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

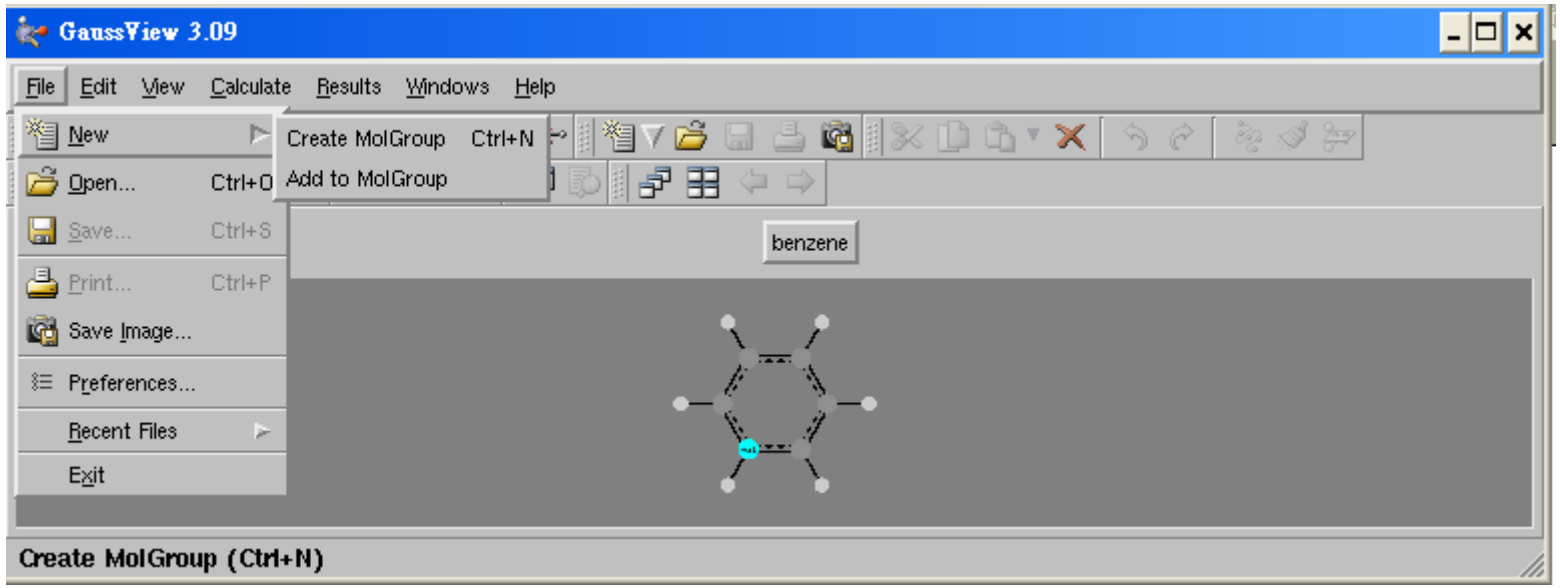
Some Useful Website

Technical Support Information

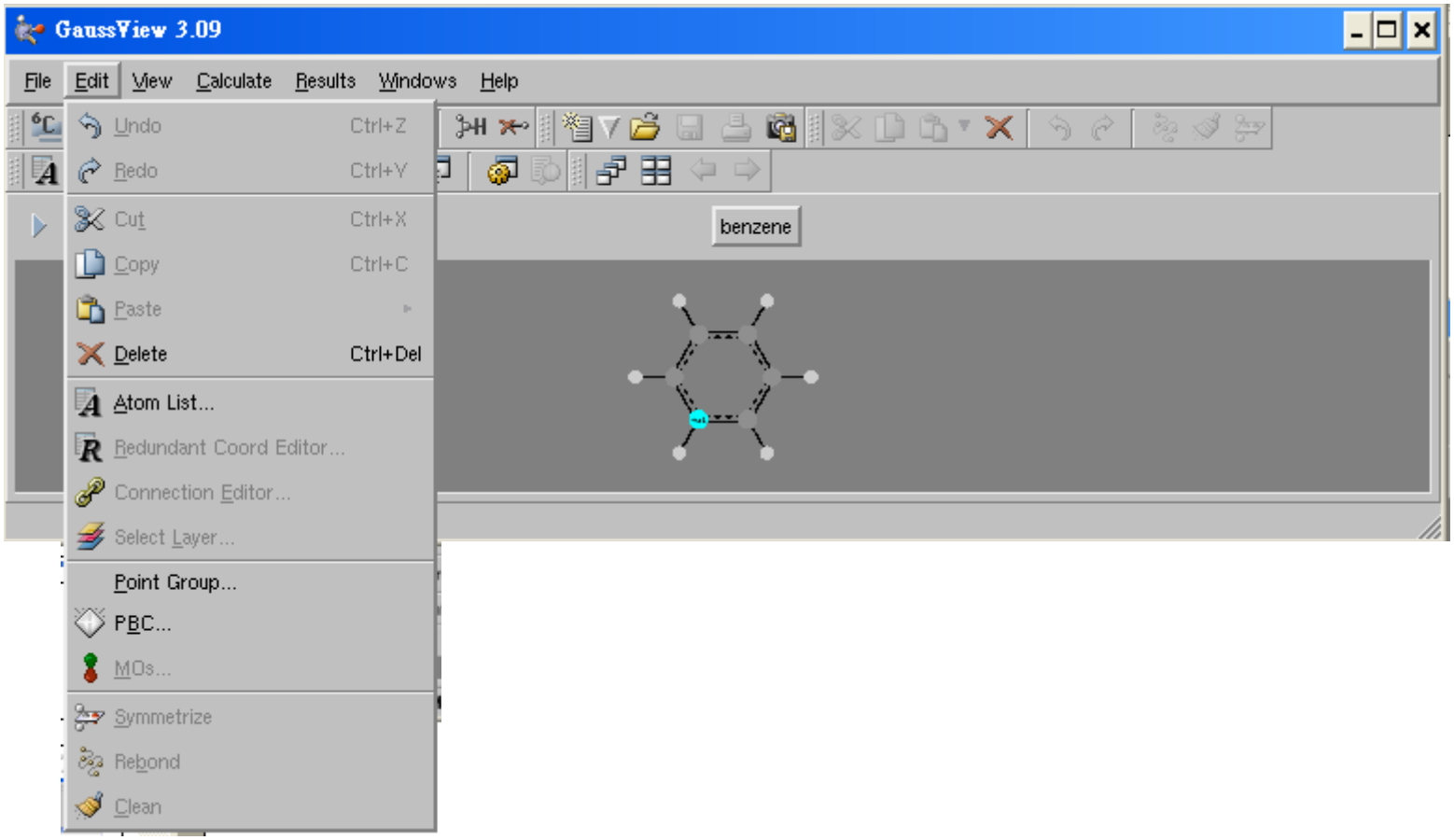
http://www.gaussian.com/tech_top_level.htm

Pull-down menu options:

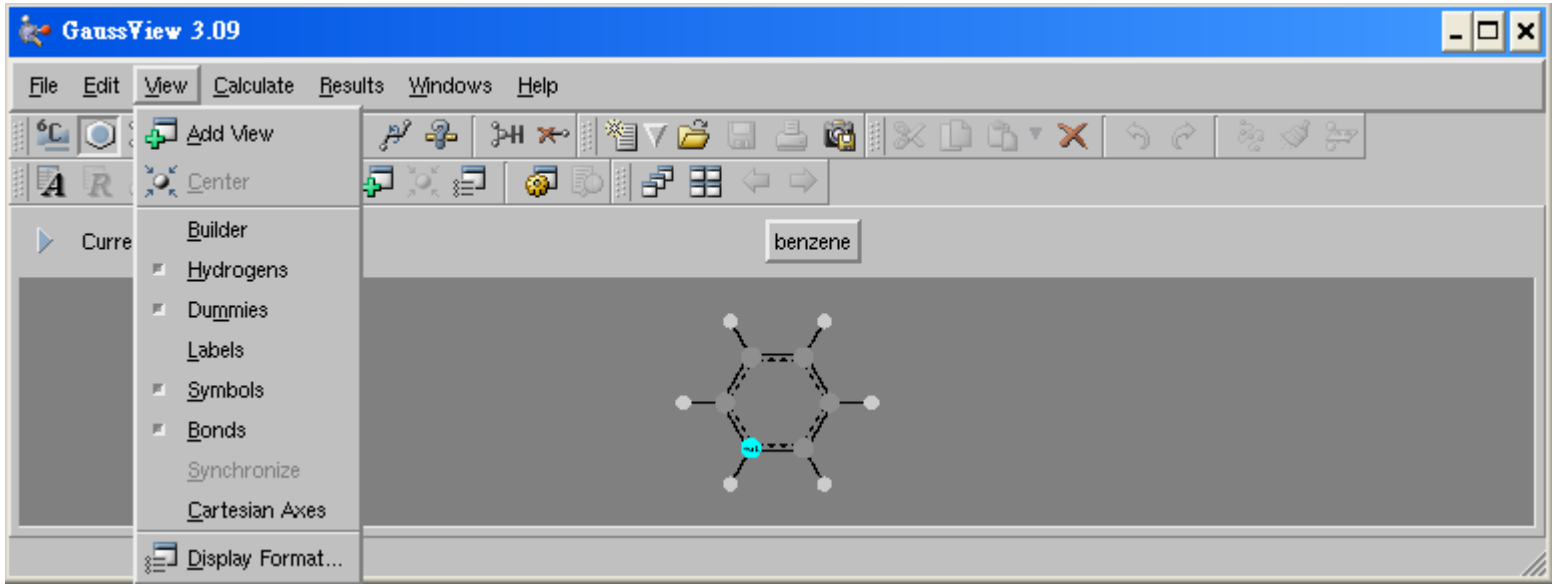
1) File:



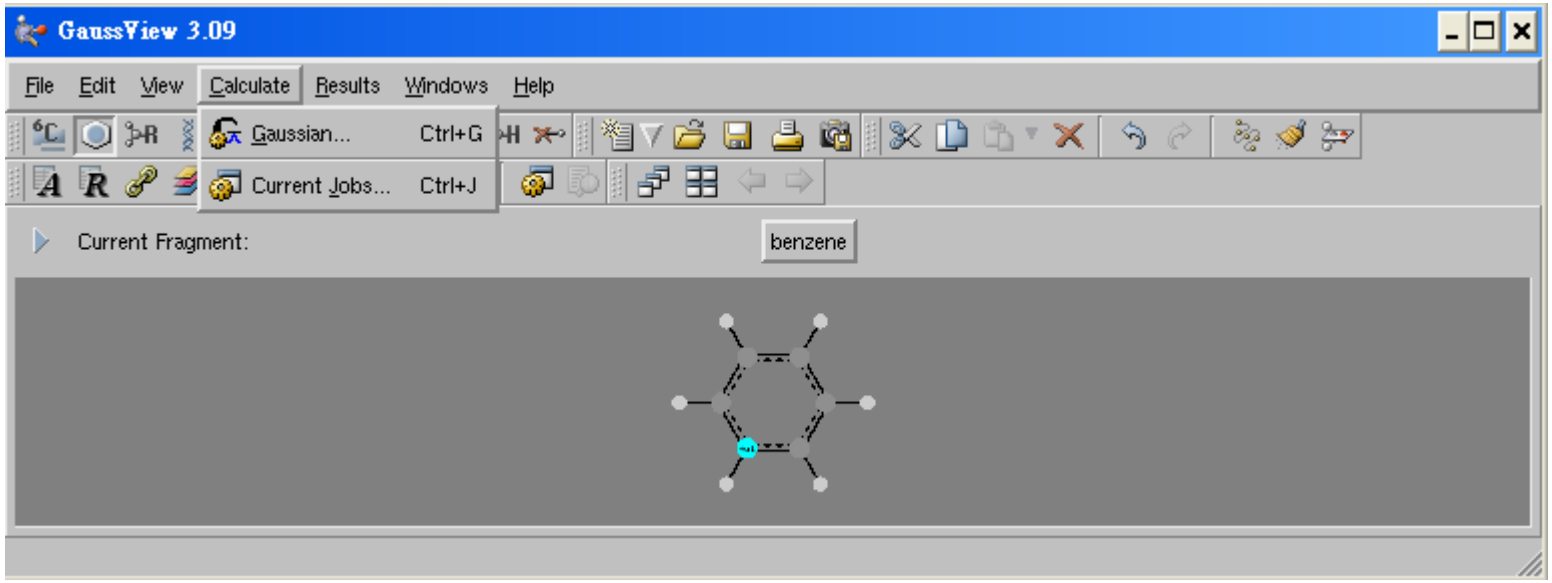
2) Edit:


GaussView 3.09
File
Edit
View
Calculate
Results
Windows
Help
Undo Ctrl+Z
Redo Ctrl+Y
Cut Ctrl+X
Copy Ctrl+C
Paste
Delete Ctrl+Del
Atom List...
Redundant Coord Editor...
Connection Editor...
Select Layer...
Point Group...
PBC...
MOs...
Symmetrize
Rebond
Clean
benzene

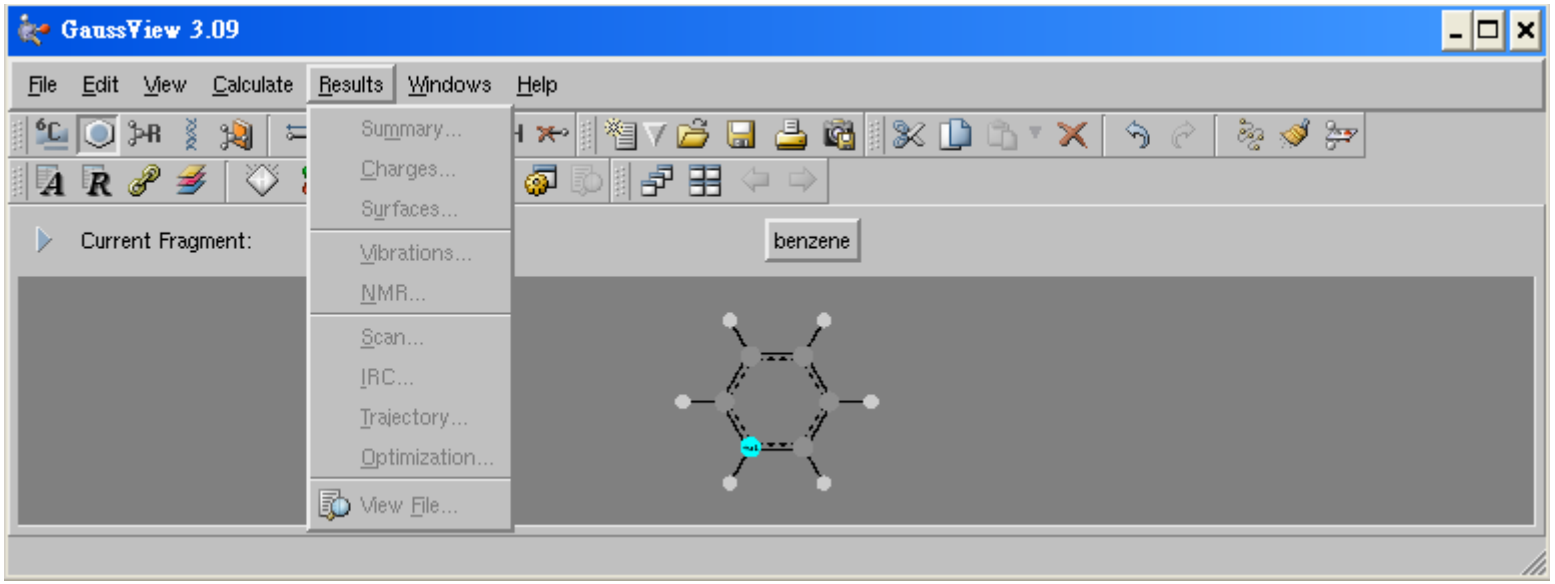
3) View:



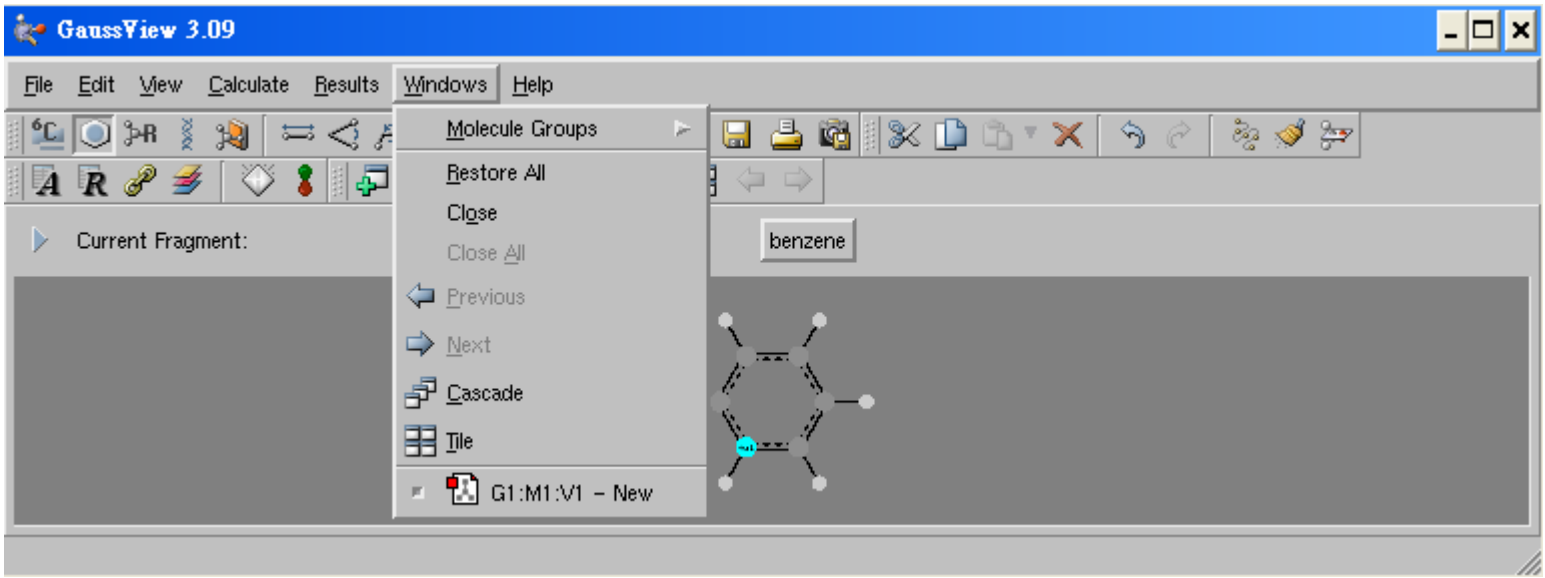
4) Calculate:



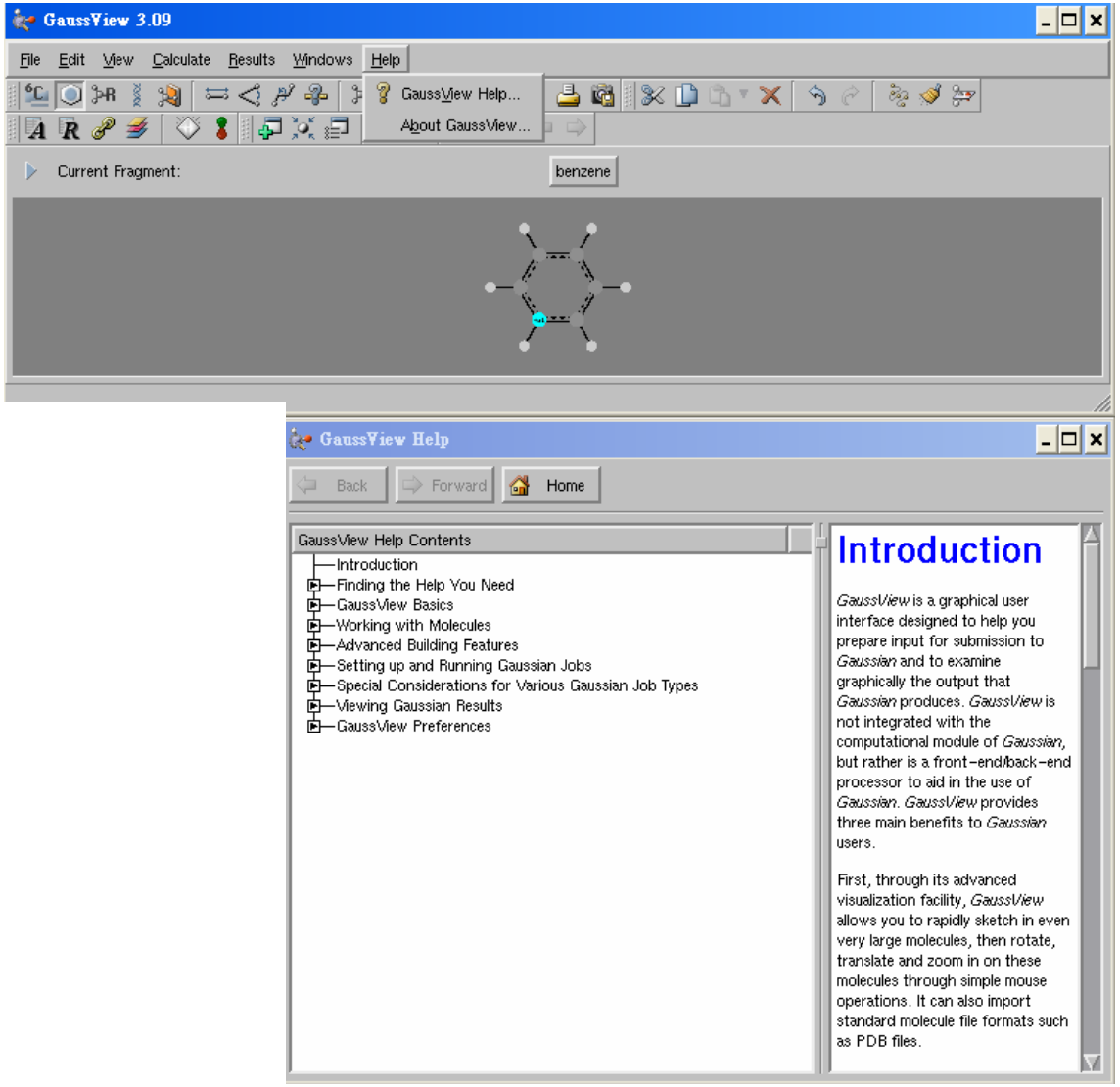
5) Results:



6) Windows:

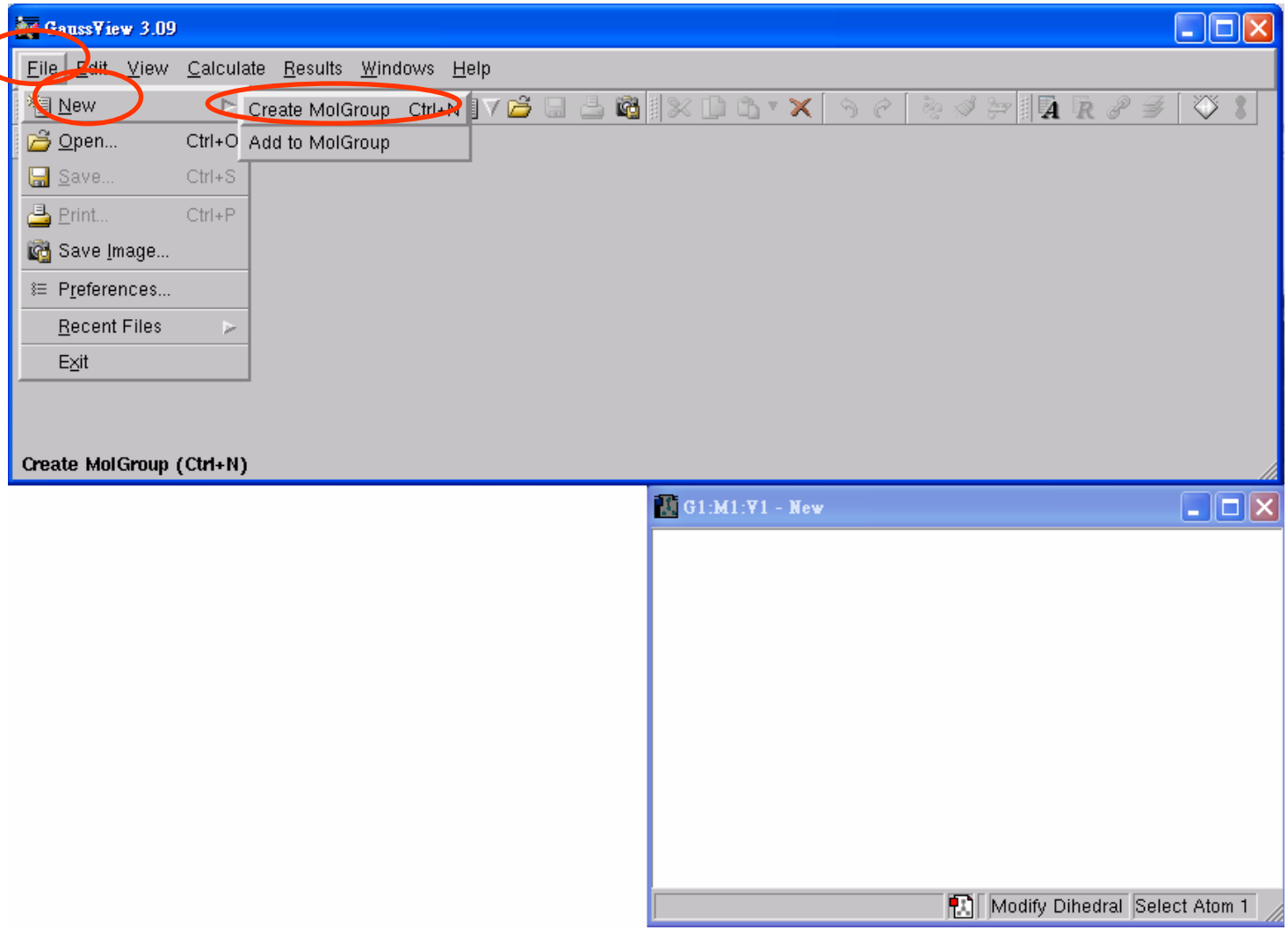


7) Help:


GaussView 3.09
File Edit View Calculate Results Windows Help
GaussView Help...
About GaussView...
Current Fragment:
benzene
GaussView Help
Back Forward Home
GaussView Help Contents
Introduction
Finding the Help You Need
GaussView Basics
Working with Molecules
Advanced Building Features
Setting up and Running Gaussian Jobs
Special Considerations for Various Gaussian Job Types
Viewing Gaussian Results
GaussView Preferences
Introduction
GaussView is a graphical user interface designed to help you prepare input for submission to Gaussian and to examine graphically the output that Gaussian produces. GaussView is not integrated with the computational module of Gaussian, but rather is a front-end/back-end processor to aid in the use of Gaussian. GaussView provides three main benefits to Gaussian users.
First, through its advanced visualization facility, GaussView allows you to rapidly sketch in even very large molecules, then rotate, translate and zoom in on these molecules through simple mouse operations. It can also import standard molecule file formats such as PDB files.

