZ= -4.2915 YYYY= 0.2050 YYYZ= 0.1215 ZZZX= 0.0903
ZZZY= -0.0133 XXYY= -6610.8029 XXZZ= -4640.1749 YYZZ= -392.9709
XXYZ= 1.0776 YYXZ= -0.3751 ZZZY= -0.1571
N-N= 2.227785506634D+03 E-N= -7.293477856766D+03 KE= 1.204919247605D+03
```

Mulliken charge

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

```
myk on jocko1: /home/myk/pentacene/CN4-2
20 C 0.000000 0.000000 -0.007952 -0.000205
21 C 0.000000 0.000000 -0.000205 -0.007951
22 C 0.000000 0.000000 0.000180 0.000028
23 C 0.000000 0.000000 0.000028 0.000181
24 C 0.000000 0.000000 -0.000006 0.000000
25 C 0.000000 0.000000 0.000000 -0.000006
26 C -0.000198 -0.008111 -0.000198 -0.008103
27 H 0.000002 0.006741 0.000000 0.000000
28 H 0.006742 0.000002 0.000000 0.000000
29 H 0.000000 0.000000 0.006766 0.000002
30 H 0.000000 0.000000 0.000002 0.006770
31 H 0.007238 0.000002 0.007249 0.000002
32 H 0.000002 0.007237 0.000002 0.007251
33 N 0.000000 0.000000 0.000000 0.000000
34 N 0.000000 0.000000 0.000000 0.000000
35 N 0.000000 0.000000 0.000000 0.000000
36 N 0.000000 0.000000 0.000000 0.000000
37 H 0.618620 0.000023 0.000001 0.000000
38 H 0.000023 0.618599 0.000000 0.000001
39 H 0.000001 0.000000 0.618464 0.000023
40 H 0.000000 0.000001 0.000023 0.618470
Mulliken atomic charges:
1
1 C 0.151659
2 C -0.244698
3 C 0.151642
4 C -0.244608
5 C 0.164229
6 C -0.324369
7 C 0.172627
8 C -0.331370
9 C 0.172448
10 C -0.324327
11 C 0.164390
12 C 0.199328
13 C 0.199319
14 C 0.172589
15 C 0.172505
16 C -0.324298
17 C -0.324338
18 C 0.164425
19 C 0.164449
20 C -0.244808
:/Mulliken
```

Thermochemistry

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

```
myk on jockol: /home/myk/pentacene/CN4-2

32 1 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.02 0.00
33 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
34 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
35 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
36 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
37 1 0.00 0.04 0.00 0.00 -0.04 0.00 0.00 -0.04 0.00
38 1 0.00 0.04 0.00 0.00 0.04 0.00 0.00 0.04 0.00
39 1 0.00 0.03 0.00 0.00 0.04 0.00 0.00 -0.04 0.00
40 1 0.00 0.03 0.00 0.00 -0.04 0.00 0.00 0.04 0.00

-----
Thermochemistry -
-----
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Atom 1 has atomic number 6 and mass 12.00000
Atom 2 has atomic number 6 and mass 12.00000
Atom 3 has atomic number 6 and mass 12.00000
Atom 4 has atomic number 6 and mass 12.00000
Atom 5 has atomic number 6 and mass 12.00000
Atom 6 has atomic number 6 and mass 12.00000
Atom 7 has atomic number 6 and mass 12.00000
Atom 8 has atomic number 6 and mass 12.00000
Atom 9 has atomic number 6 and mass 12.00000

14437,2 87%
```

Zero-point energy

Press **Page Down**

$$E_0 = E_{\text{elec}} + \text{ZPE}$$

$$E = E_0 + E_{\text{vib}} +$$

$$E_{\text{rot}} + E_{\text{transl}}$$

$$H = E + RT$$

$$G = H - TS$$

entropy

```
myk on jockol: /home/myk/pentacene/CN4-2
4500.65 4600.66 4602.45 4602.58
Zero-point correction= 0.278439 (Hartree/Particle)
Thermal correction to Energy= 0.300940
Thermal correction to enthalpy= 0.301884
Thermal correction to Gibbs Free Energy= 0.225643
Sum of electronic and zero-point Energies= -1215.581916
Sum of electronic and thermal Energies= -1215.559416
Sum of electronic and thermal Enthalpies= -1215.558477
Sum of electronic and thermal Free Energies= -1215.634718
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.843	89.464	160.464
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.682
Rotational	0.889	2.981	36.627
Vibrational	187.065	83.502	78.777
Vibration 1	0.593	1.985	6.418
Vibration 2	0.594	1.982	5.486
Vibration 3	0.597	1.974	4.476
Vibration 4	0.597	1.971	4.306
Vibration 5	0.599	1.967	4.081
			14519.30

87%

► Zero-point energy and other thermodynamic quantities (enthalpy, entropy, free energy) are obtained through frequency calculation.