Step1 : Coarse Optimization

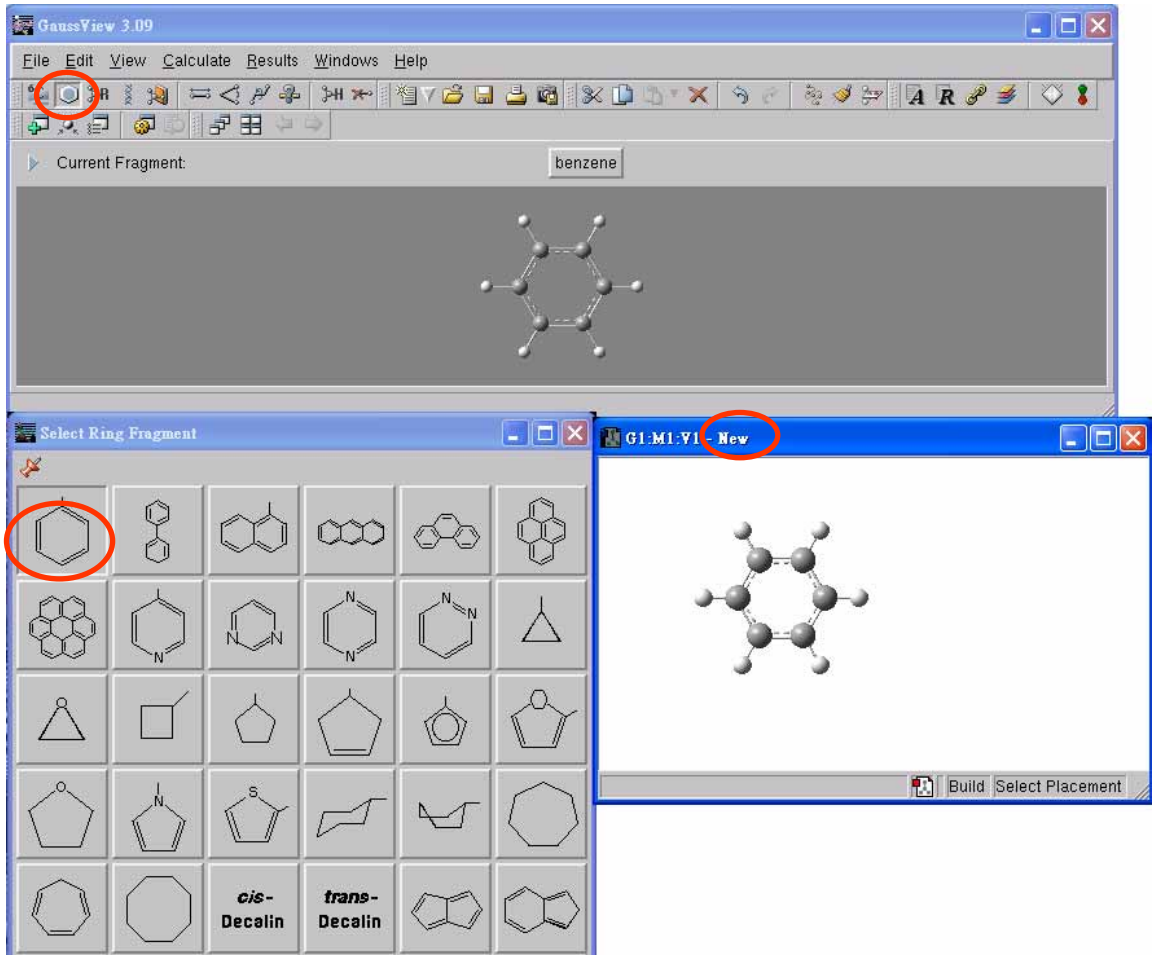
Open new file → File → New → Create MolGroup



Create Molecule : CN-PPV

Double Click at Ring Fragment →

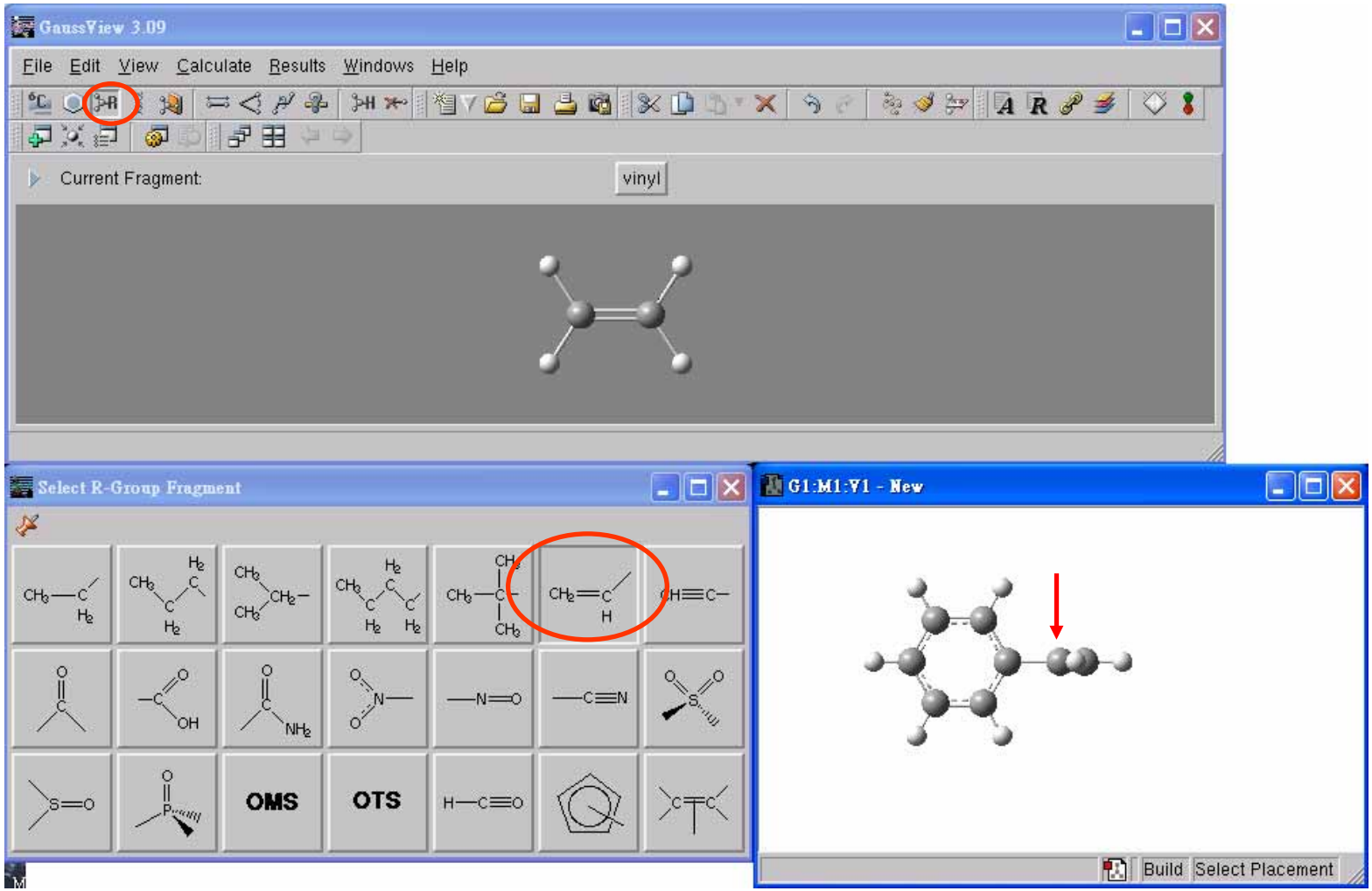
Select Benzene →Click at new window



Create Molecule : CN-PPV

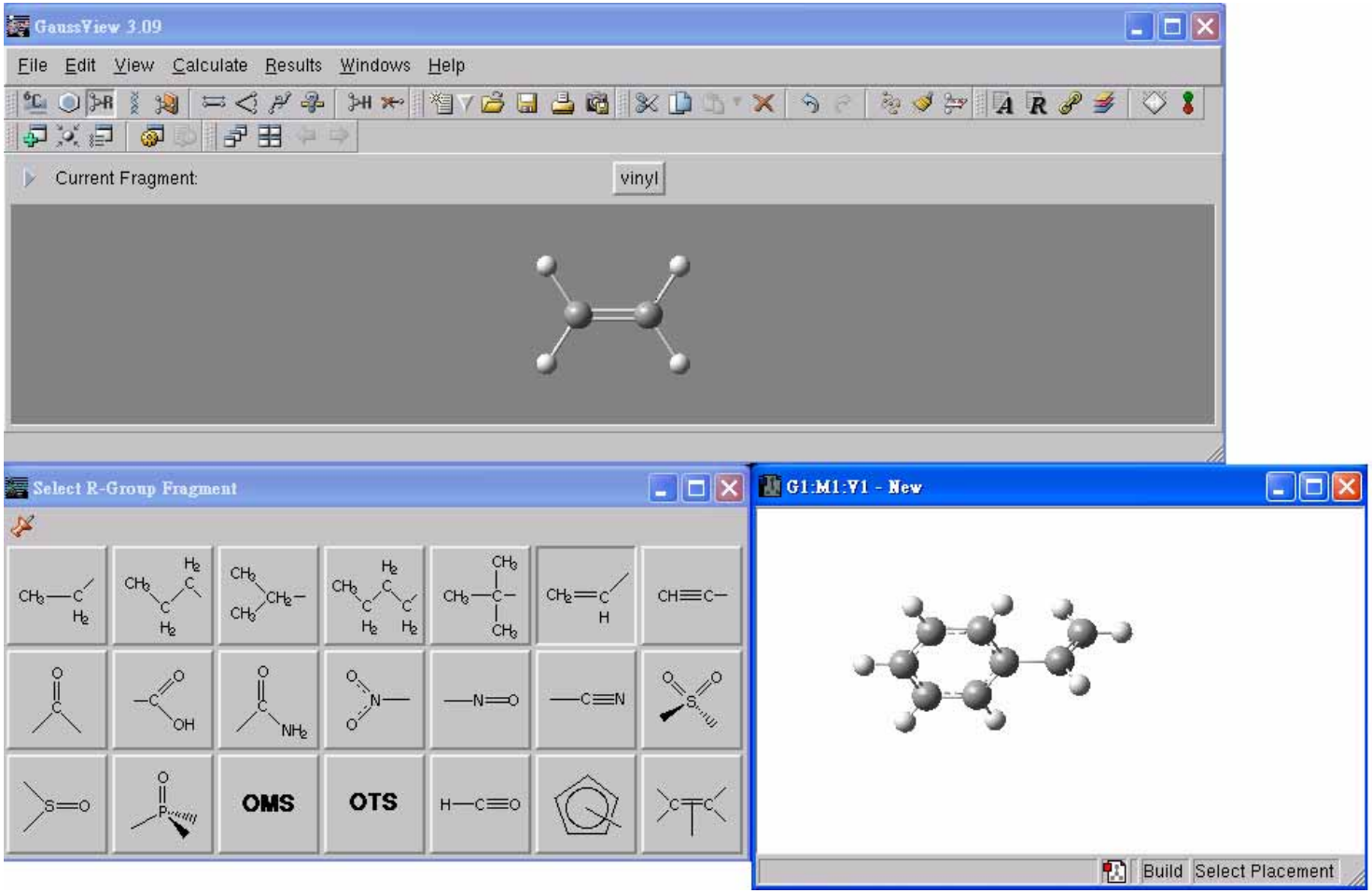
Double Click at R-Group Fragment →

Select vinyl →Click at H atom



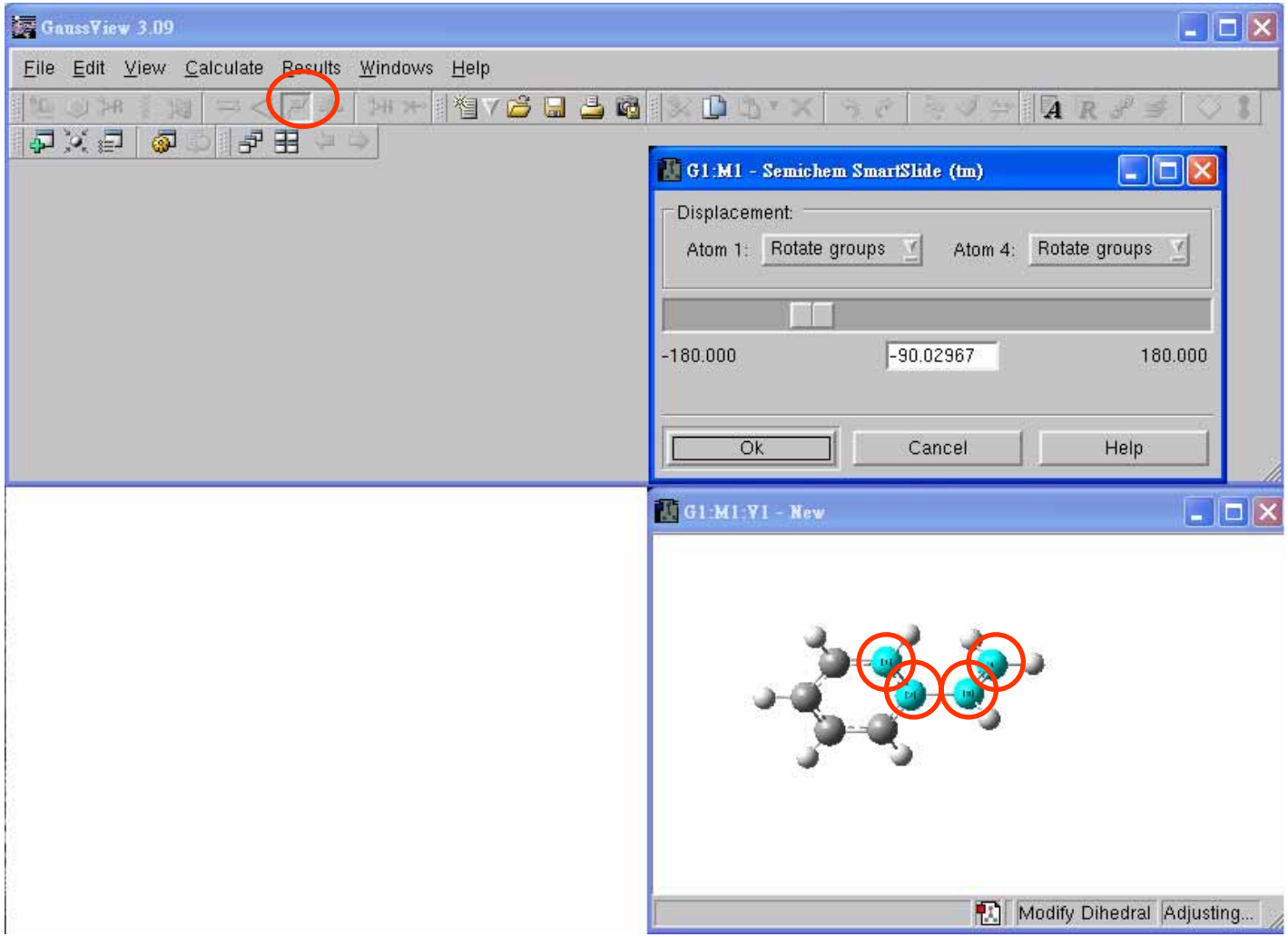
Rotate the molecule

Rotate the molecule using left button



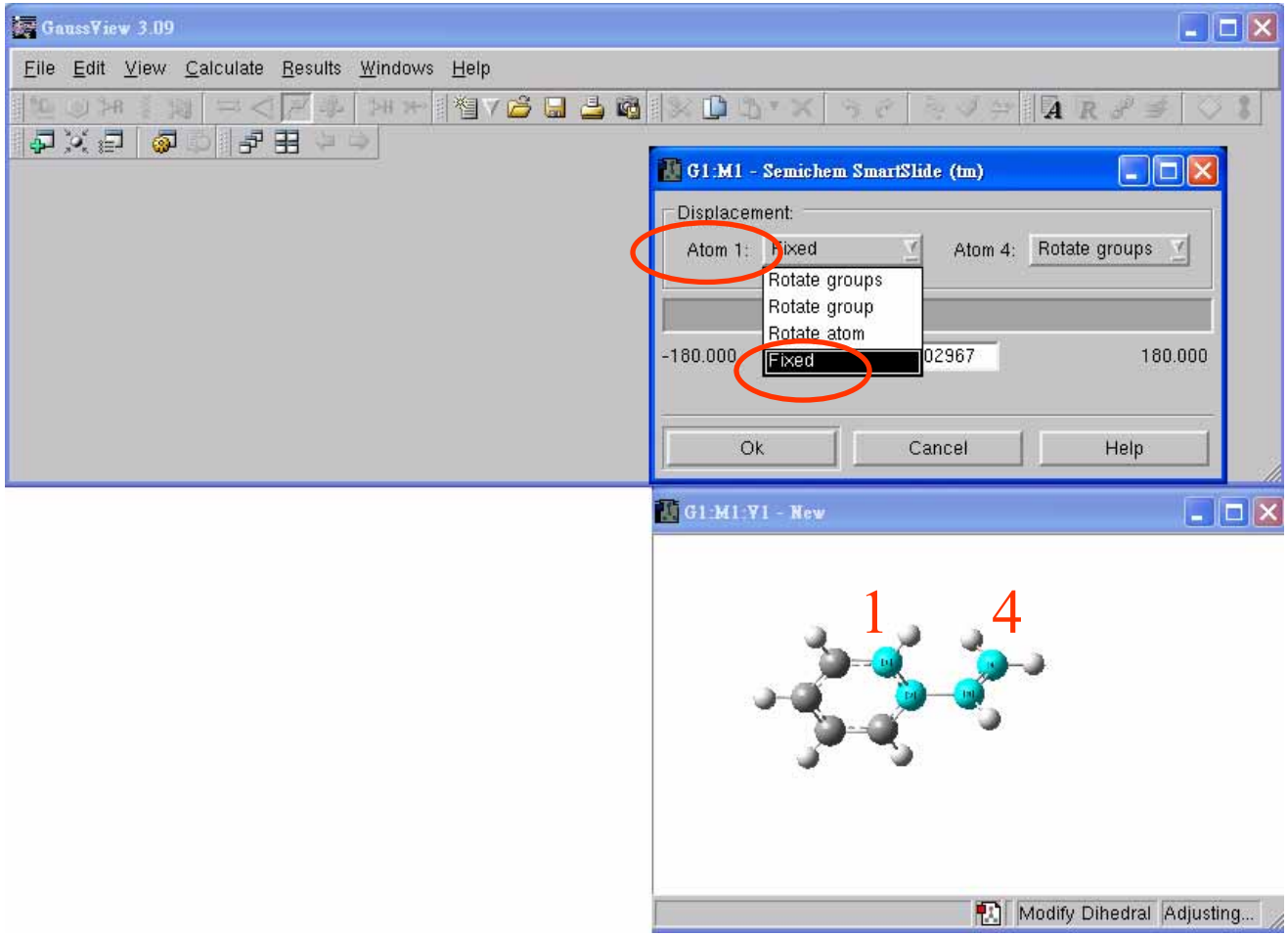
Modify Dihedral Angle

Click Modify dihedral → Select atoms



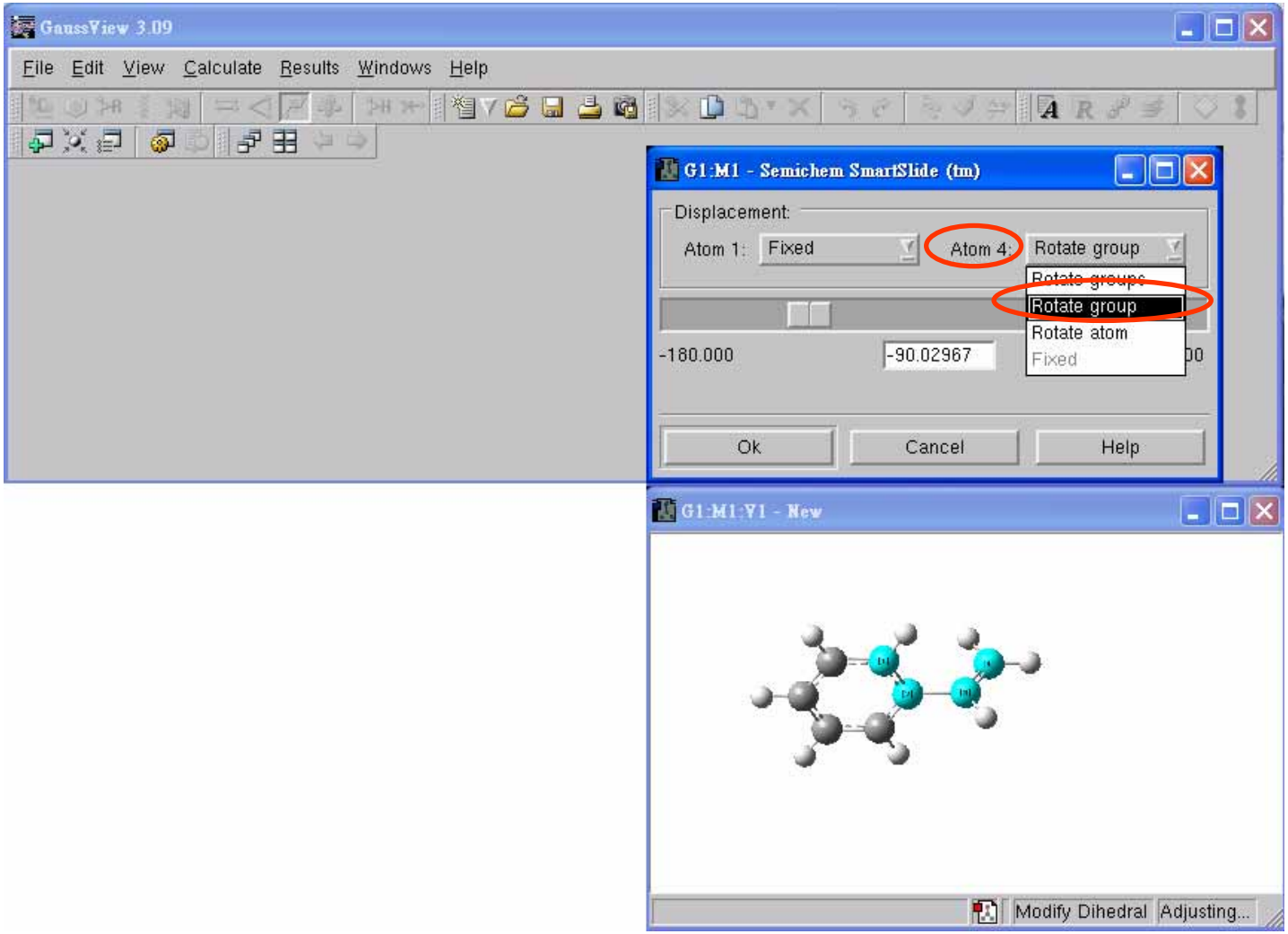
Coplanrity

Fixed atom1



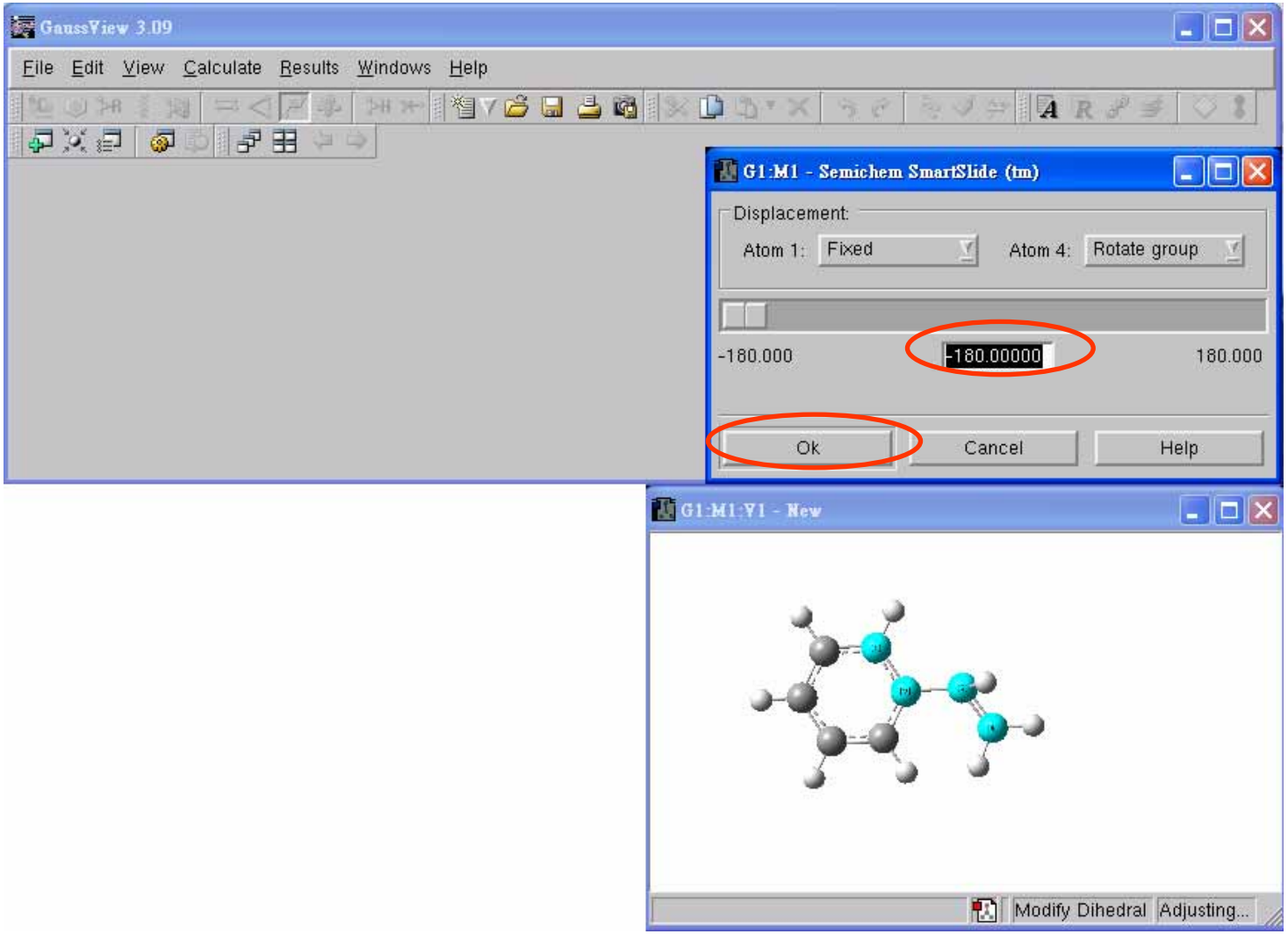
Coplanrity

Rotate atom4 → select Rotate group

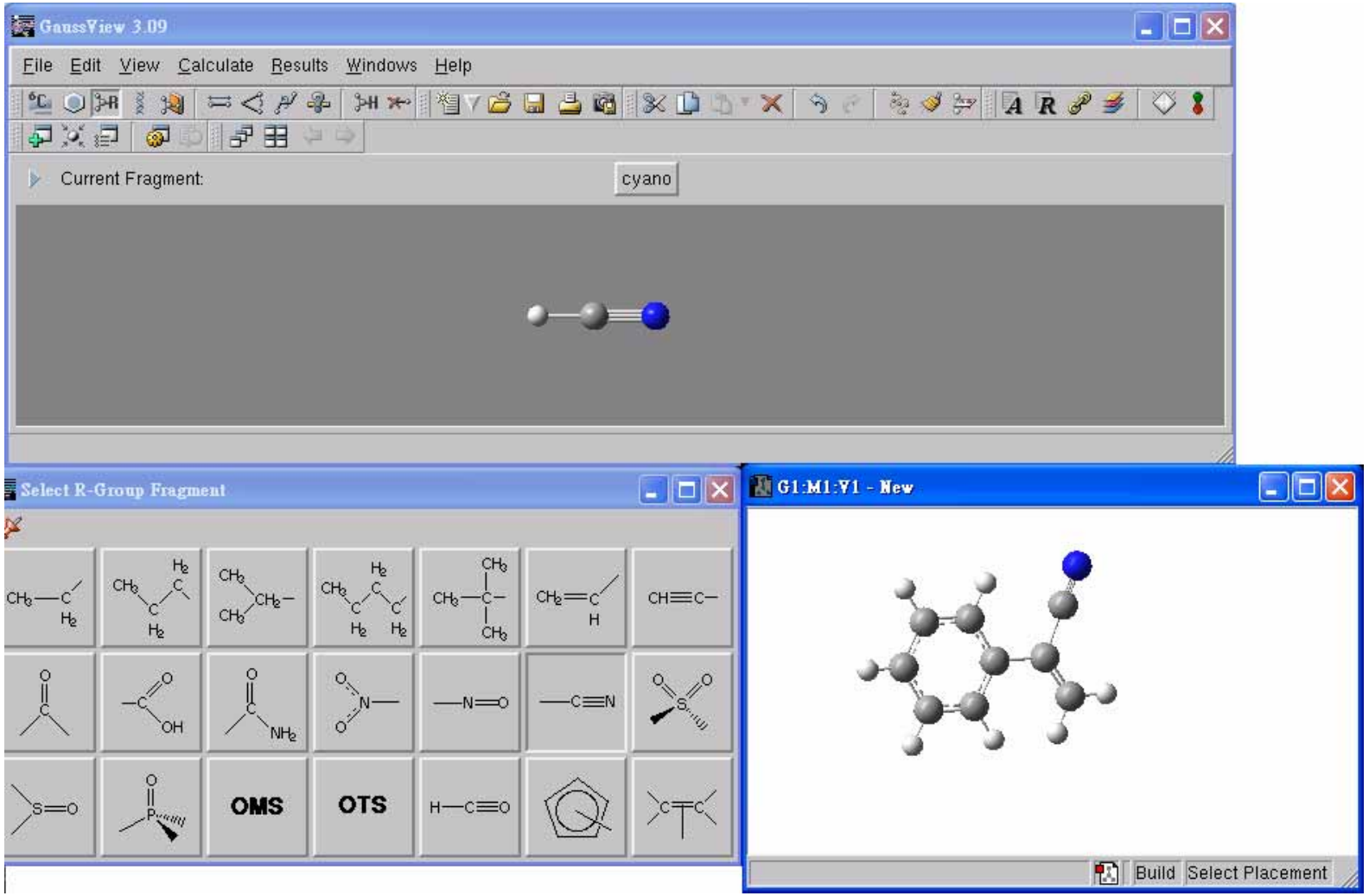


Coplanrity

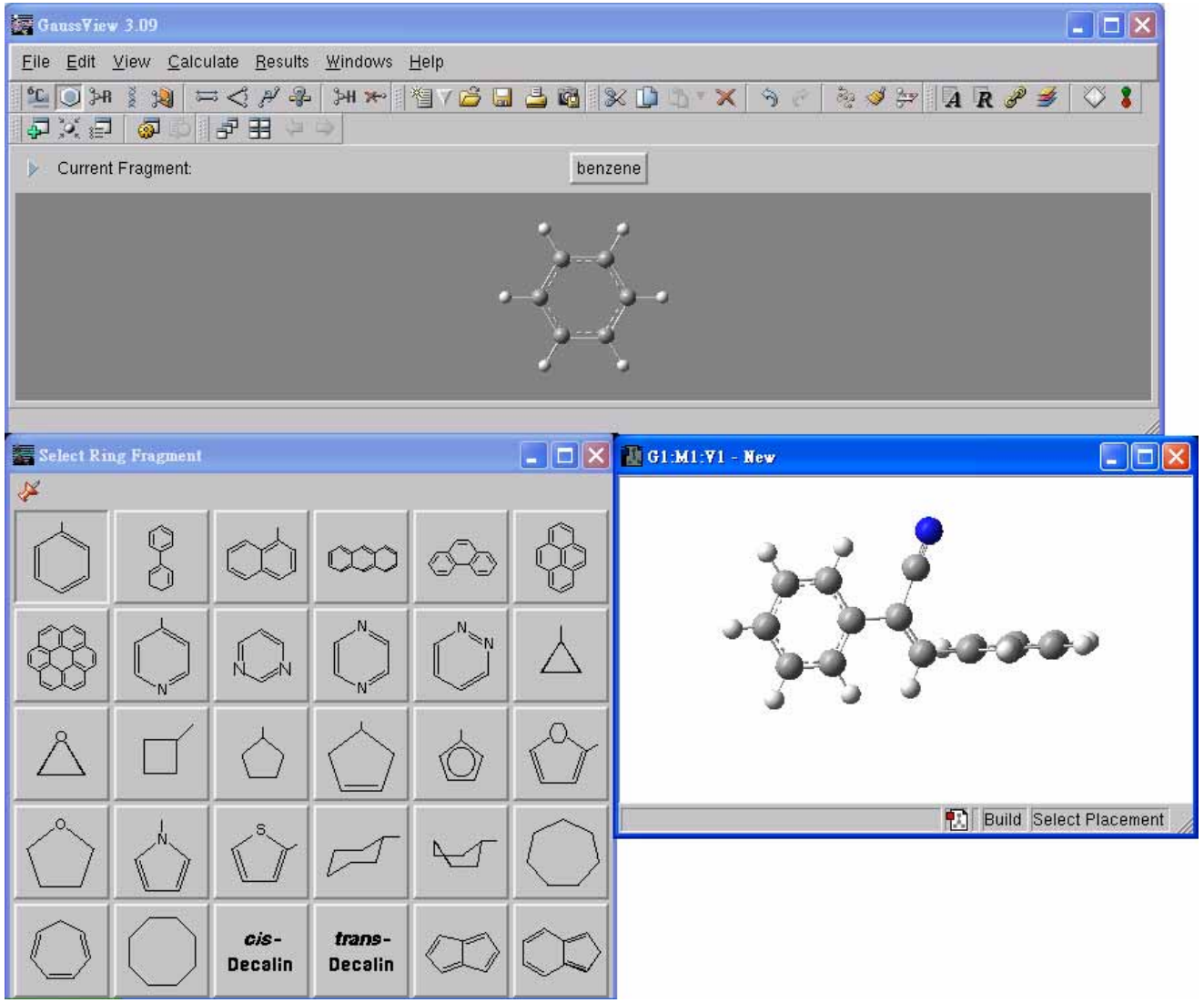
Key in the angle → Click OK



Add CN group

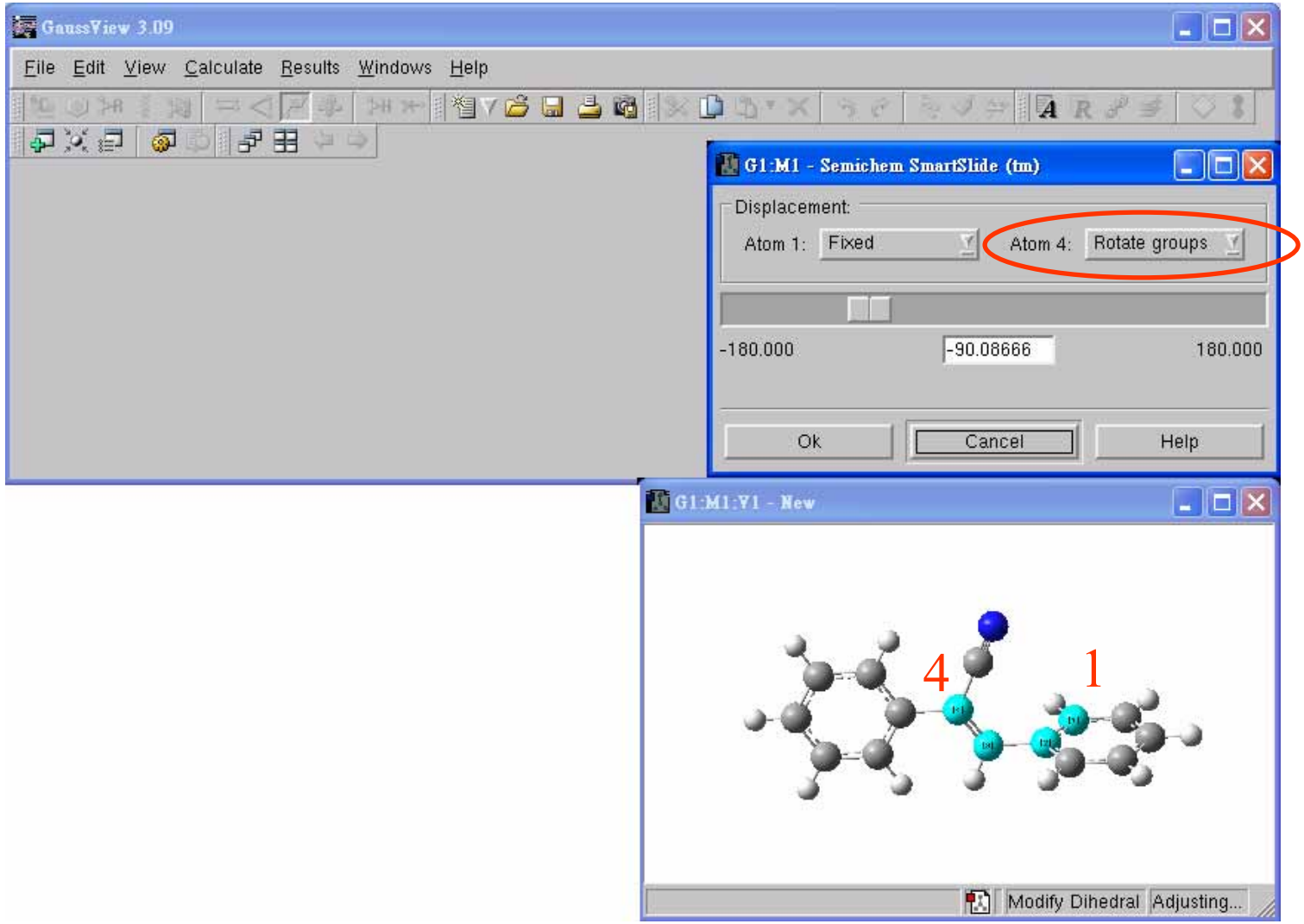

GaussView 3.09
File Edit View Calculate Results Windows Help
Current Fragment:
cyano
Select R-Group Fragment
OMS
OTS
G1:M1:V1 - New
Build
Select Placement

Add Benzene

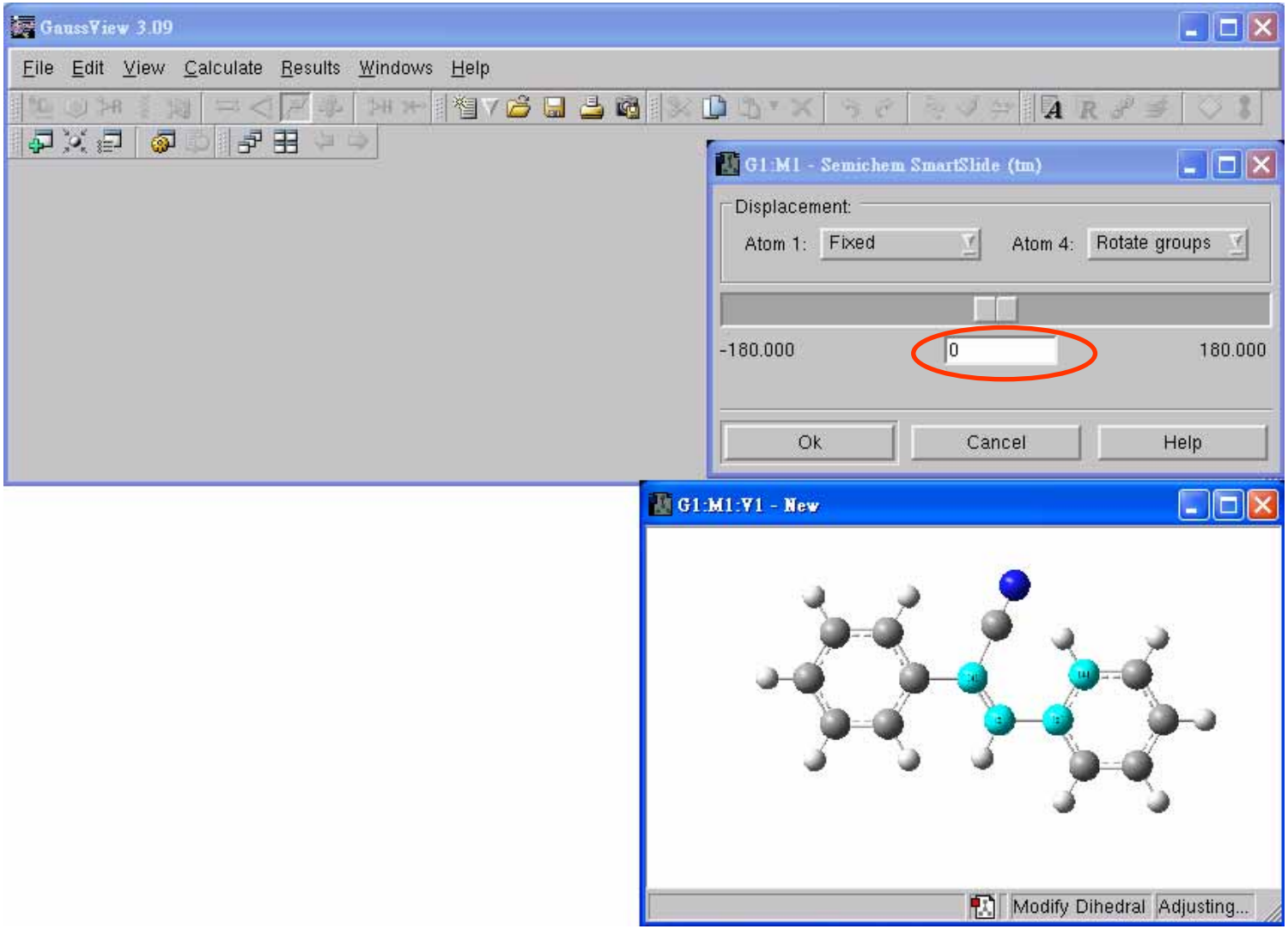

GaussView 3.09
File Edit View Calculate Results Windows Help
Current Fragment:
benzene
Select Ring Fragment
cis-
Decalin
trans-
Decalin
G1:M1:V1 - New
Build
Select Placement