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
1\INGING-JOCKO1\F0pt\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)]\@

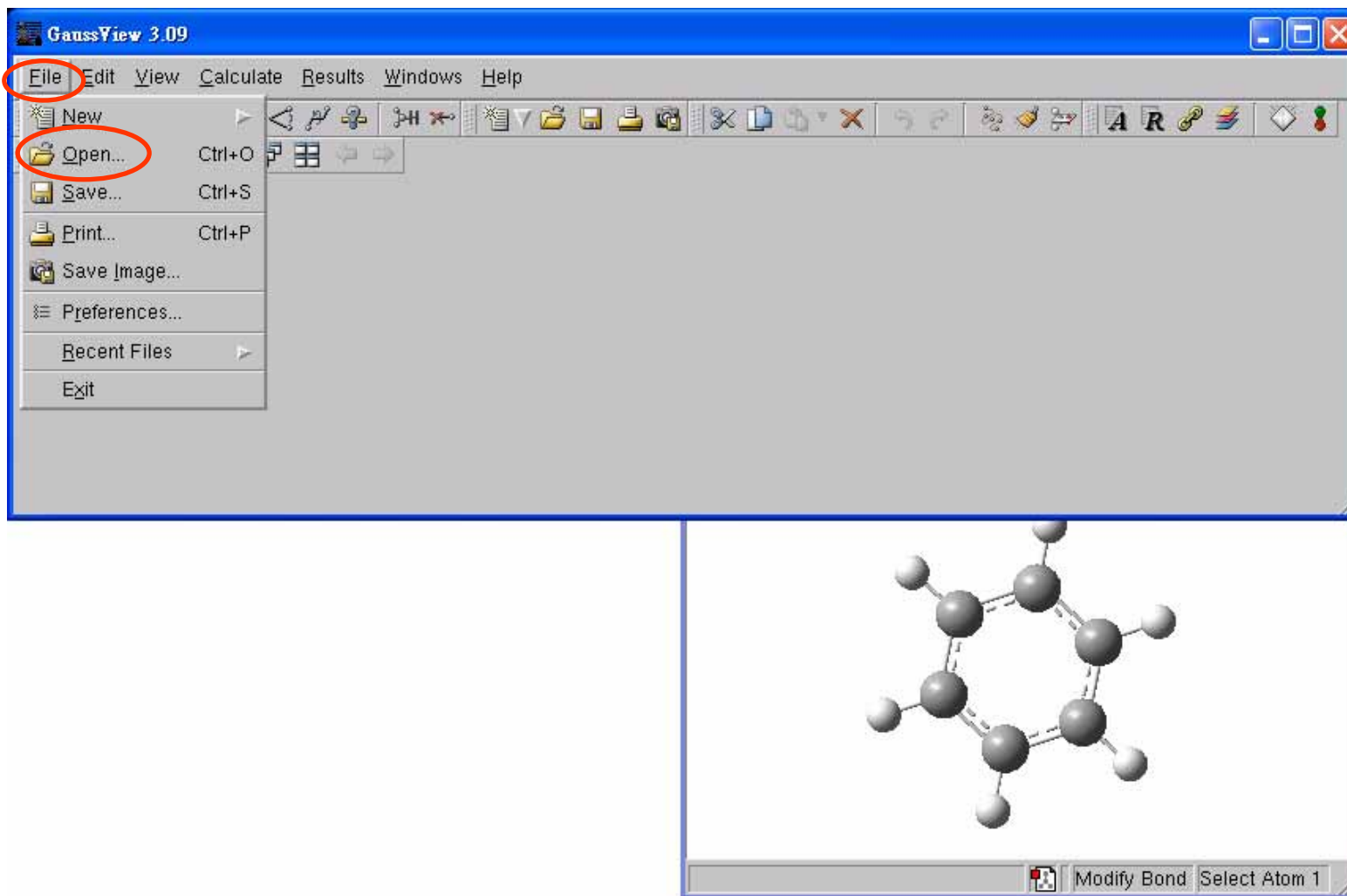
ALL MY ATTEMPTS TO ADAPT THE THEORETICAL FOUNDATIONS OF PHYSICS
TO THESE NEW NOTIONS FAILED COMPLETELY. IT WAS AS IF THE GROUND HAD
BEEN PULLED OUT FROM UNDER ONE WITH NO FIRM FOUNDATION TO BE SEEN ANYWHERE,
UPON WHICH ONE COULD HAVE BUILT. -- A. EINSTEIN
Job cpu time: 0 days 0 hours 0 minutes 2.0 seconds.