Rotate Benzene

Atom4 → Select Groups

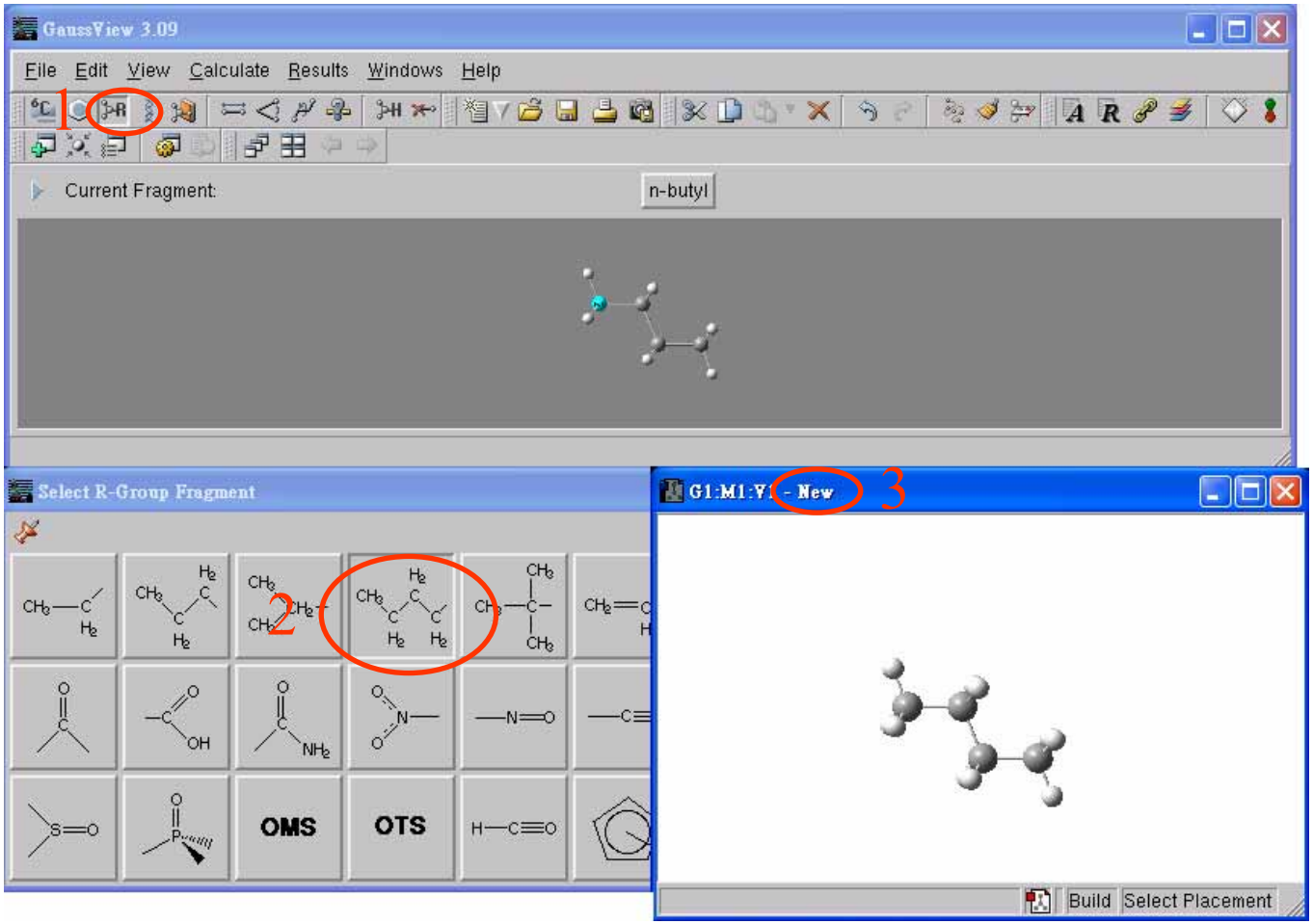


Key in the angle



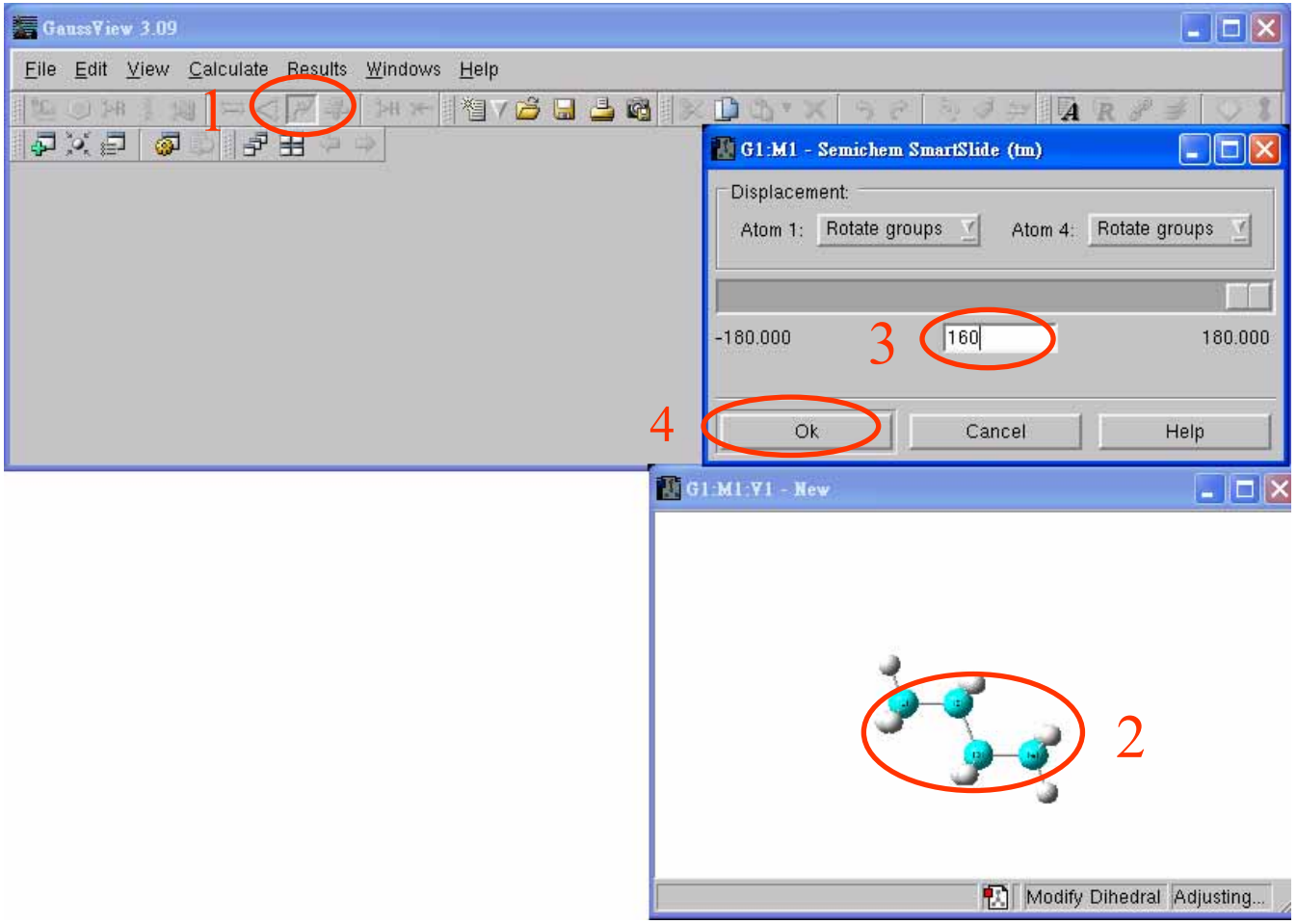
Mechanics Minimization

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



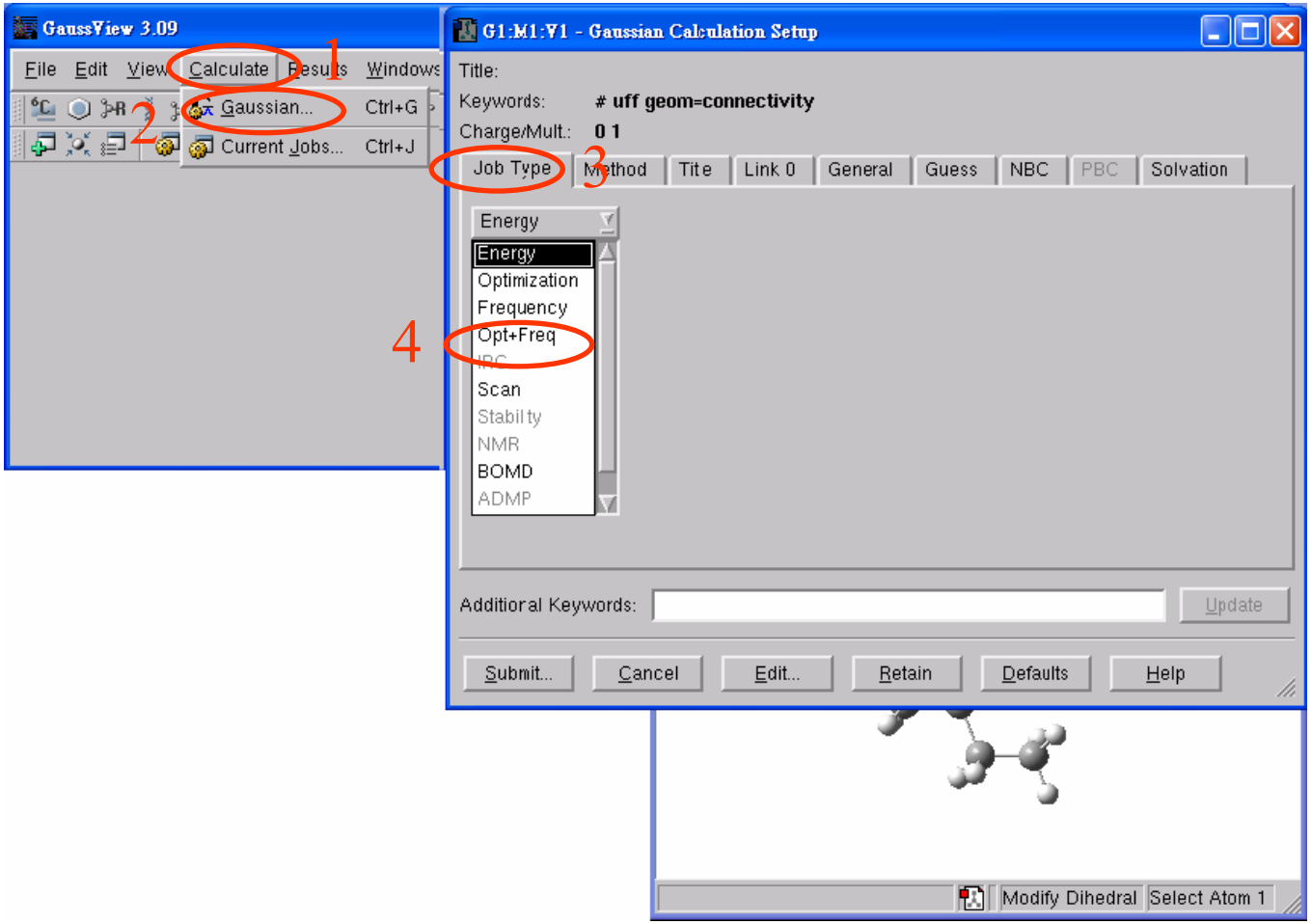
Modify dihedral angle

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



Minimization

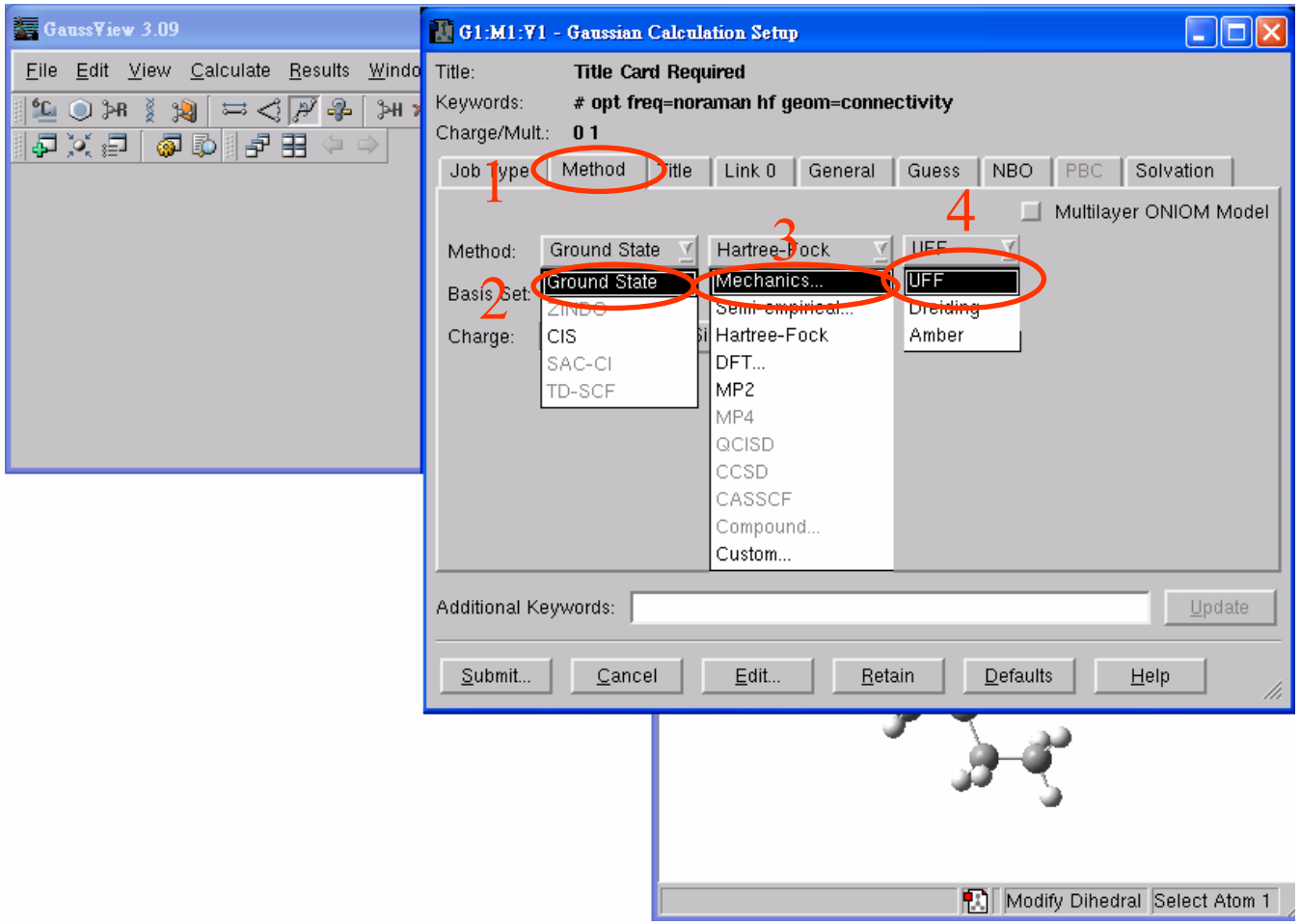
Click Calculate → Select Gaussian →
Click Job Type → Select Opt + Freq



Method

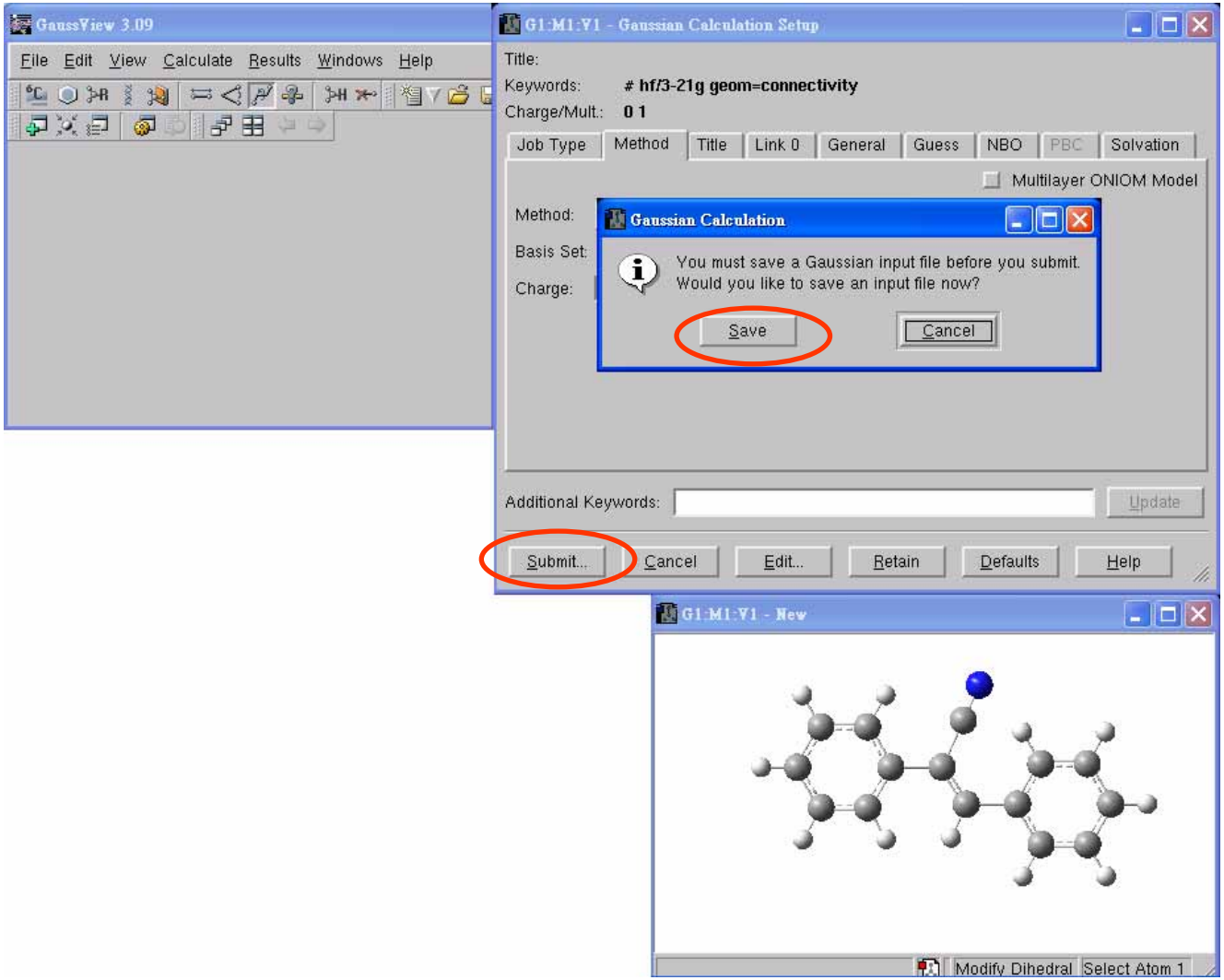
Click Method → Select Ground State →

Select Mechanics → Select Force Field



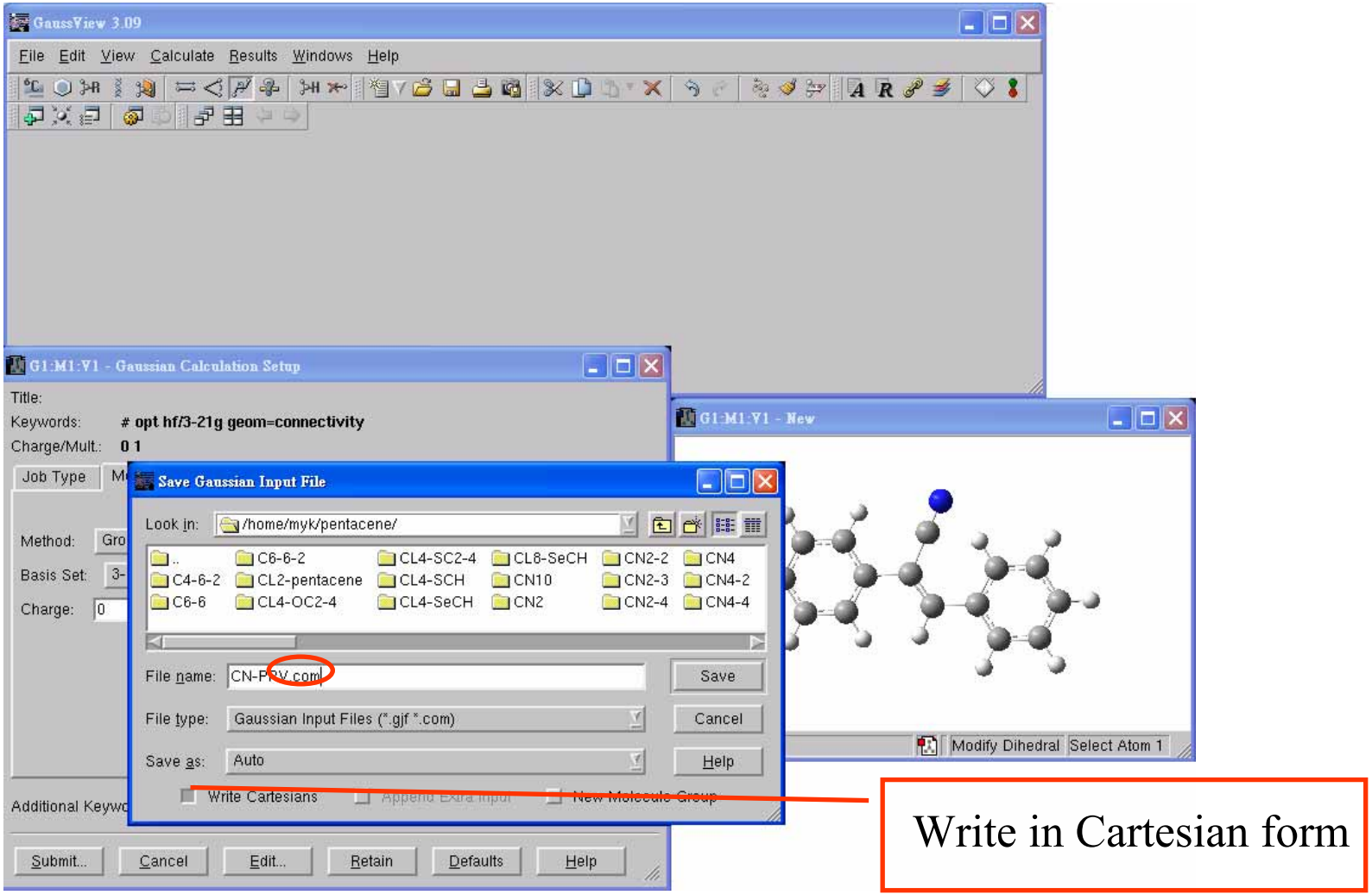
Submit the job

Click Submit → Save the job

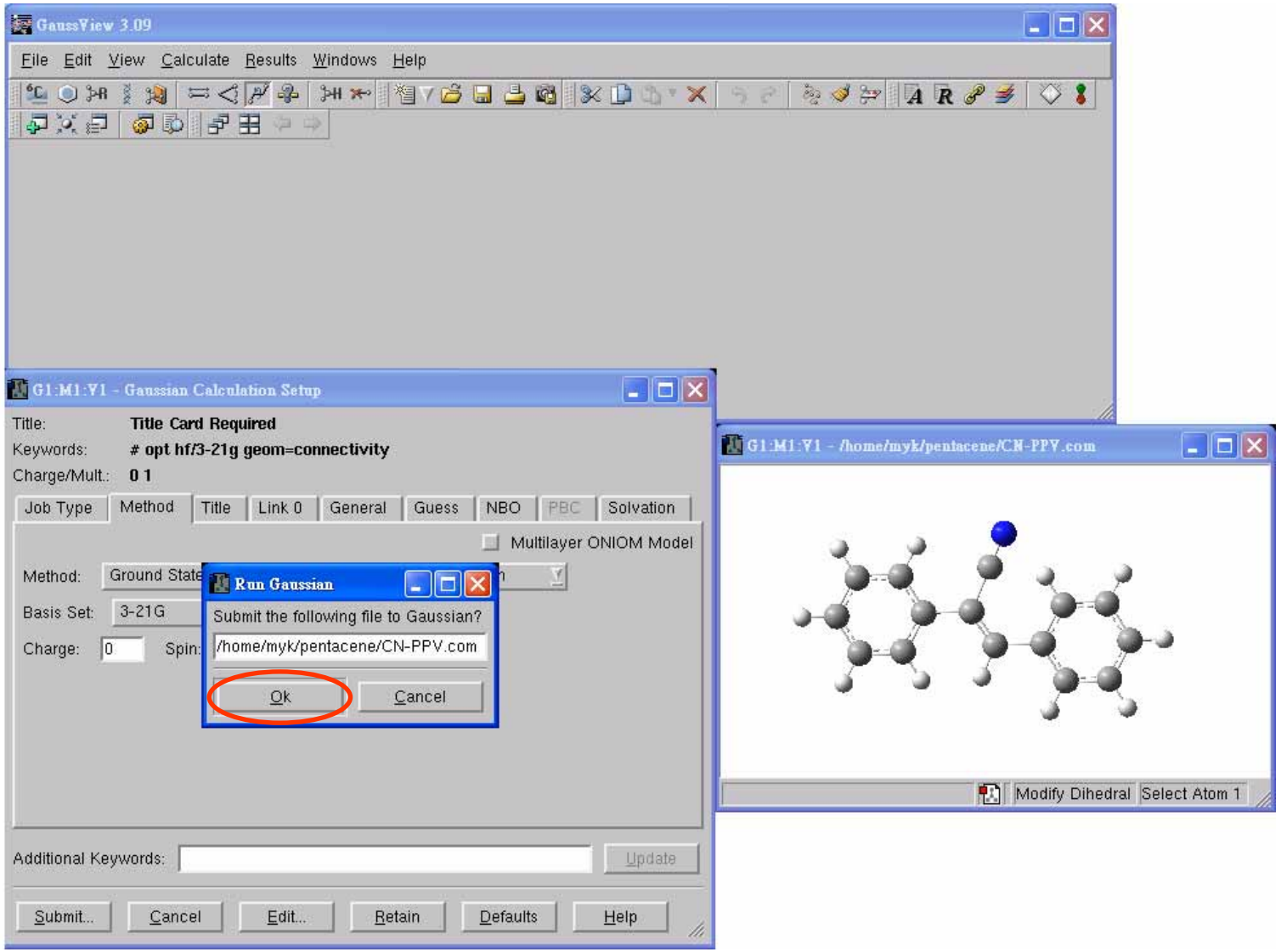


Save the job

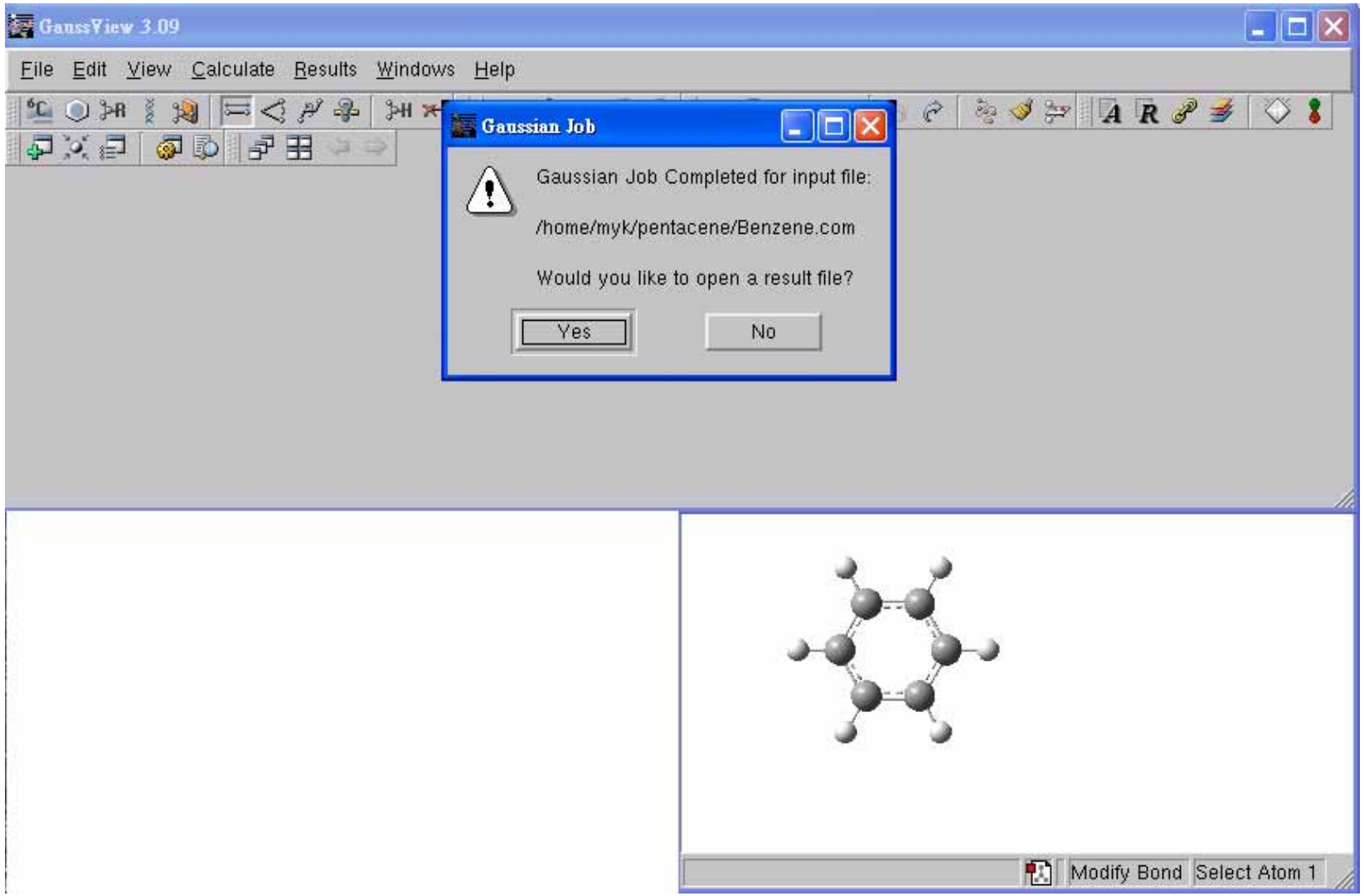
File type *.com



Run the Job


GaussView 3.09
File Edit View Calculate Results Windows Help
G1:M1:V1 - Gaussian Calculation Setup
Title: Title Card Required
Keywords: # opt hf/3-21g geom=connectivity
Charge/Mult.: 0 1
Job Type Method Title Link 0 General Guess NBO PBC Solvation
Multilayer ONIOM Model
Method: Ground State
Basis Set: 3-21G
Charge: 0 Spin:
Run Gaussian
Submit the following file to Gaussian?
/home/myk/pentacene/CN-PPV.com
Ok Cancel
Additional Keywords:
Update
Submit... Cancel Edit... Retain Defaults Help
G1:M1:V1 - /home/myk/pentacene/CN-PPV.com
Modify Dihedral Select Atom 1

Finish Optimization

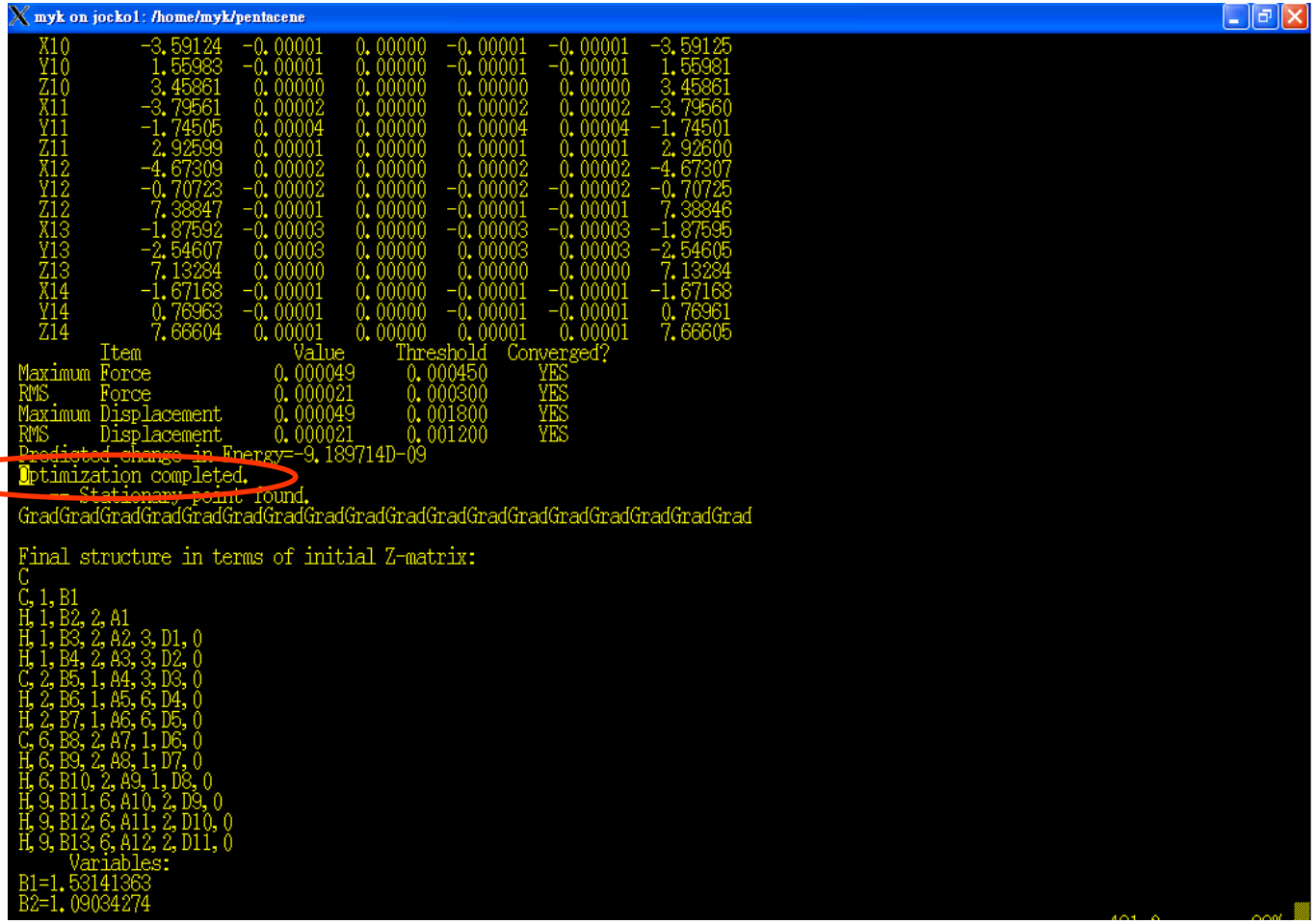


Check output *.log from startxwin

Type vi *.log → Enter

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

Then press Page Up to find the final Geometry



Final geometry

myk on jocko1: /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:

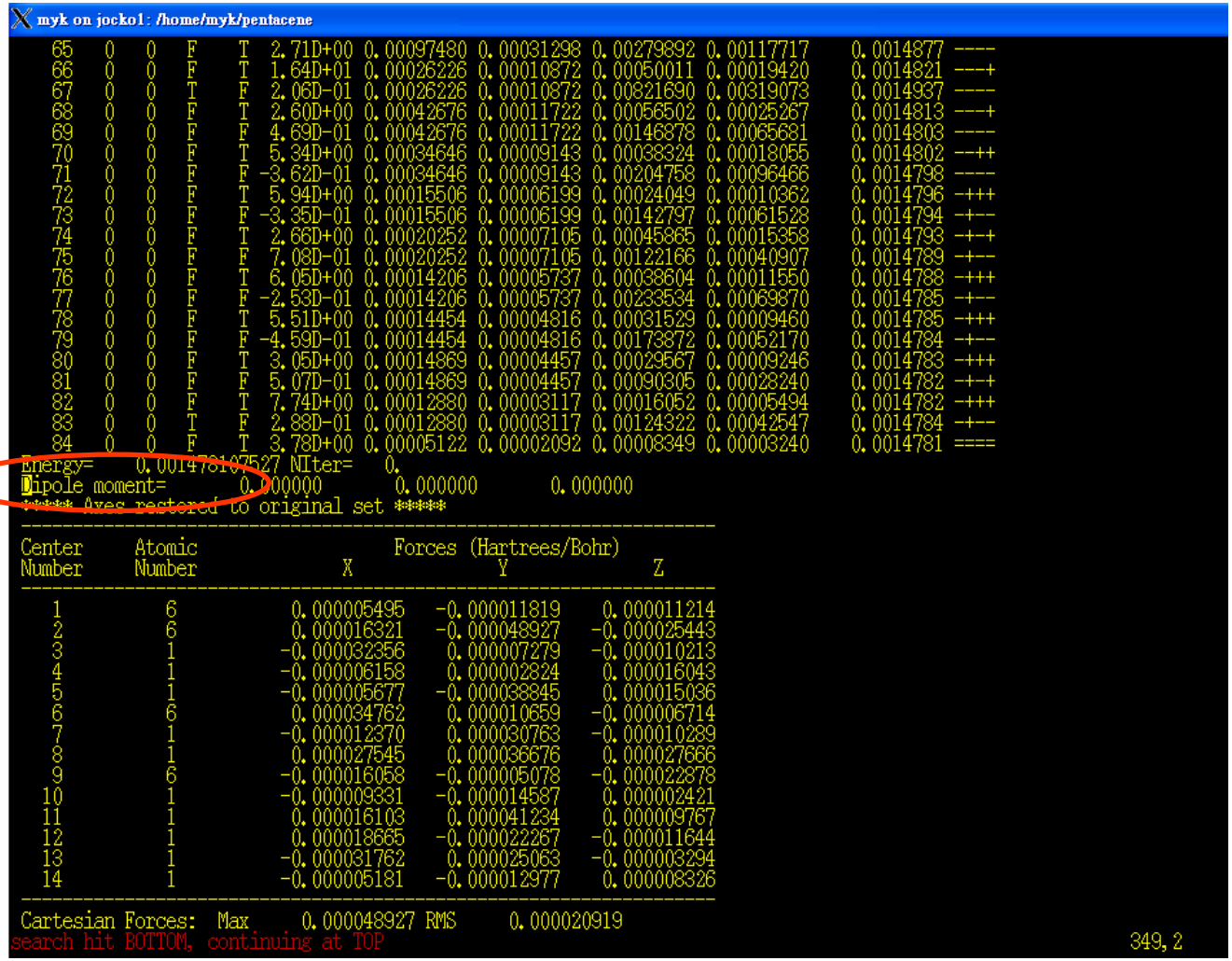
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	20001001	0.000000	0.000000	0.000000
2	6	20001001	0.000000	0.000000	1.506718
3	1	20001034	1.046893	0.000000	-0.388611
4	1	20001034	-0.522633	-0.904842	-0.394513
5	1	20001034	-0.522499	0.904976	-0.394435
6	6	20001001	-1.407851	0.000178	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

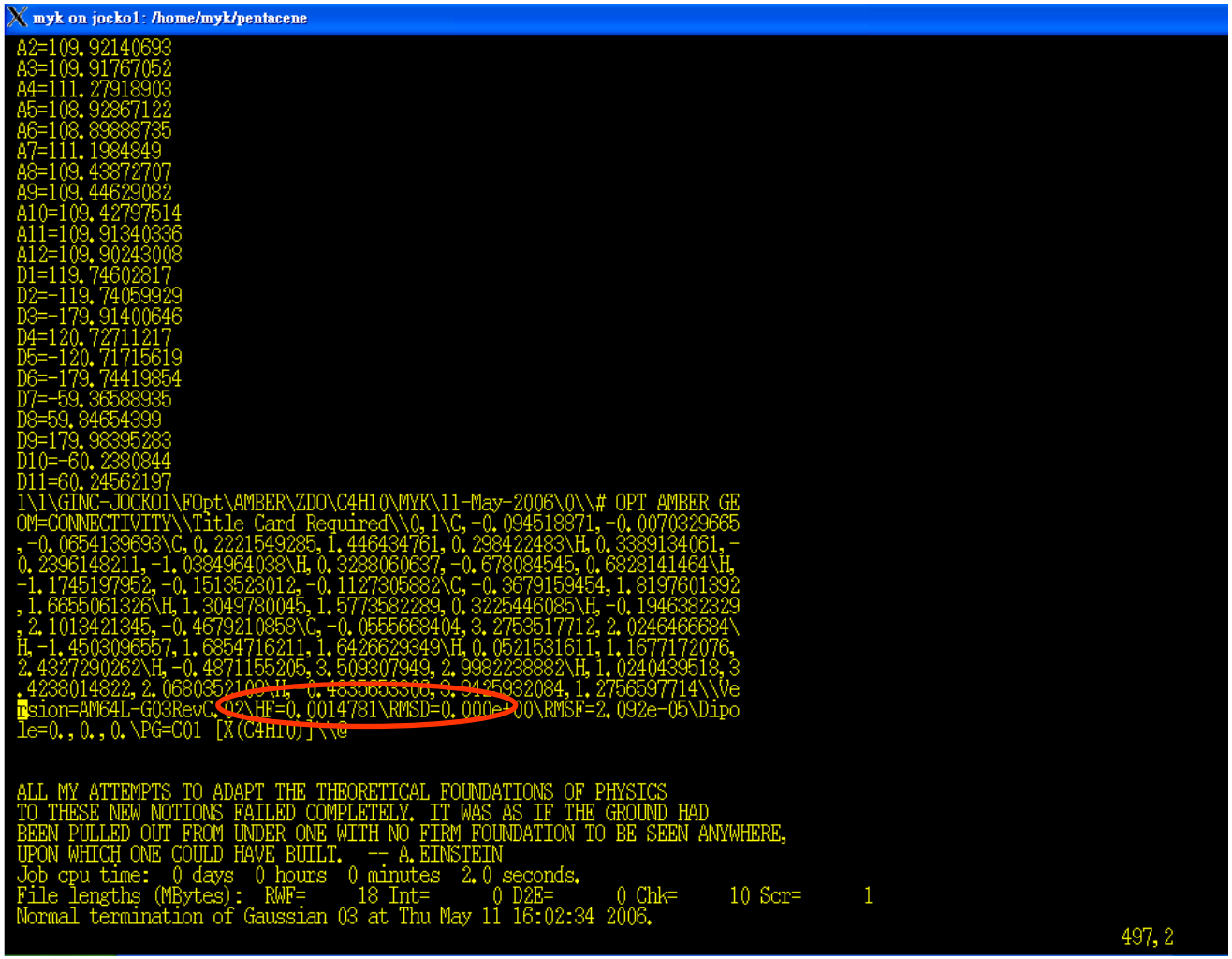
Dipole moment

Press Esc → type :/Dipole → Enter



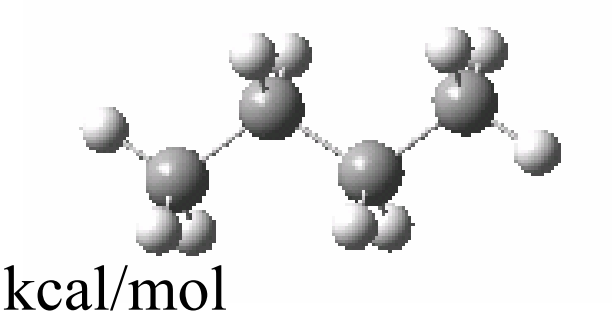
Energy

Press Esc → type :/HF= → Enter



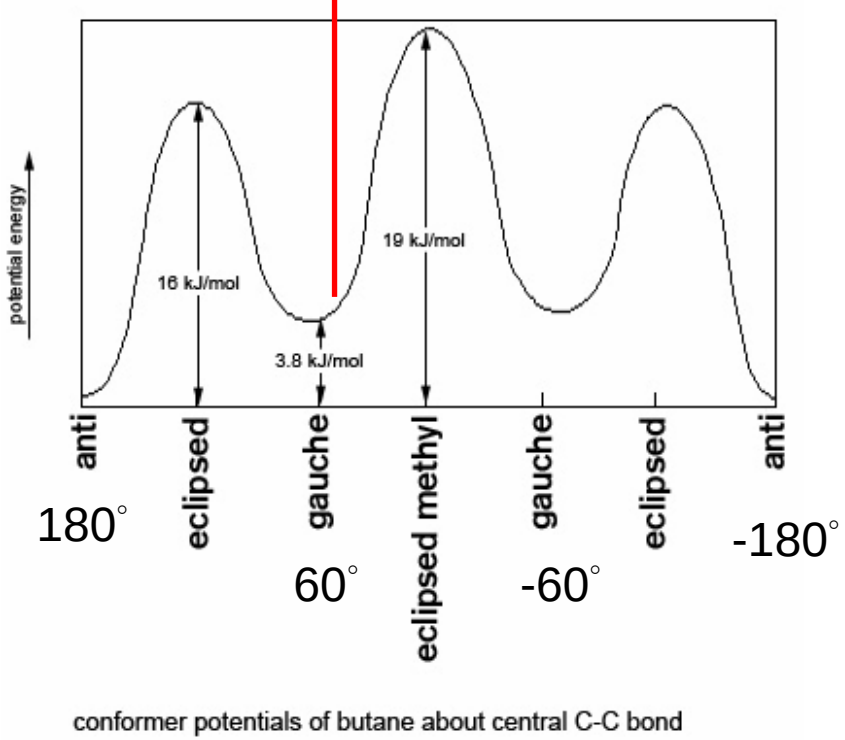
Different Force Field

UFF 4.81
Dreiding 3.05
Amber 3.01



1 Hartree = 627.50956 kcal/mol

1 cal = 4.18 J



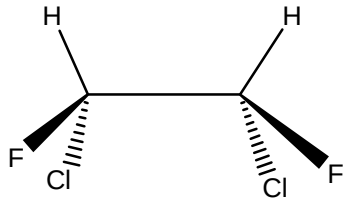
conformer potentials of butane about central C-C bond

Torsion Angle

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

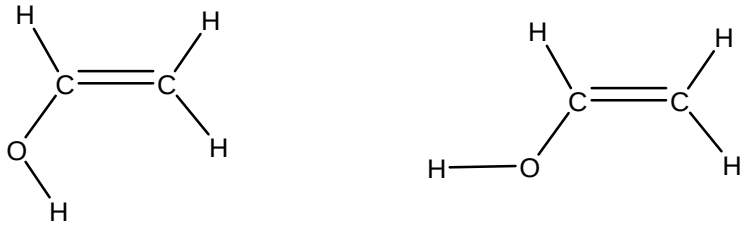
Exercises:

1) Build molecule 1 and manipulate to different stereoisomers.



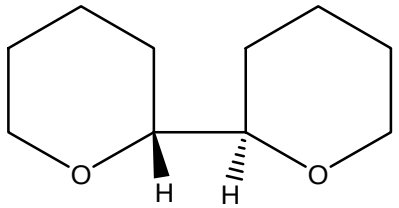
1

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



2

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



3

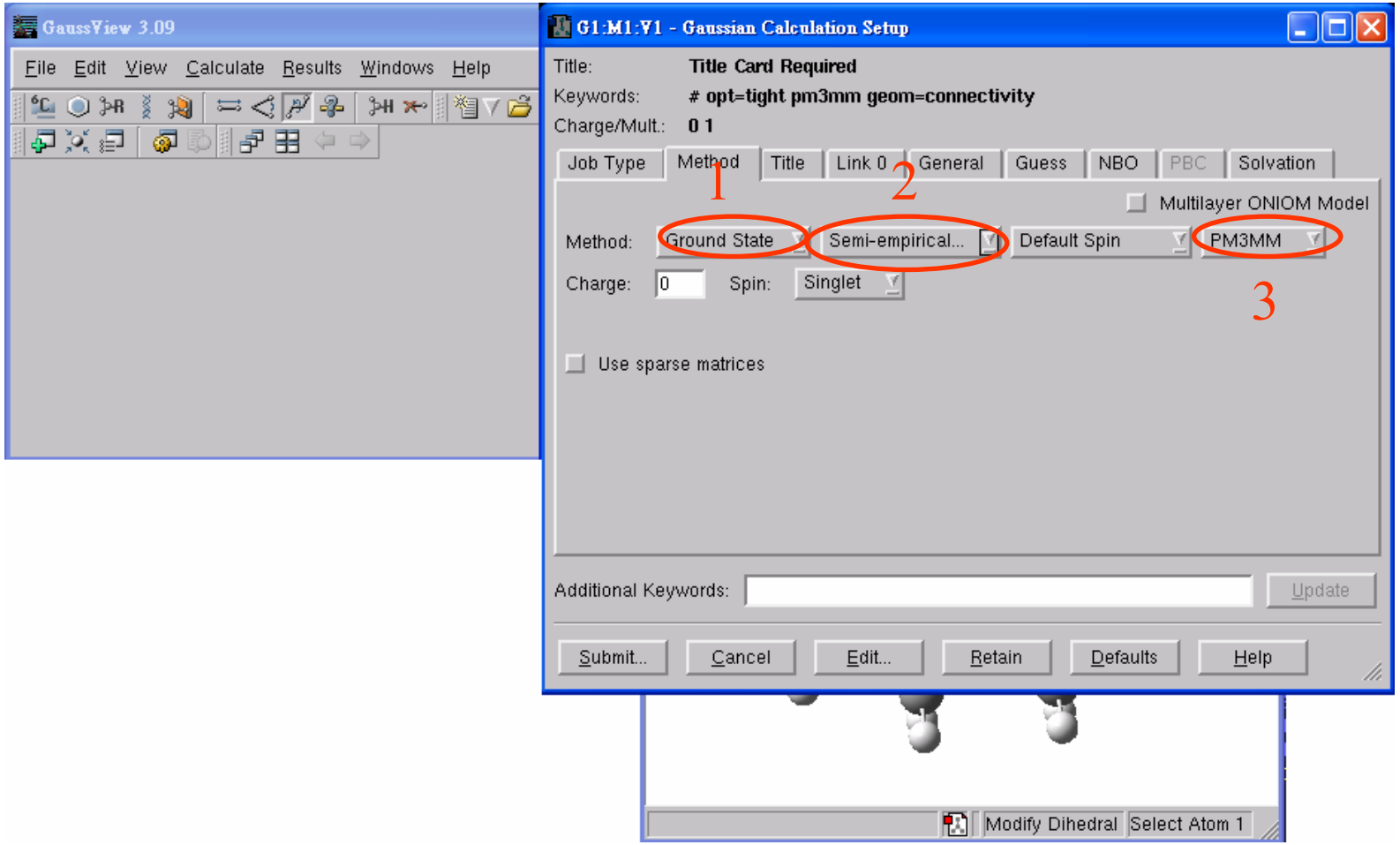
4) Conformational Search:

Build a butane molecule (CH_3-CH_2-CH_2-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.

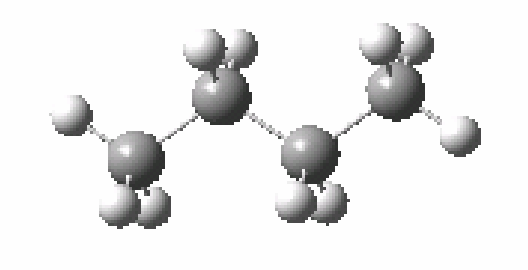
5) Build a water dimer, and try to manipulate them at different binding orientations.