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.

497,2
```

► This is the total electronic energy reported in the literature.

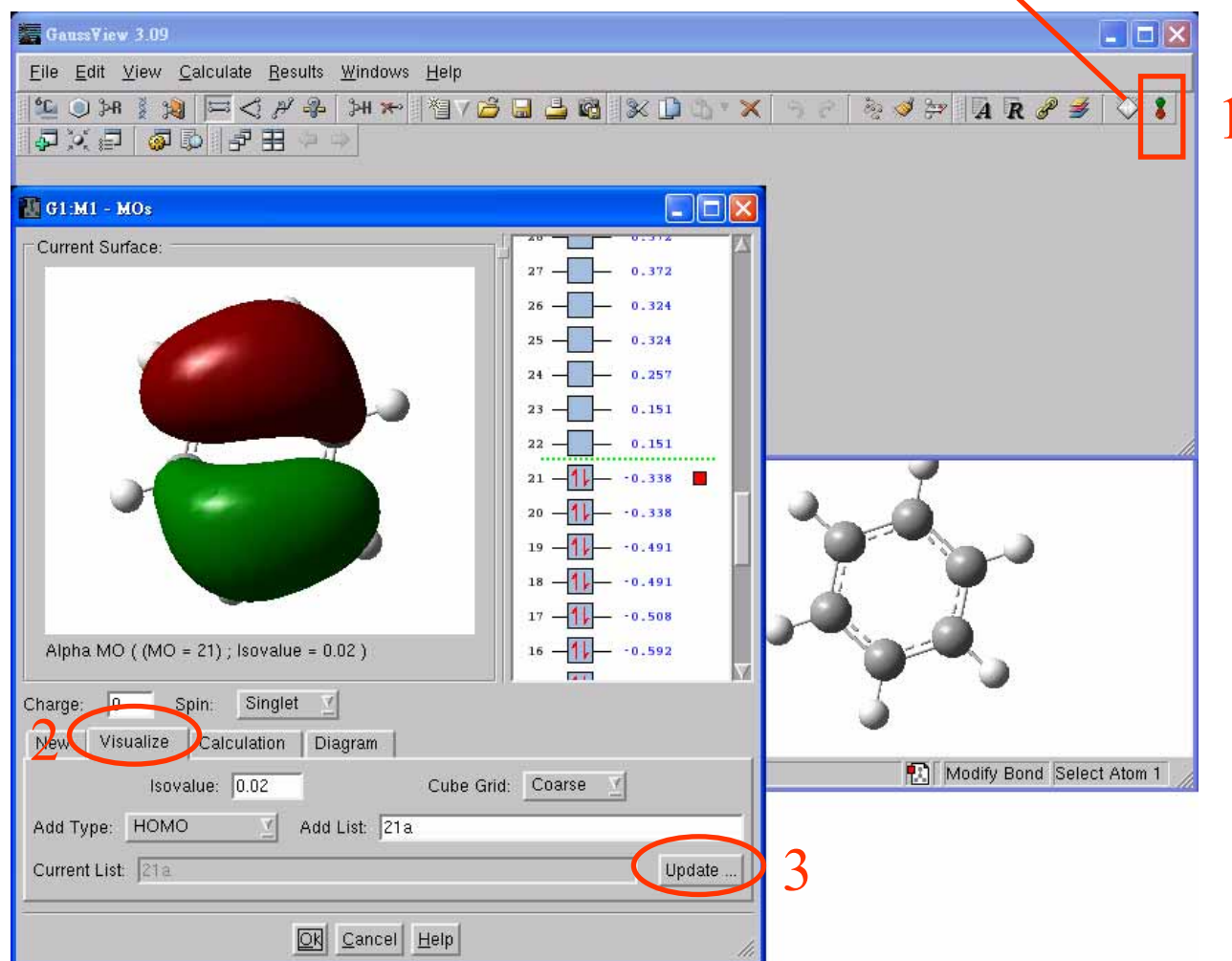
Check HOMO

Using GaussView → File → Open *.chk



Check HOMO

Press **Molecular Orbital Editor** →
Select **Visualize** → Press **Update**



IR Spectrum

Click **File** to open *.chk → Click **Result** →
Select **Vibration** → Click **Spectrum**

1

2

3

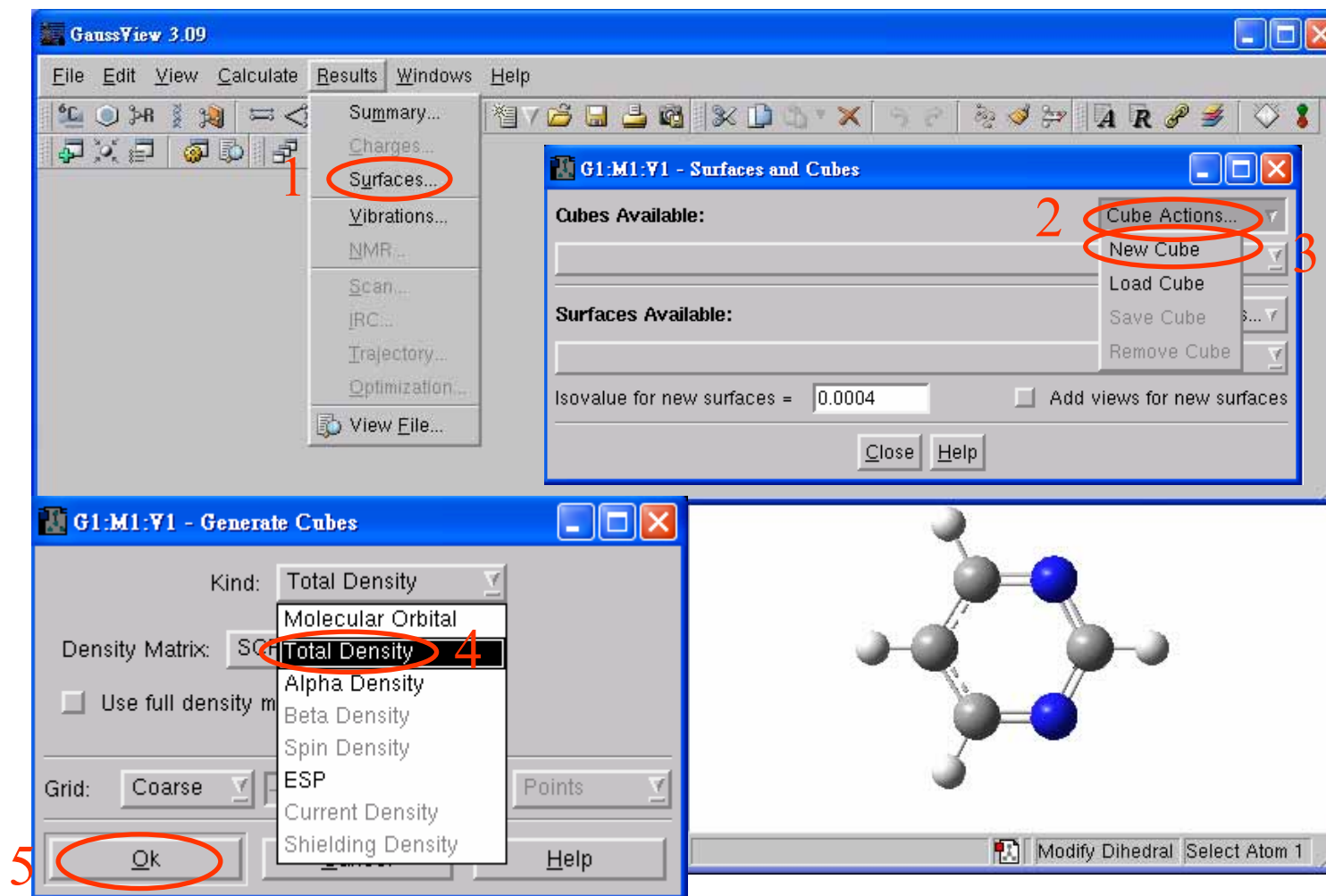
4

The screenshot displays the GaussView 3.09 software interface. The main window shows the 'Infrared Spectrum' plot with Intensity on the y-axis (ranging from -20 to 120) and Frequency on the x-axis (ranging from 0 to 3500 cm⁻¹). The spectrum shows several sharp peaks, with the most prominent ones