Semi-empirical Optimization

Select Group State → Select Semi-empirical → Select Method



Different Method

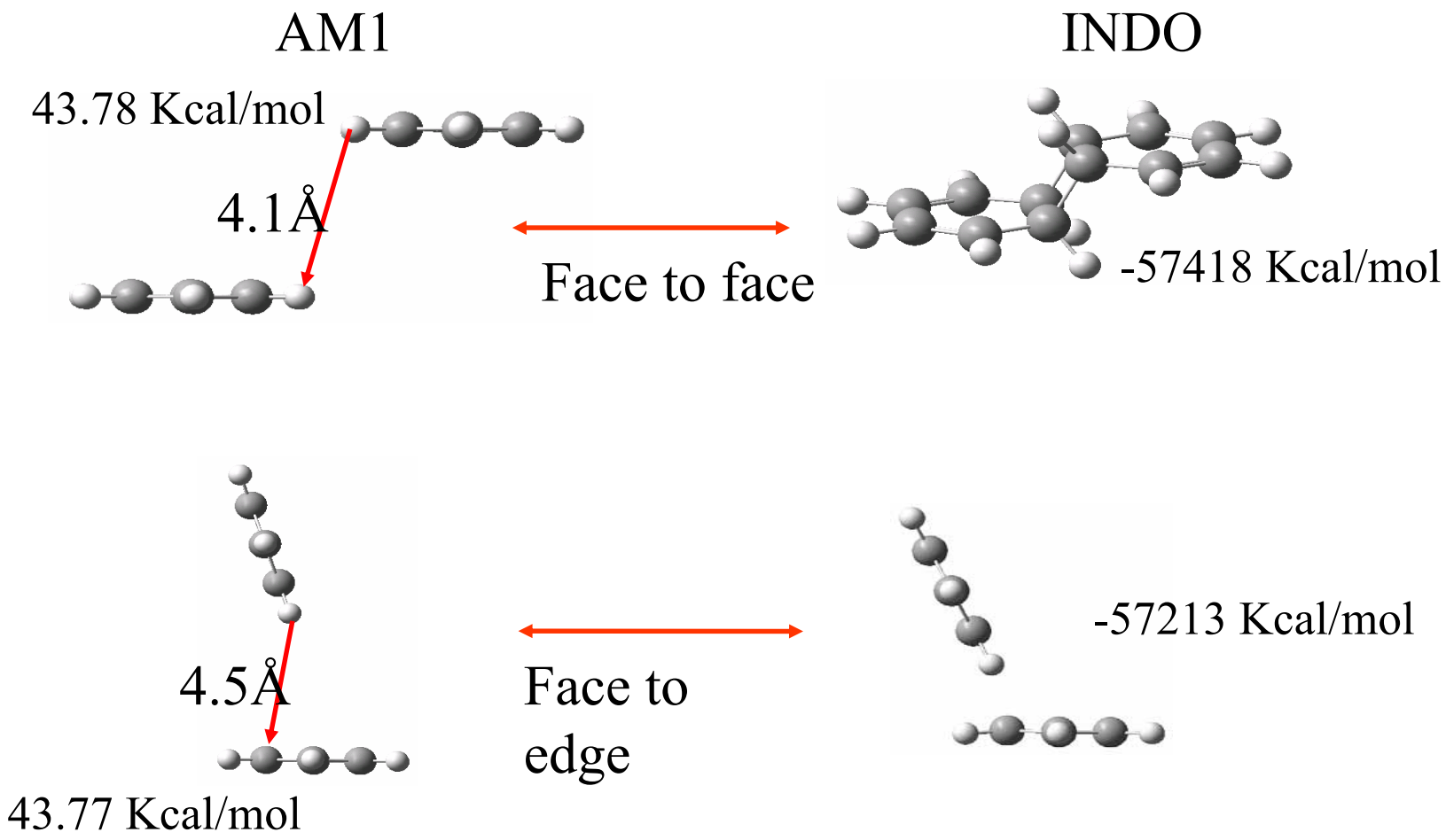


Torsion Angle

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

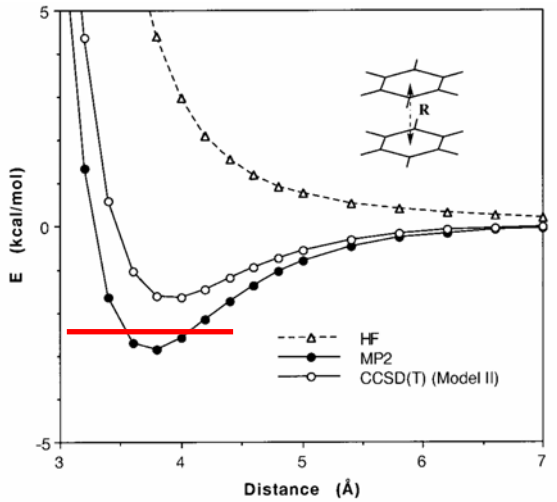


Figure 3. The HF, MP2, and CCSD(T) interaction energies of the benzene dimer A. The HF and MP2 interaction energies were calculated with the aug(d,p)-6-311G** basis set. The CCSD(T) interaction energy was calculated by the AIMI Model II. See text.

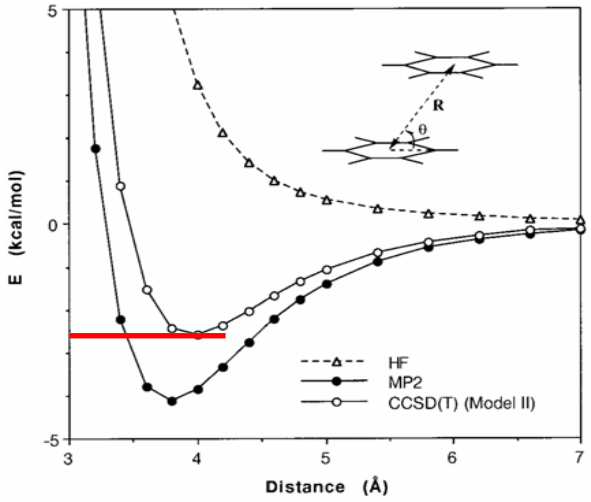


Figure 5. The HF, MP2, and CCSD(T) interaction energies of the benzene dimer C. The HF and MP2 interaction energies were calculated with the aug(d,p)-6-311G** basis set. The CCSD(T) interaction energy was calculated by the AIMI Model II. See text. The angle θ was fixed at 63°. The angle θ is 63° when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

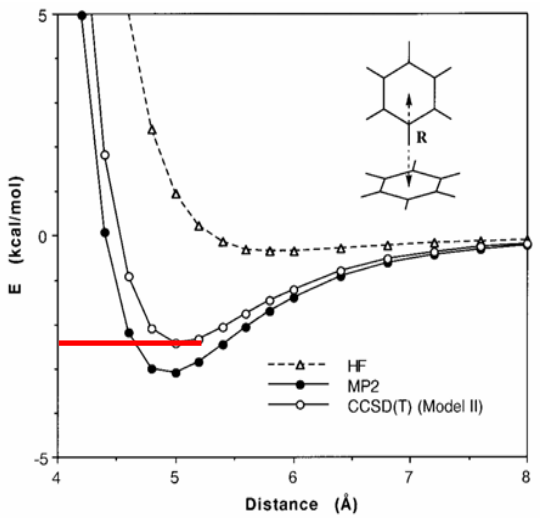


Figure 4. The HF, MP2, and CCSD(T) interaction energies of the benzene dimer B. The HF and MP2 interaction energies were calculated with the aug(d,p)-6-311G** basis set. The CCSD(T) interaction energy was calculated by the AIMI Model II. See text.

►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.

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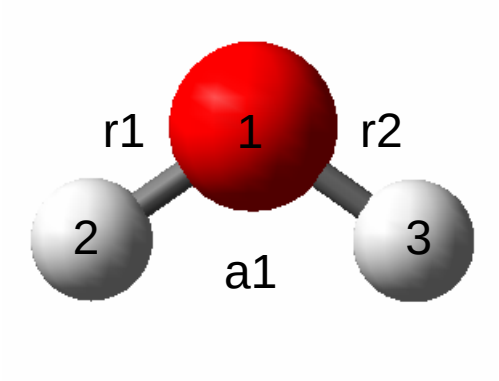
Coordinate: Cartesian vs Z-matrix



Cartesian

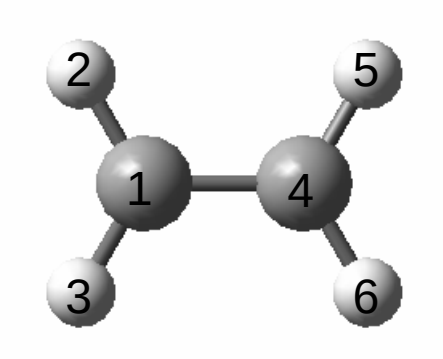
O	0.0000	0.0000	-0.1108
H	0.0000	-0.7840	0.4432
H	0.0000	0.7849	0.4432

Z-matrix

O
H 1 r1
H 1 r2 2 a1
Variables:
r1=0.96
r2=0.96
a1=109.5

3N – 6 = 3

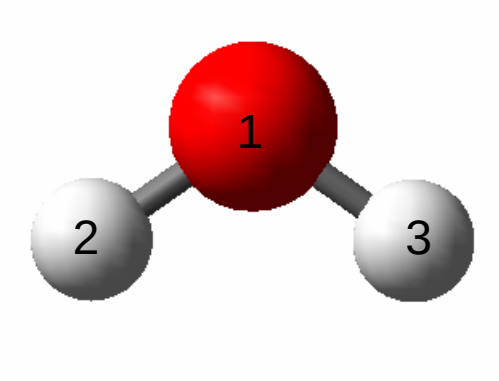
Z-matrix for more than 3 atoms




```
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

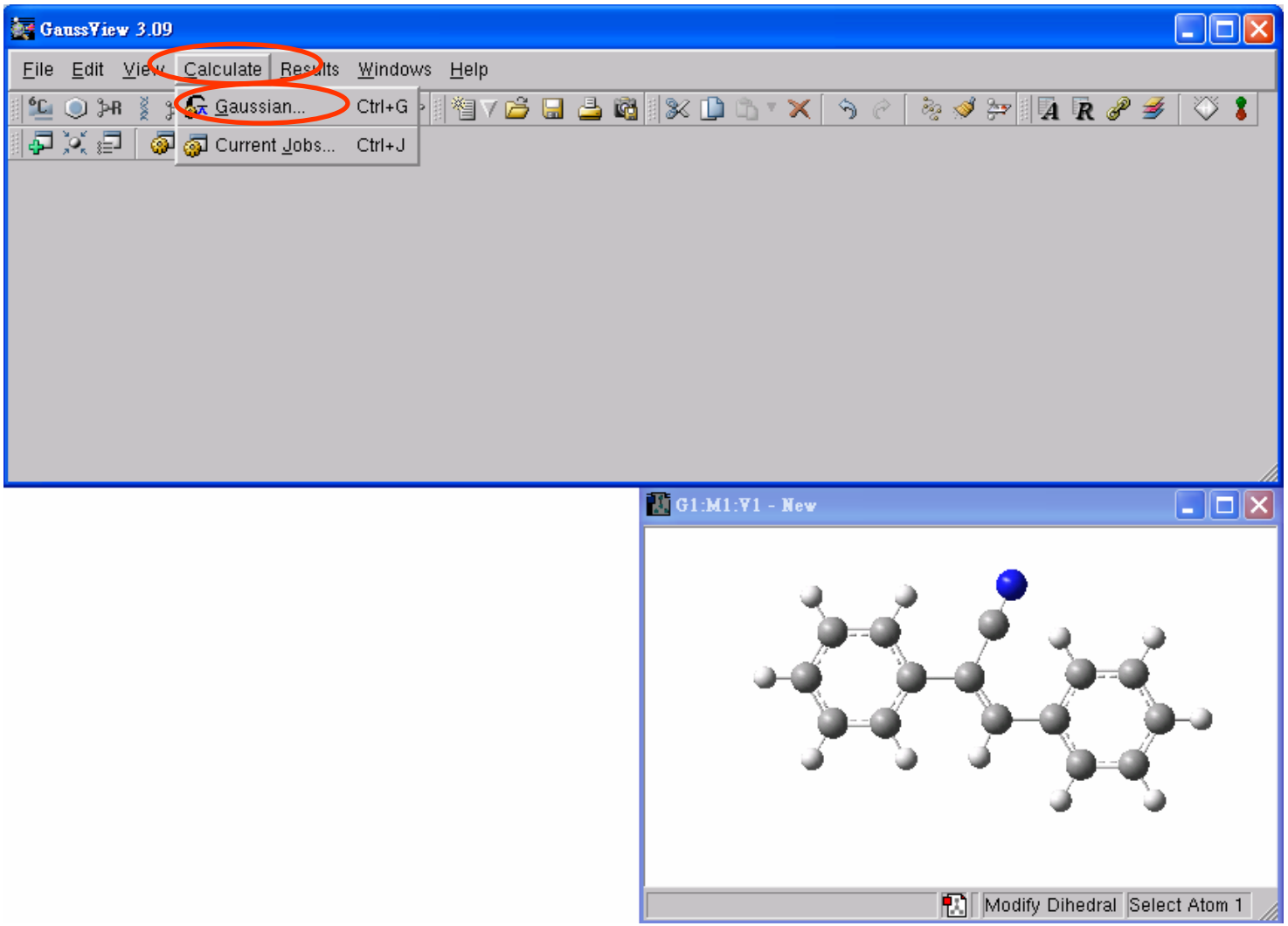
O
H 1 r1
H 1 r2 2 a1
Variables:
r1=0.960
r2=0.961
a1=109.5

C_{2v} symmetry

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

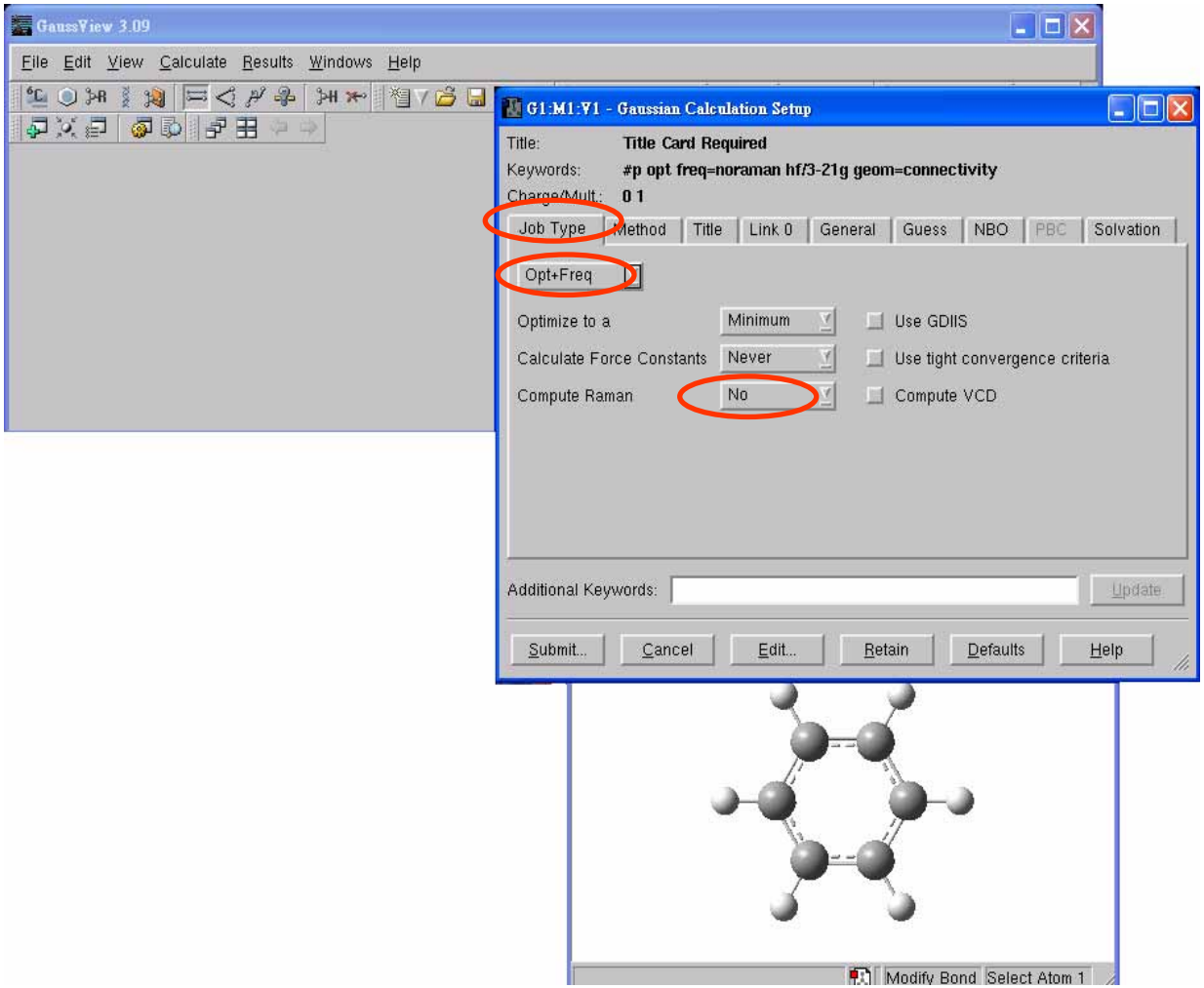
Optimization and Frequency

Click Calculate → Select Gaussian



Job Type

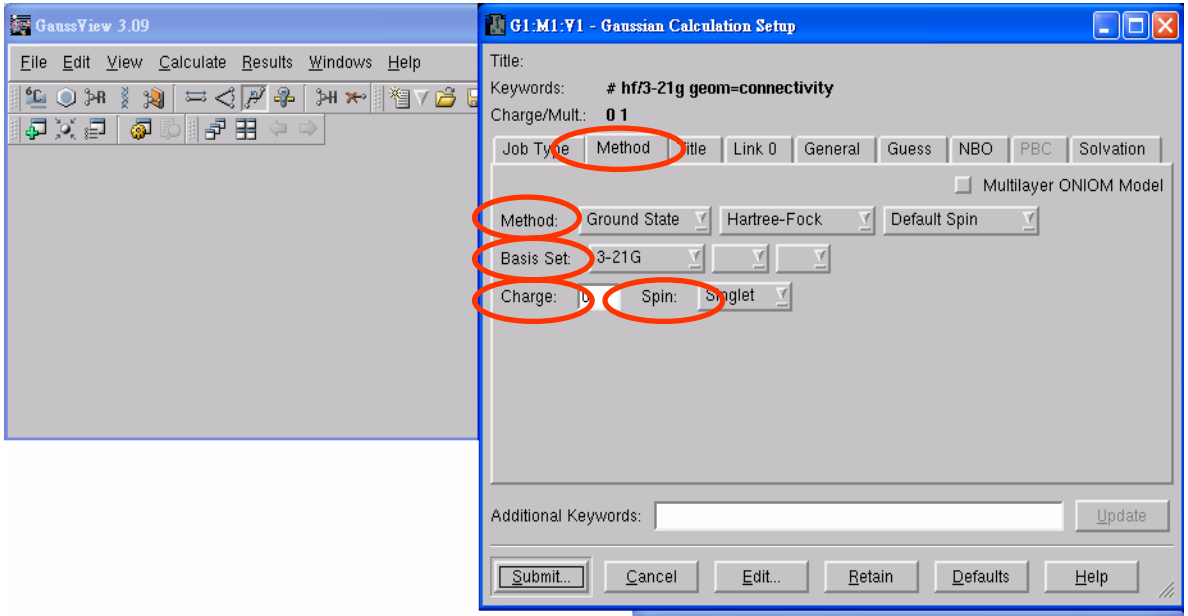
Job type → Opt + freq → Noraman



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

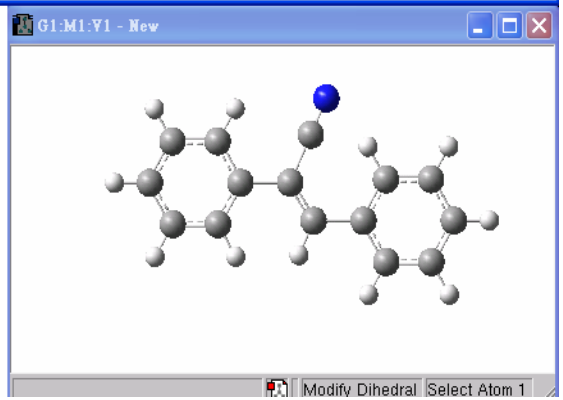
Methods

Select Method → Basis set → Charge → Spin

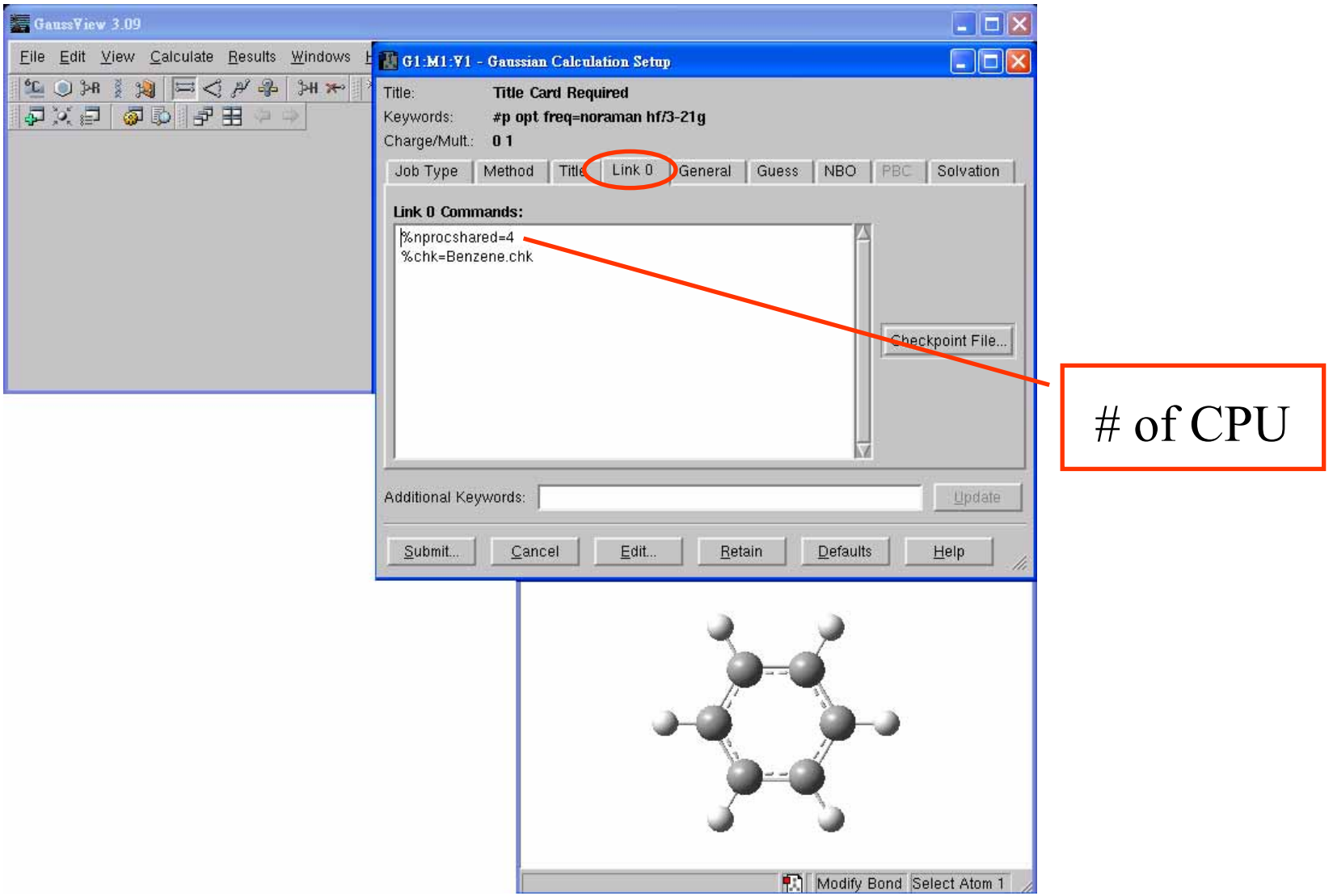


Spin multiplicity (2S+1):

Singlet: 1 (S=0)
Doublet: 2 (S= ½)
Triplet: 3 (S= 1)
Quartet: 4 (S= 1.5)

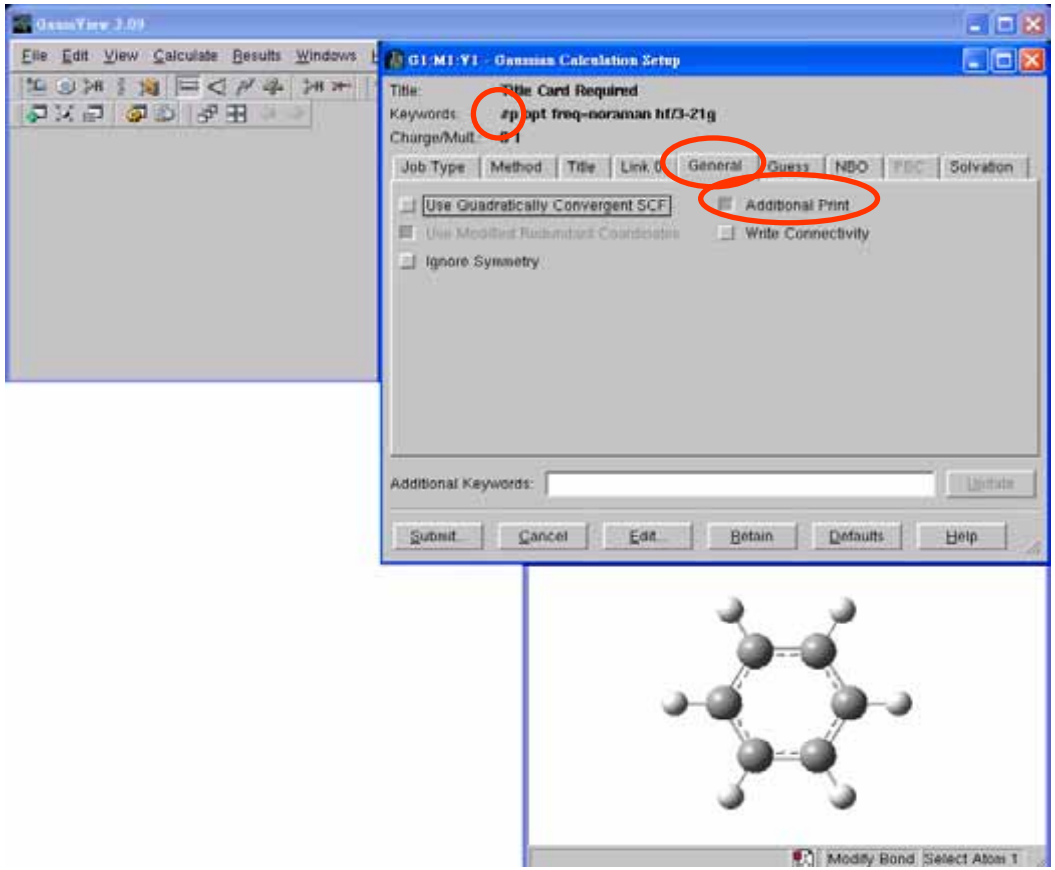


Link


GaussView 3.09
File Edit View Calculate Results Windows
G1:M1:Y1 - Gaussian Calculation Setup
Title: Title Card Required
Keywords: #p opt freq=noraman hf/3-21g
Charge/Mult.: 0 1
Job Type Method Title Link 0 General Guess NBO PBC Solvation
Link 0 Commands:
%nprocshared=4
%chk=Benzene.chk
Checkpoint File...
Additional Keywords:
Update
Submit... Cancel Edit... Retain Defaults Help
Modify Bond Select Atom 1
# of CPU

General

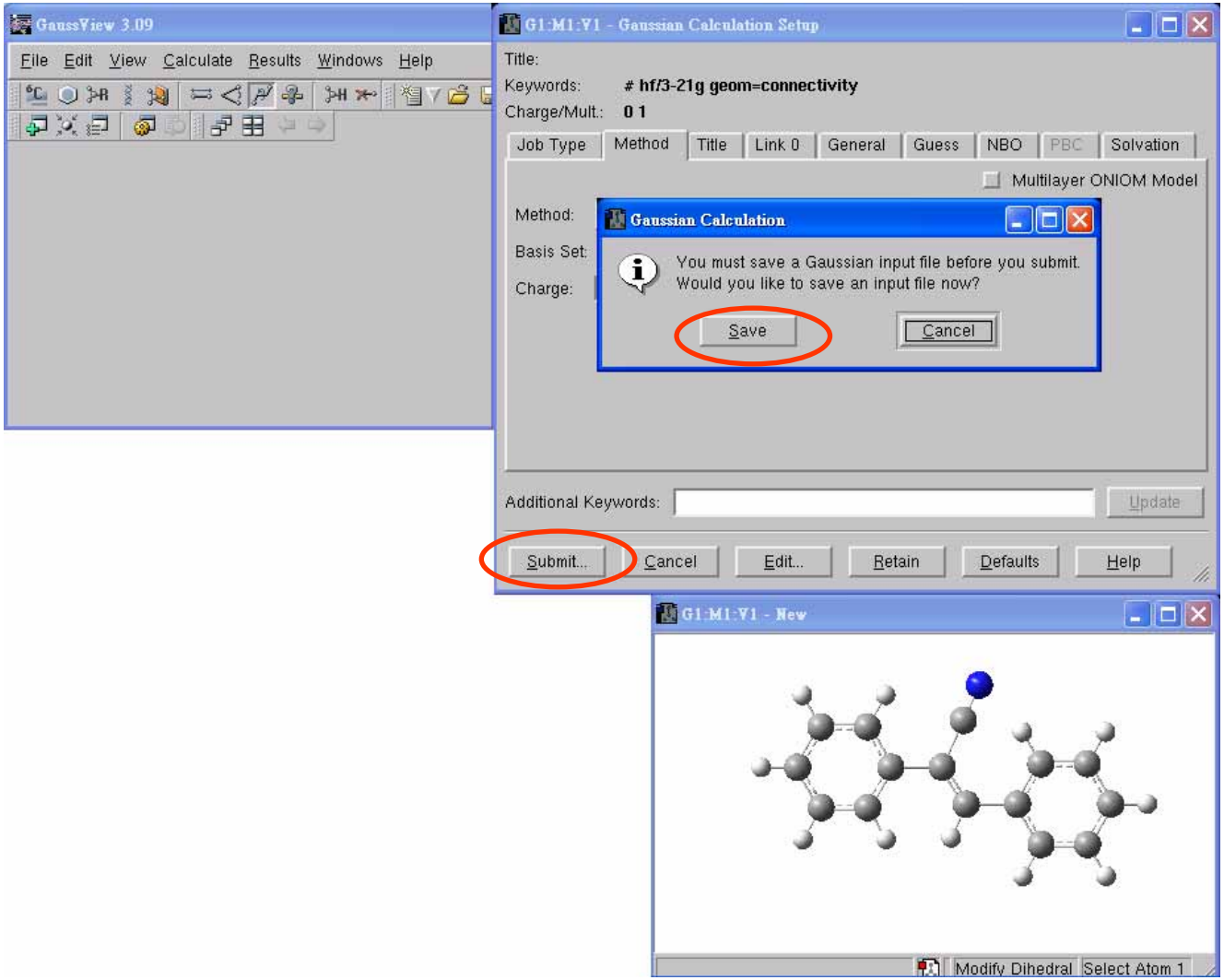
Click General → Select Additional print



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

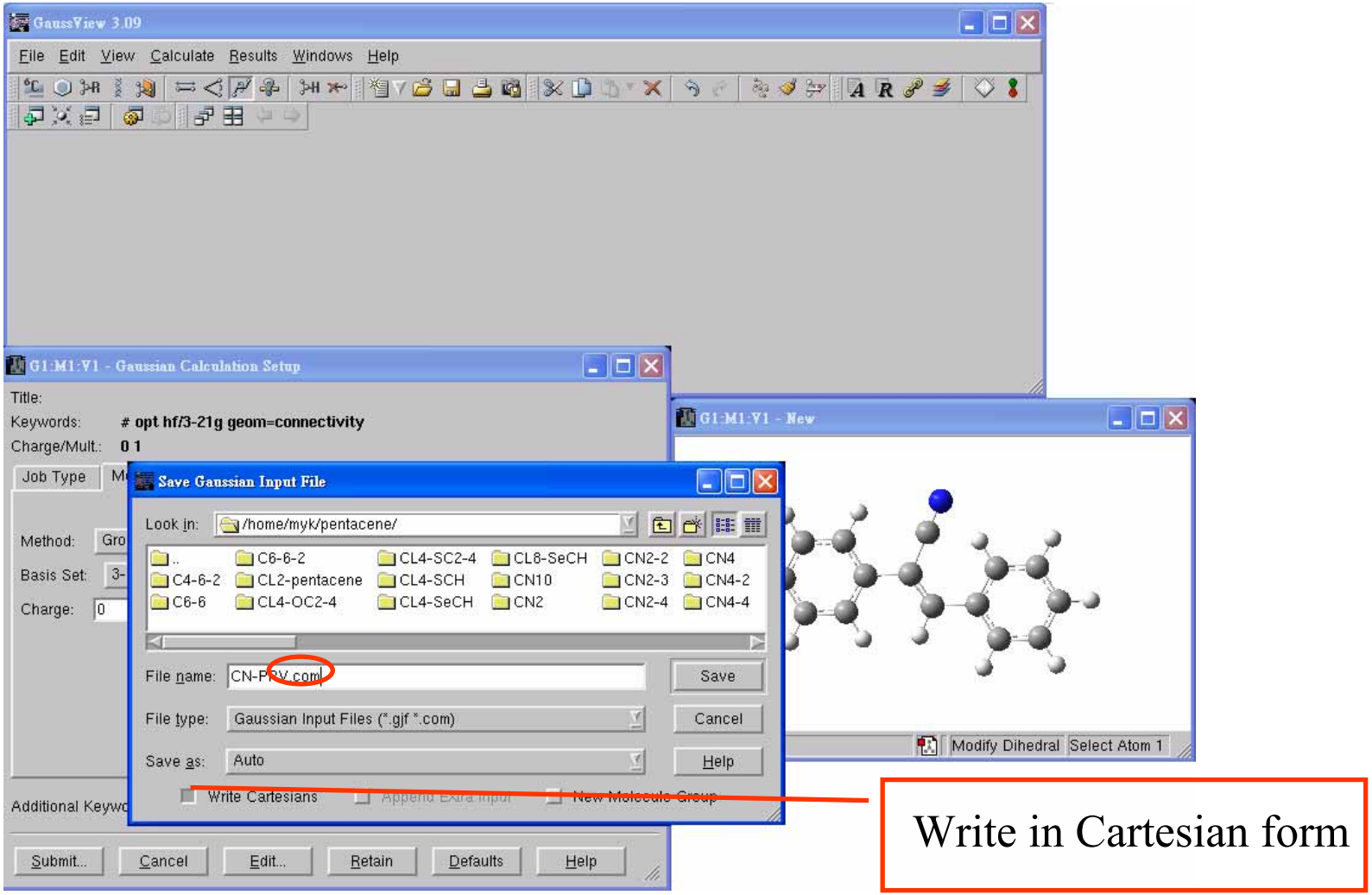
Submit the job

Click Submit → Save the job

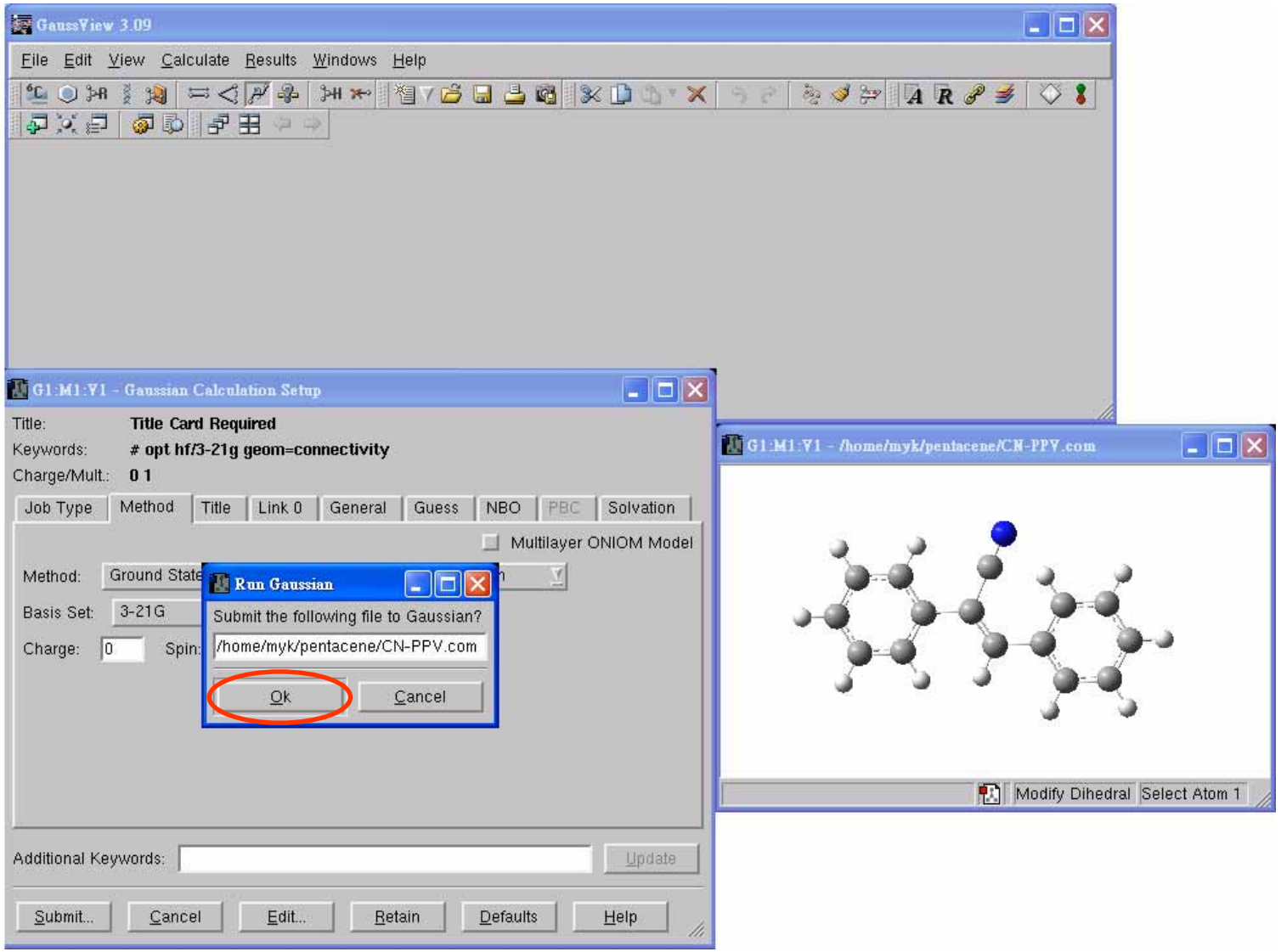


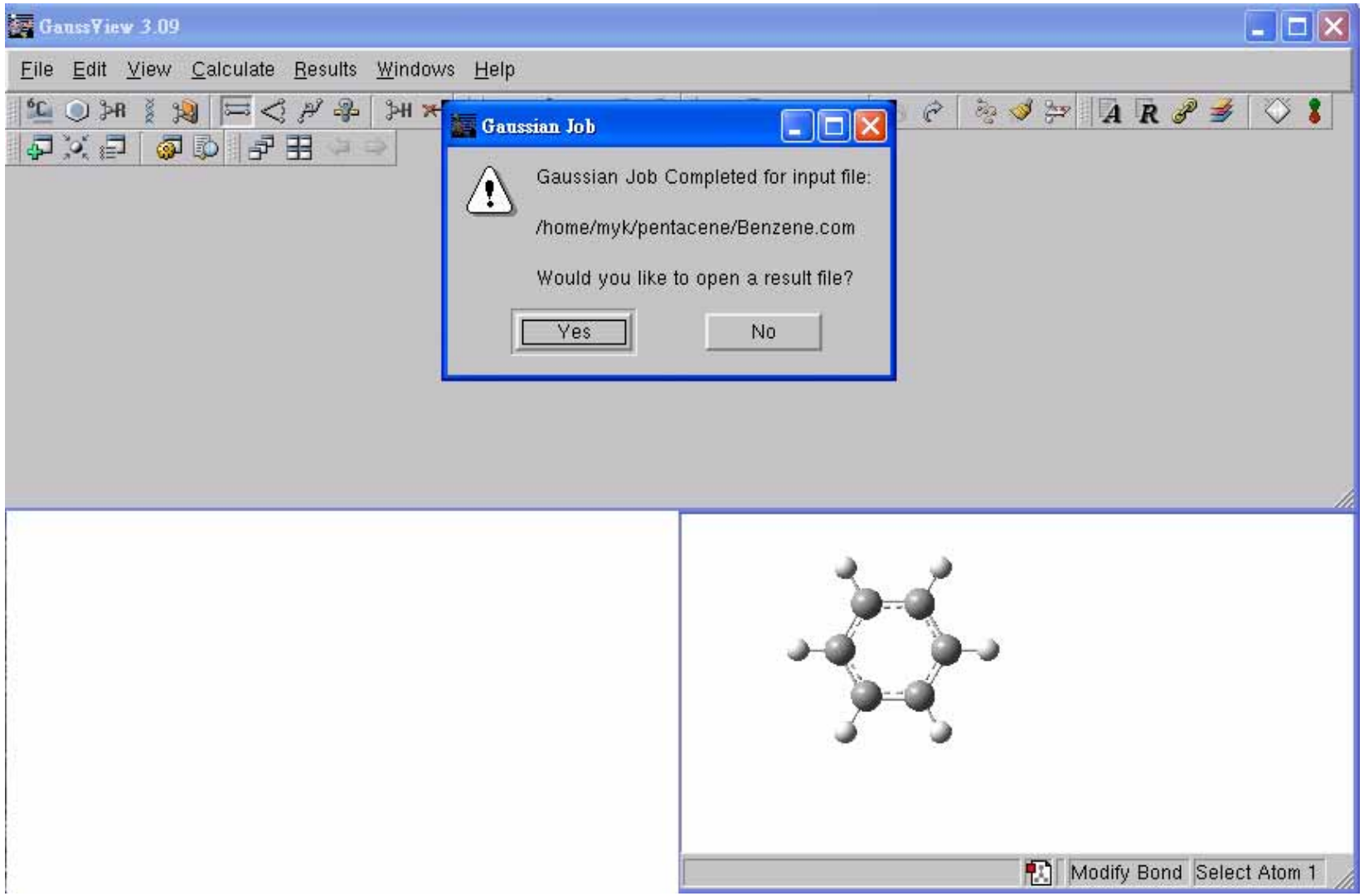
Save the job

File type *.com