around 1600 and 1500 cm⁻¹. Below the main window, a smaller window titled 'G1:M1:Y1 - Display Vibrations' is open, showing a table of vibrational frequencies and infrared intensities. The table has columns for #, Freq, and Infrared. The first row shows a frequency of 446.469 and an infrared intensity of 4.955. The second row shows a frequency of 490.34 and an infrared intensity of 0. The third row shows a frequency of 706.638 and an infrared intensity of 17.0459. The fourth row shows a frequency of 772.352 and an infrared intensity of 6.4578. The fifth row shows a frequency of 837.109 and an infrared intensity of 68.5069. The sixth row shows a frequency of 949.562 and an infrared intensity of 8.9429. The seventh row shows a frequency of 1078.86 and an infrared intensity of 2.8261. The eighth row shows a frequency of 1124.28 and an infrared intensity of 1.4547. The ninth row shows a frequency of 1145.36 and an infrared intensity of 0.6071. The tenth row shows a frequency of 1160.17 and an infrared intensity of 0. Below the table, there are checkboxes for 'Show Displacement Vectors' and 'Show Dipole Derivative Unit Vector', both of which are currently unchecked. At the bottom of the dialog, there are buttons for 'Close', 'Cancel', 'Start', 'Spectrum', and 'Help'. The 'Spectrum' button is highlighted with a red circle and the number 4.

#	Freq	Infrared
1	446.469	4.955
2	490.34	0
3	706.638	17.0459
4	772.352	6.4578
5	837.109	68.5069
6	949.562	8.9429
7	1078.86	2.8261
8	1124.28	1.4547
9	1145.36	0.6071
10	1160.17	0

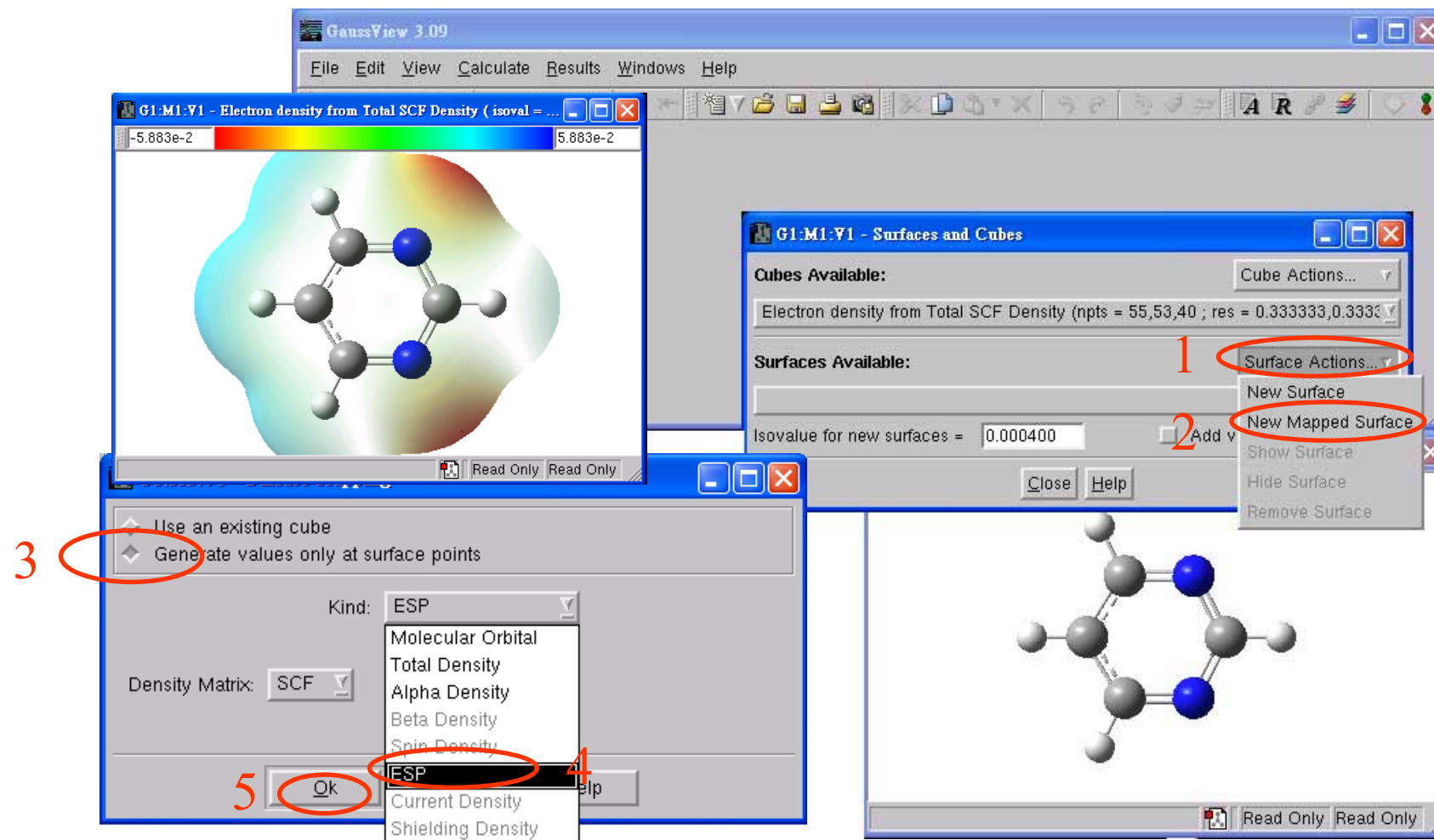
Total density

Select **Surface** → Click **Cube Actions** → Select **New Cube** → Select **Total Density** → Click **OK**

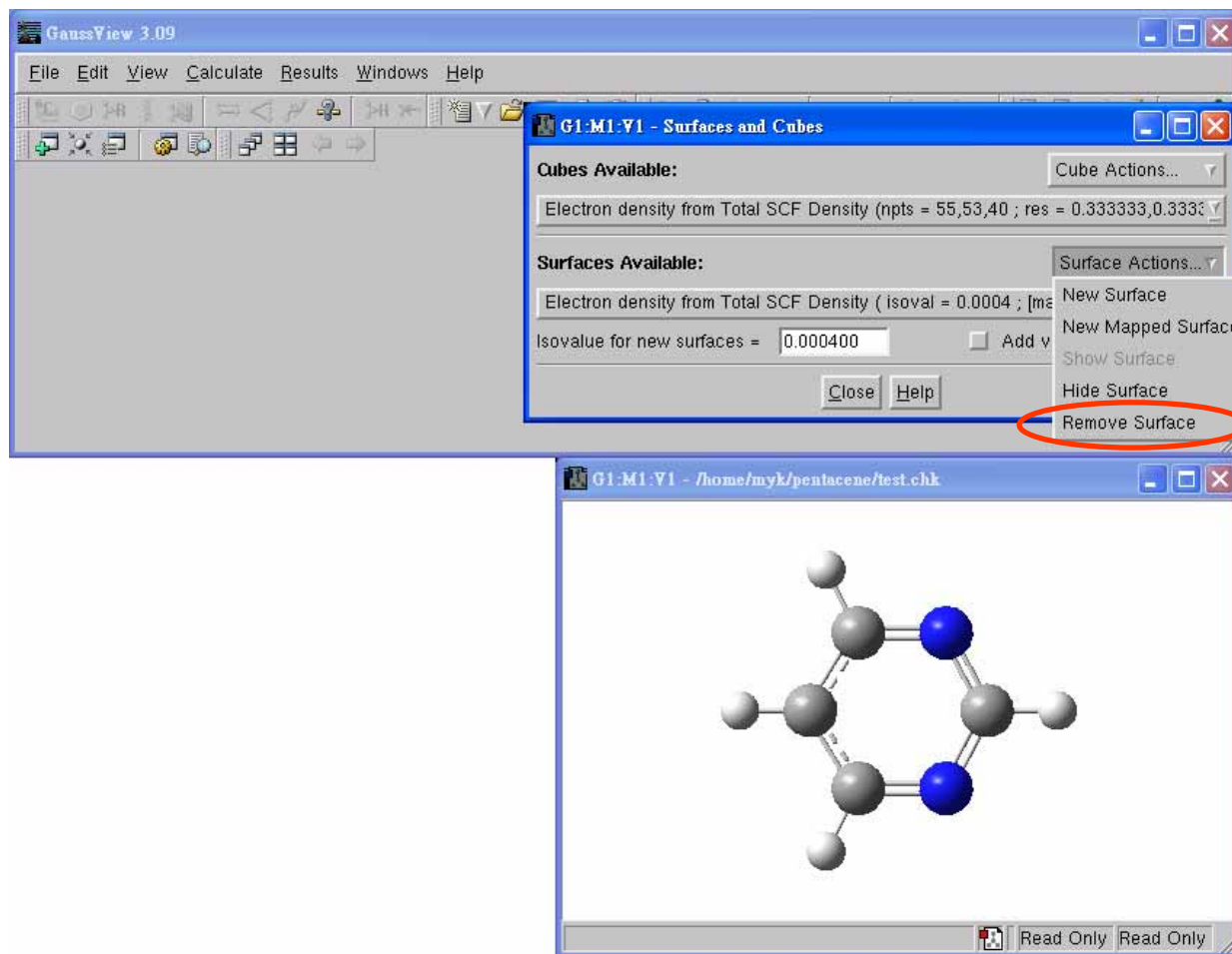


Mapping the MEP

Click **Surface Actions** → Select **New Mapped Surface**
Surface → Select **ESP** → Click **OK**



Remove MEP Mapping



HOMO Mapping

Click **Surface Actions** → Select **New Mapped Surface**
Surface → Select **Molecular Orbital** → Click **OK**

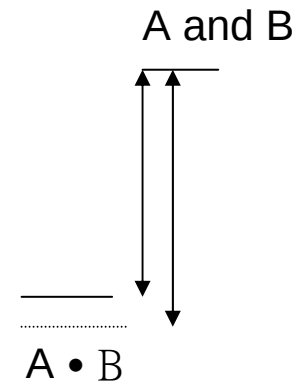
The screenshot displays the GaussView 3.09 interface with several windows and dialog boxes illustrating the HOMO mapping process:

- G1:M1:Y1 - Electron density from Total SCF Density (isoval = ...)**: Shows a 3D molecular model with electron density isosurfaces. A color scale at the top ranges from $-1.178\text{e-}2$ to $1.178\text{e-}2$.
- G1:M1:Y1 - Surfaces and Cubes**:
 - Cubes Available:** Electron density from Total SCF Density (npts = 55,53,40 ; res = 0.333333,0.333333).
 - Surfaces Available:** A red circle labeled '1' highlights the **Surface Actions...** button.
 - Isovalue for new surfaces =** 0.000400. A red circle labeled '2' highlights the **Add v** checkbox.
 - A context menu is open, showing **New Mapped Surface** circled in red.
- G1:M1:Y1 - Surface Mapping**:
 - Use an existing cube** (checked).
 - Generate values only at surface points** (checked). A red circle labeled '3' highlights this option.
 - Kind:** Molecular Orbital (selected). A red circle labeled '4' highlights the **Molecular Orbital** option in the dropdown menu.
 - Orbitals:** HOMO (selected), 21. Below it, 21 Occ and 41 Virt are displayed.
 - Alpha** (dropdown menu).
 - OK** button circled in red, with a red circle labeled '5' next to it.
- Main Viewport**: Shows a ball-and-stick model of the molecule.

Basis Set Superposition Error (BSSE)

$$\Delta E_{\text{bind}} = E_{\text{HF}}^{\text{a}\cup\text{b}}(\text{A}\bullet\text{B}) - E_{\text{HF}}^{\text{a}}(\text{A}) - E_{\text{HF}}^{\text{b}}(\text{B})$$

For finite basis sets calculations, the monomer energies in A•B are artificially lowered



Counterpoise correction for BSSE

$$\begin{aligned} \Delta E_{\text{BIND}}^{\text{CP}} = & E_{\text{HF}}^{\text{a}\cup\text{b}}(\text{A}\bullet\text{B})_{\text{A}\bullet\text{B}} - E_{\text{HF}}^{\text{a}}(\text{A})_{\text{A}} - E_{\text{HF}}^{\text{b}}(\text{B})_{\text{B}} \\ & + \underbrace{[E_{\text{HF}}^{\text{a}}(\text{A})_{\text{A}\bullet\text{B}} - E_{\text{HF}}^{\text{a}\cup\text{b}}(\text{A})_{\text{A}\bullet\text{B}}]}_{\text{BSSE correction for A}} + \underbrace{[E_{\text{HF}}^{\text{b}}(\text{B})_{\text{A}\bullet\text{B}} - E_{\text{HF}}^{\text{a}\cup\text{b}}(\text{B})_{\text{A}\bullet\text{B}}]}_{\text{BSSE correction for B}} \end{aligned}$$

How to Setup Counterpoise Correction in G03

```
shin on jockol: /home/shin
#p hf/sto-3g counterpoise=2 scf=tight
BSSE correction for water dimer
0 1
O          -1.43153078   -0.11125867   -0.02862199   1
H          -0.47444833   -0.04005002   -0.05148040   1
H          -1.80875365    0.72723635    0.24747405   1
H          1.74256759   -0.42527451    0.65281084   2
O          1.21951501    0.08013940    0.02625456   2
H          1.55770605   -0.06113768   -0.86102646   2
~
~
~
~
~
~
~
~
~
~
11 fewer lines
12, 0-1
All
```


Counterpoise Calculation Results

```
shin on jocko1: /home/shin
Leave Link 601 at Fri May 19 12:56:50 2006, MaxMem= 6291456 cpu:
(Enter /package/g03/l122.exe)
Restoring MOs from calculation 1 to rwf.
Counterpoise: corrected energy = -149.920319535212
Counterpoise: BSSE energy = 0.011534051052
Leave Link 122 at Fri May 19 12:56:50 2006, MaxMem= 6291456 cpu: 0.0
(Enter /package/g03/l9999.exe)
1\1\GINC-JOCKO1\SP\RHF\STO-3G\H402\SHIN\19-May-2006\0\#\#P HF/STO-3G CO
UNTERPOISE=2 SCF=TIGHT\BSSE correction for water dimer\0,1\0,0,-1.43
153078,-0.11125867,-0.02862199\H,0,-0.47444833,-0.04005002,-0.0514804\
H,0,-1.80875365,0.72723635,0.24747405\H,0,1.74256759,-0.42527451,0.652
81084\0,0,1.21951501,0.0801394,0.02625456\H,0,1.55770605,-0.06113768,-
0.86102646\Version=AM64L-G03RevC.02\State=1-A\HF=-74.9607025\RMSD=2.5
29e-09\Dipole=1.1101794,0.1142007,-0.0207793\PG=C01 [X(H402)]\@

You don't have to suffer to be a poet.
Adolescence is enough suffering for anyone.
-- John Ciardi
Job cpu time: 0 days 0 hours 0 minutes 5.6 seconds.
File lengths (MBytes): RWF= 17 Int= 0 D2E= 0 Chk= 10 Scr=
1
Normal termination of Gaussian 03 at Fri May 19 12:56:51 2006.
1310,2 Bot
```