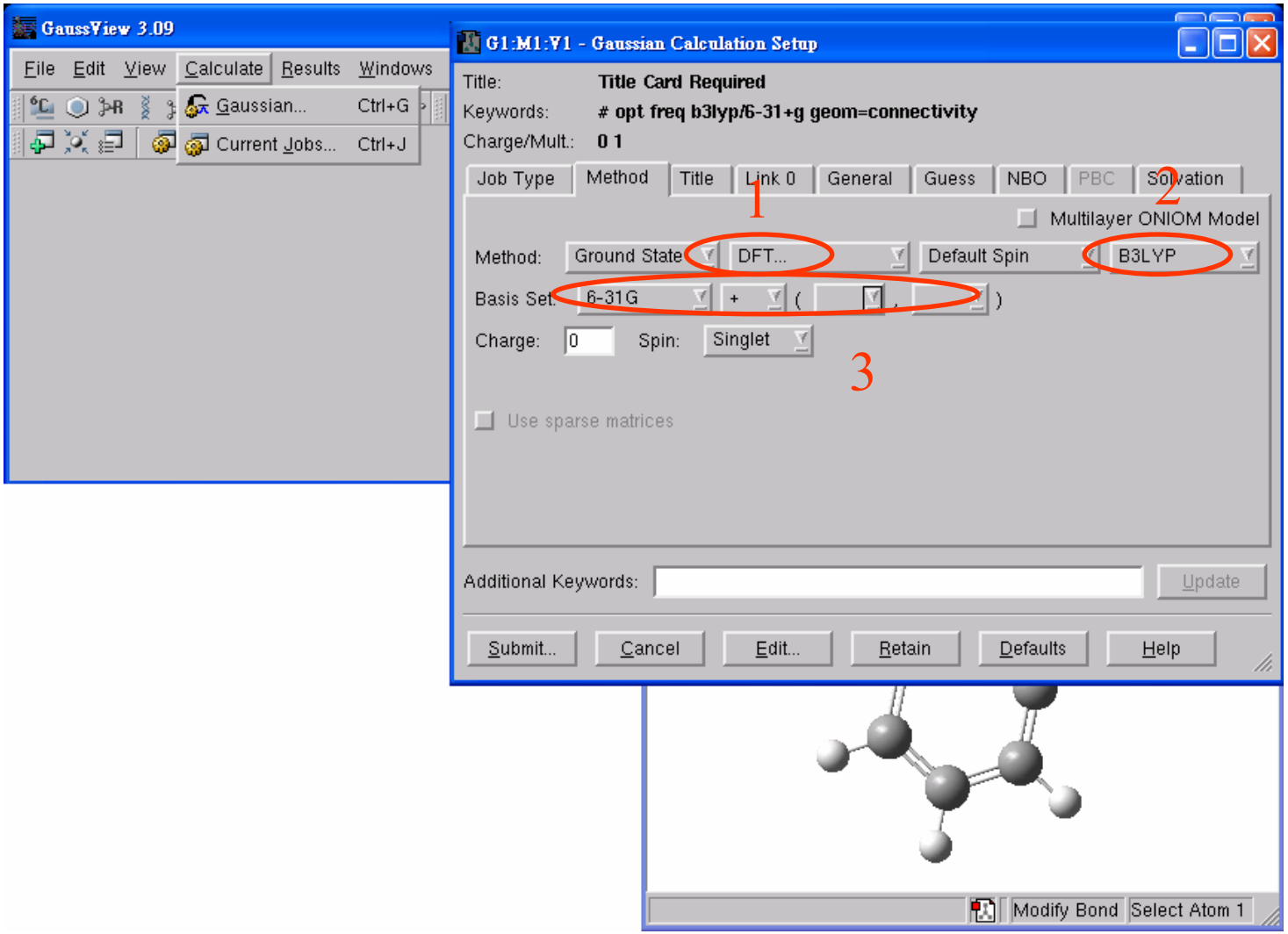
Run the Job


GaussView 3.09
File Edit View Calculate Results Windows Help
G1:M1:V1 - Gaussian Calculation Setup
Title: Title Card Required
Keywords: # opt hf/3-21g geom=connectivity
Charge/Mult.: 0 1
Job Type Method Title Link 0 General Guess NBO PBC Solvation
Multilayer ONIOM Model
Method: Ground State
Basis Set: 3-21G
Charge: 0 Spin:
Run Gaussian
Submit the following file to Gaussian?
/home/myk/pentacene/CN-PPV.com
Ok Cancel
Additional Keywords:
Update
Submit... Cancel Edit... Retain Defaults Help
G1:M1:V1 - /home/myk/pentacene/CN-PPV.com
Modify Dihedral Select Atom 1

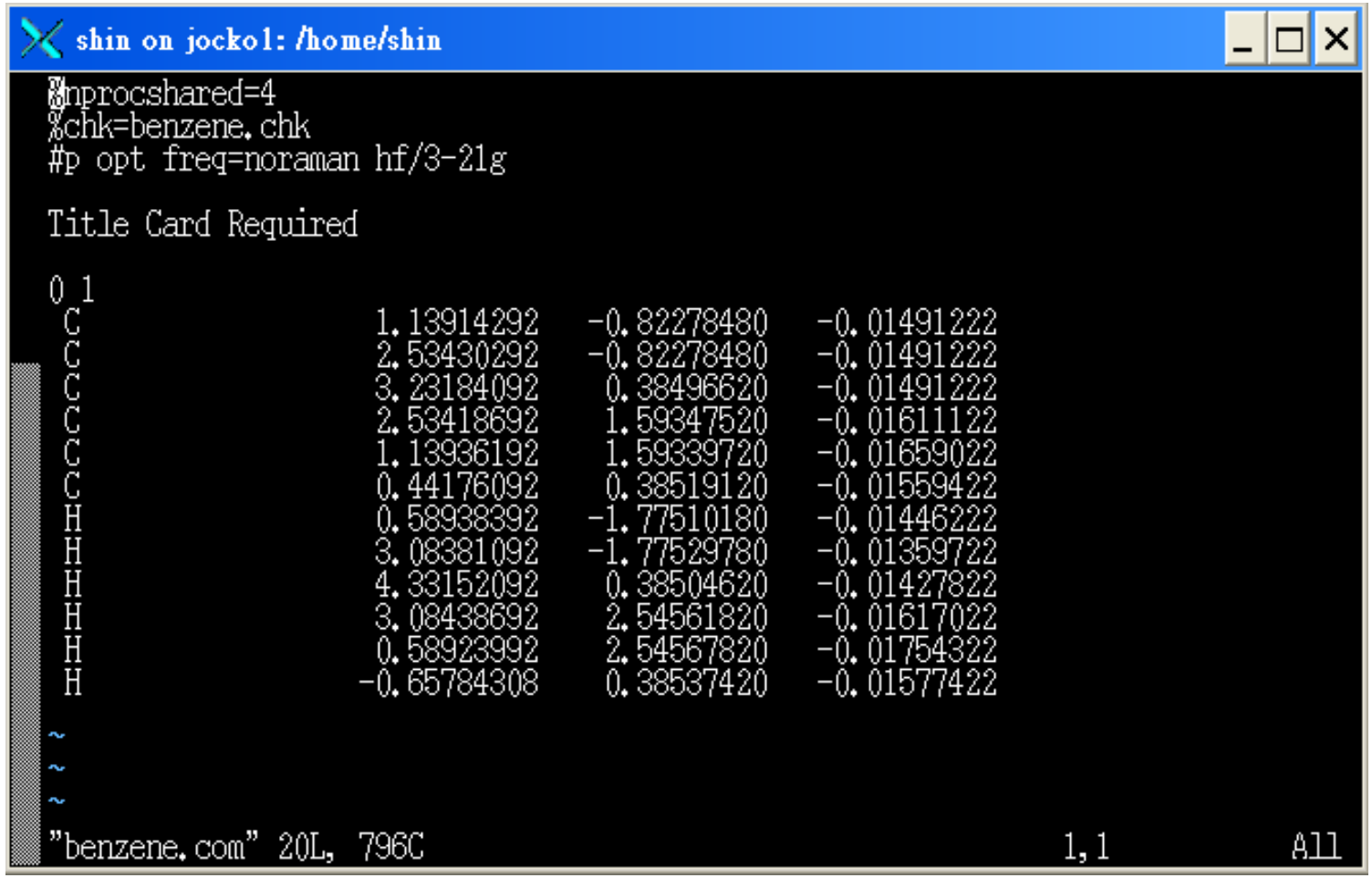

GaussView 3.09
File Edit View Calculate Results Windows Help
Gaussian Job
Gaussian Job Completed for input file:
/home/myk/pentacene/Benzene.com
Would you like to open a result file?
Yes
No
Modify Bond
Select Atom 1

Again : Job type → Method → Link → General

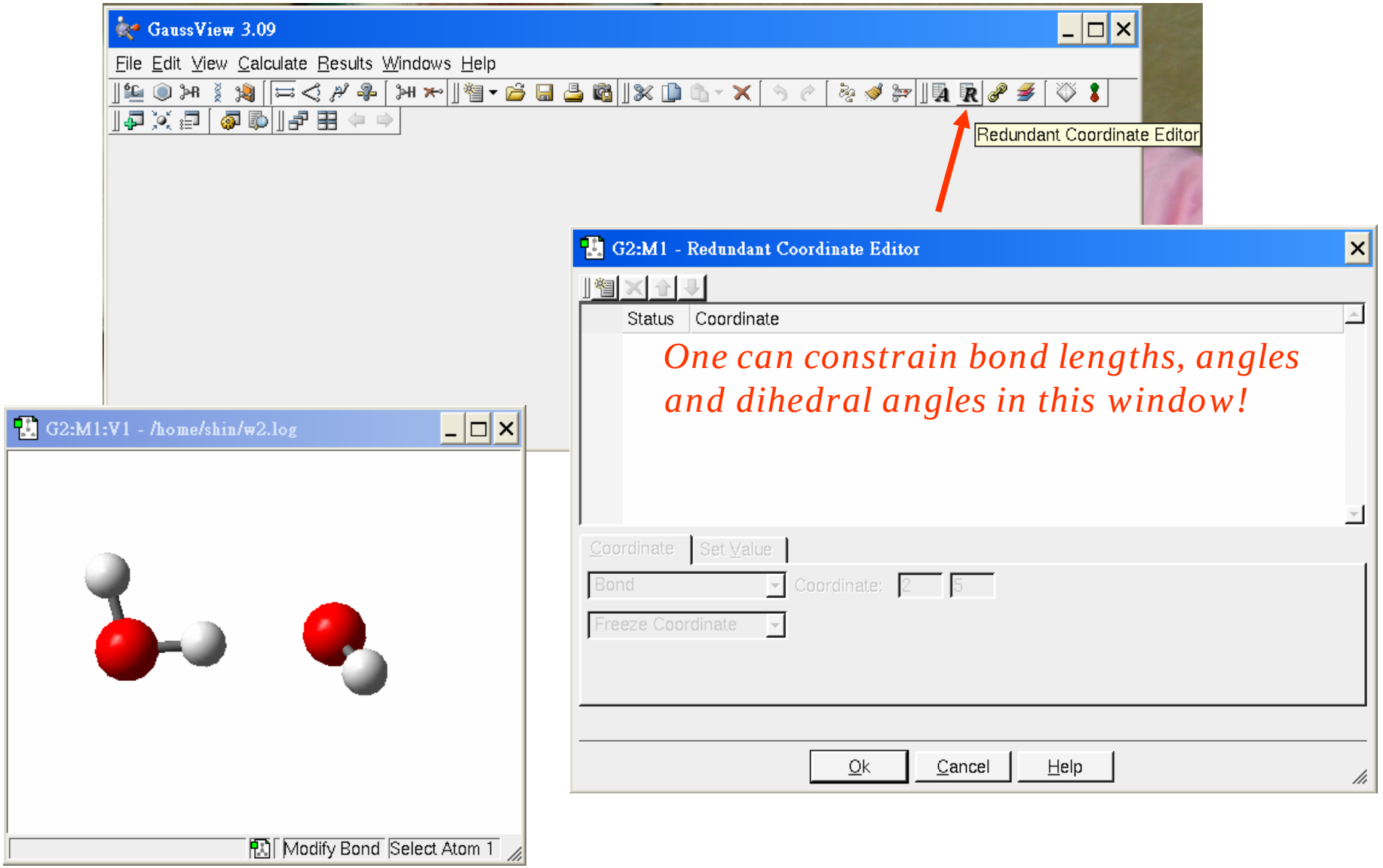
Method (DFT) → Exchange-Correlation (B3LYP) → Basis set



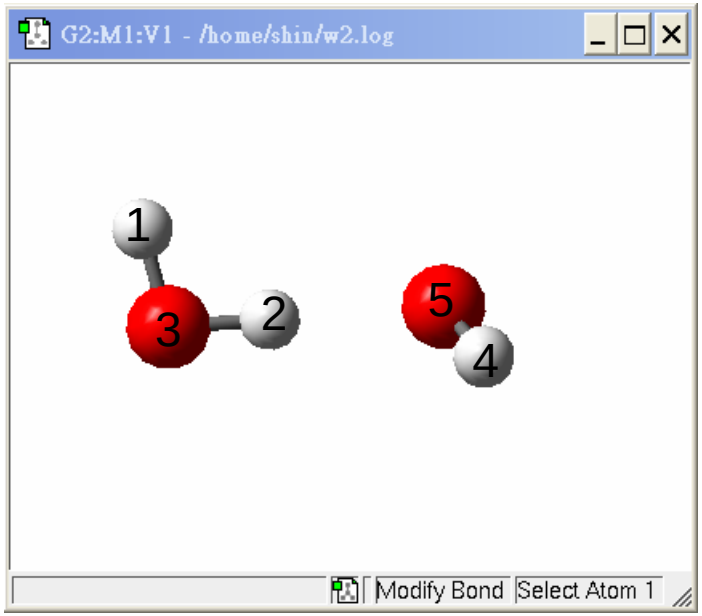
Input File XXX.com of Gaussian

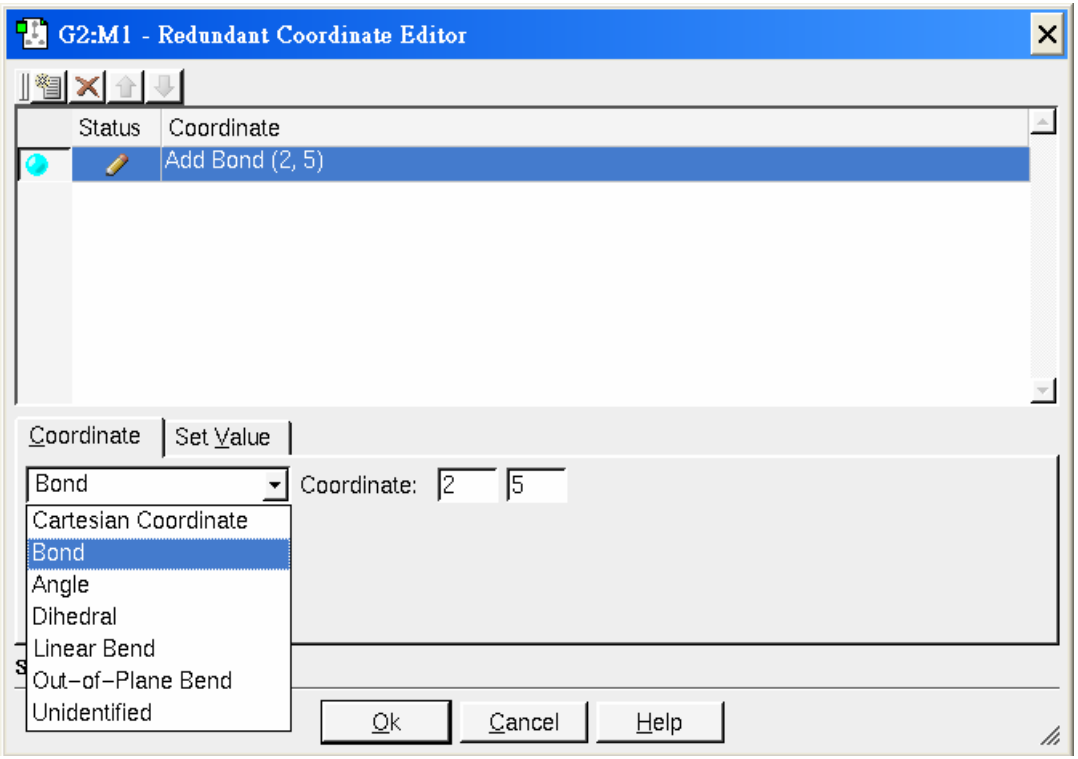


Partial Optimization: How to Constrain Coordinates

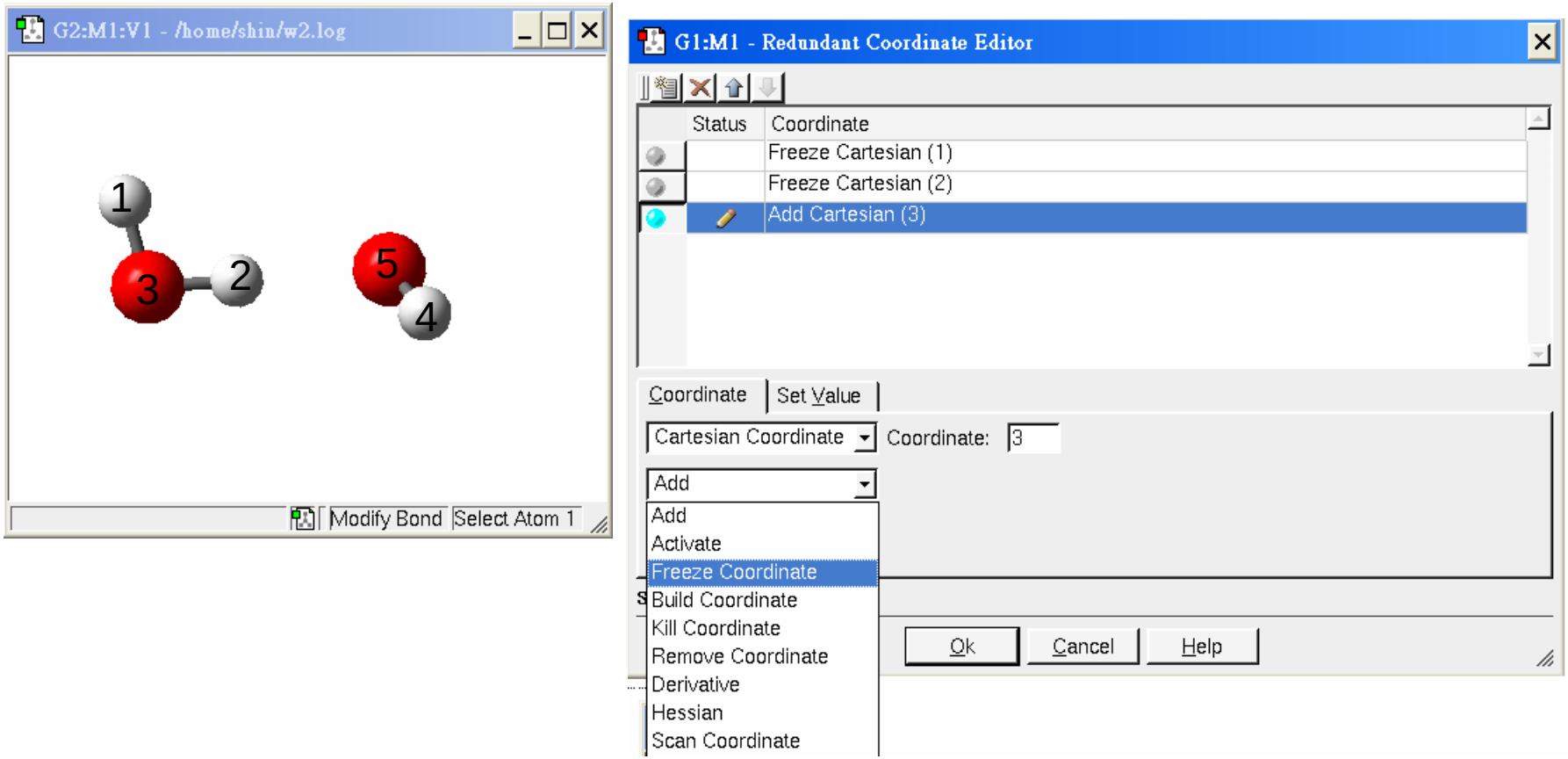


Constrain Bond Length





Freeze Atom Positions

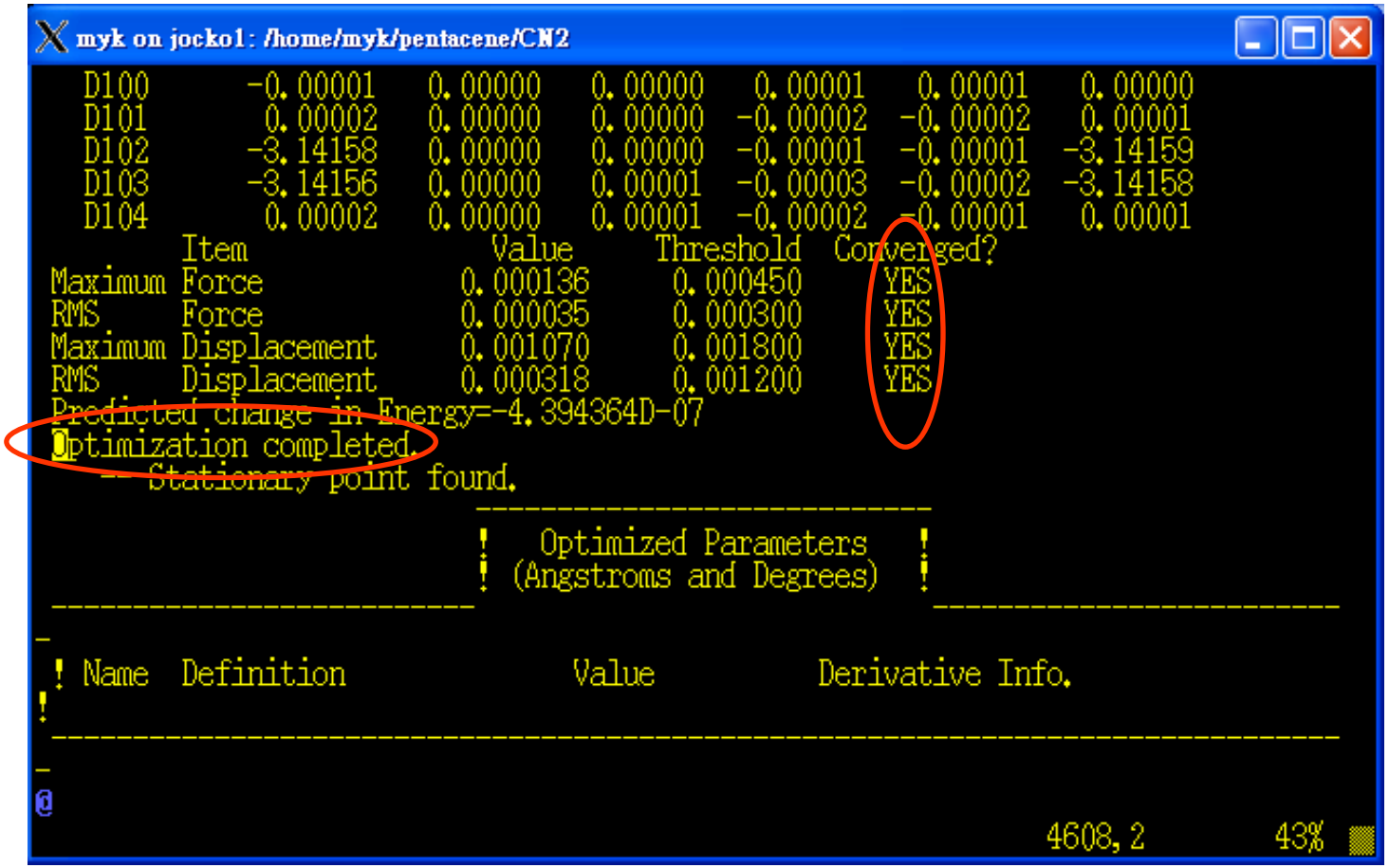


Check output *.log from startxwin

Type vi *.log → Enter

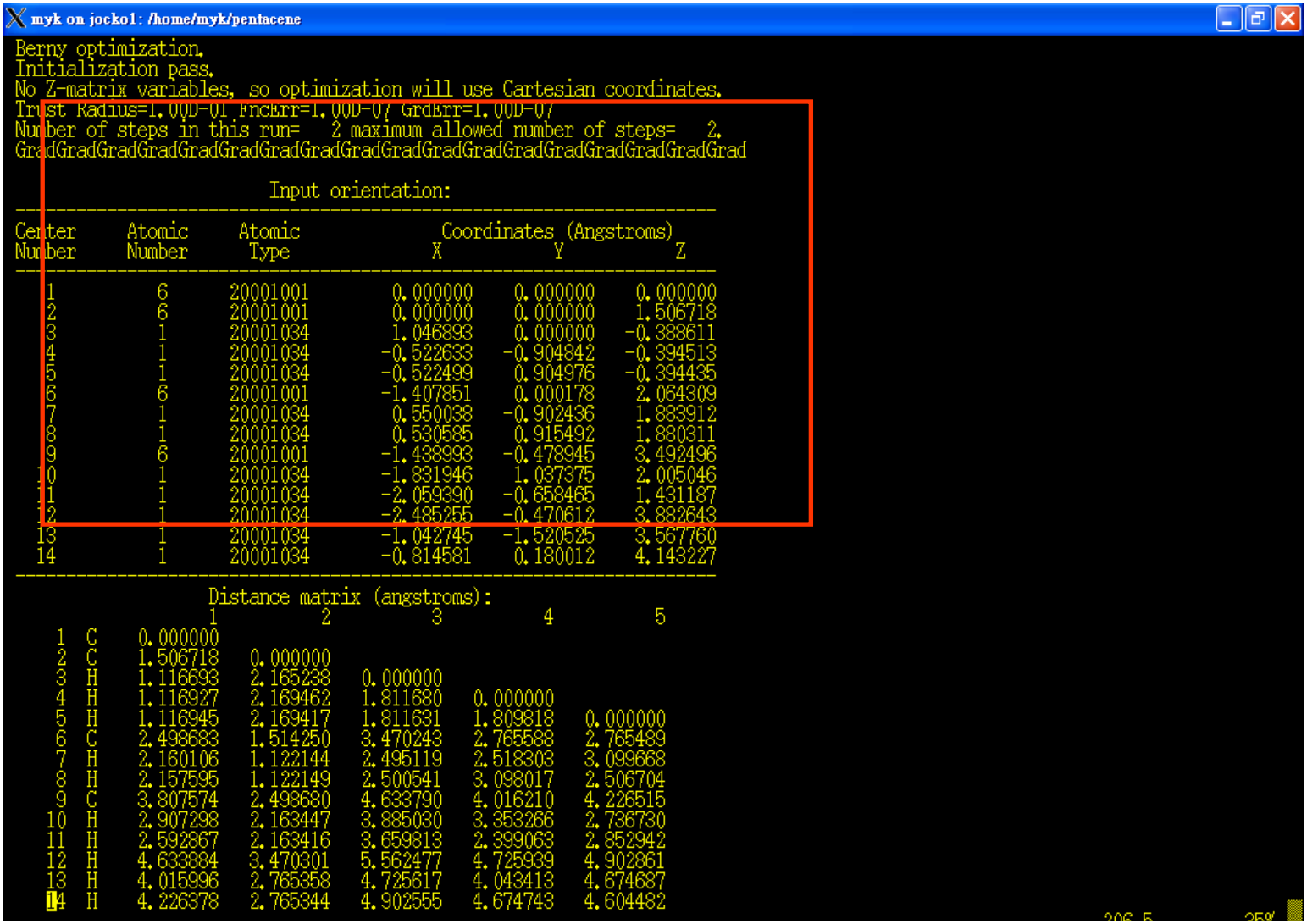
Check Optimization : Press Esc → type :/Optimization → Enter

Then press Page Up to find the final Geometry



Final geometry

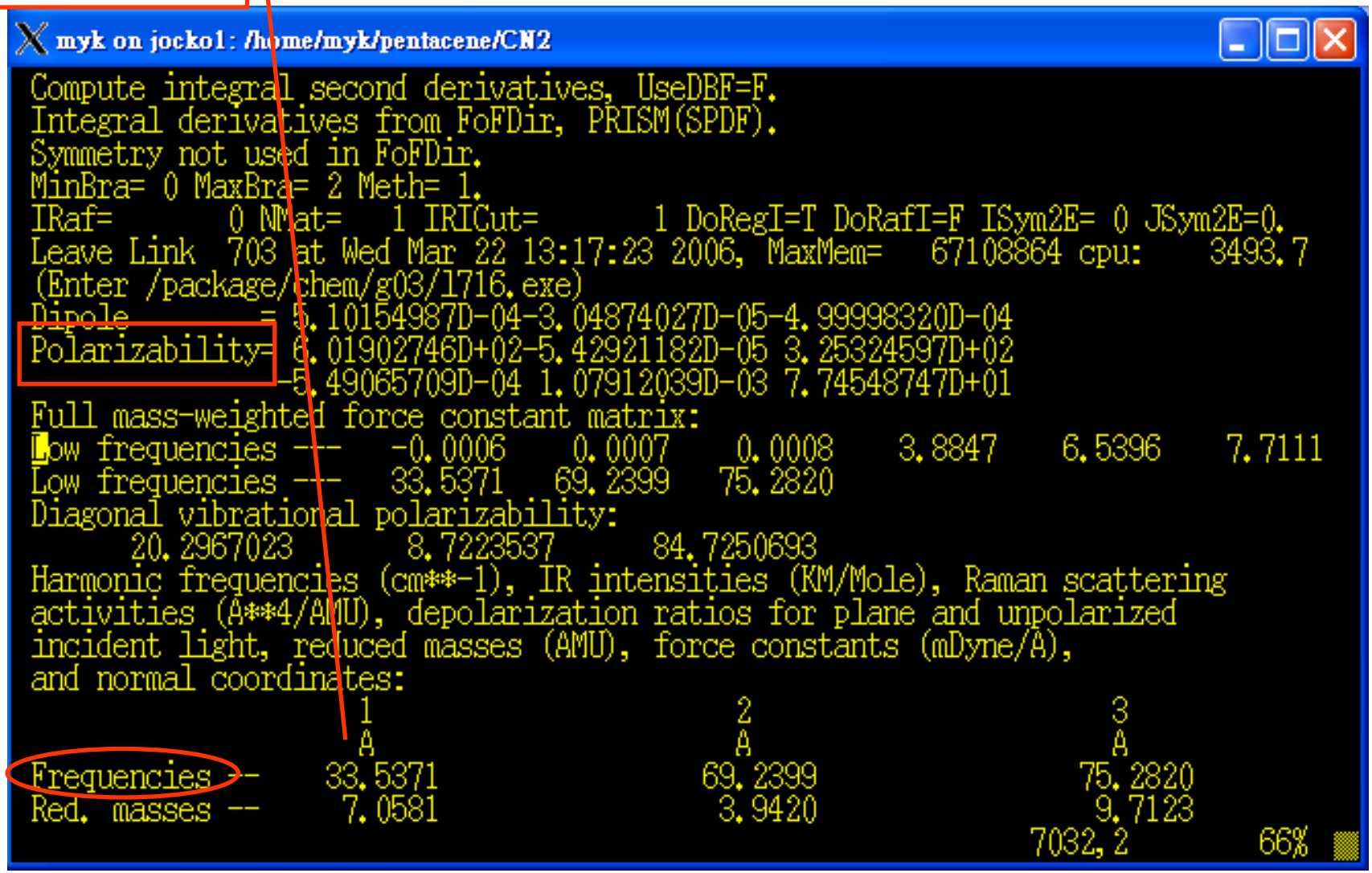
Remember to search upward from the string “Optimization completed”



Check Frequency and Polarizability

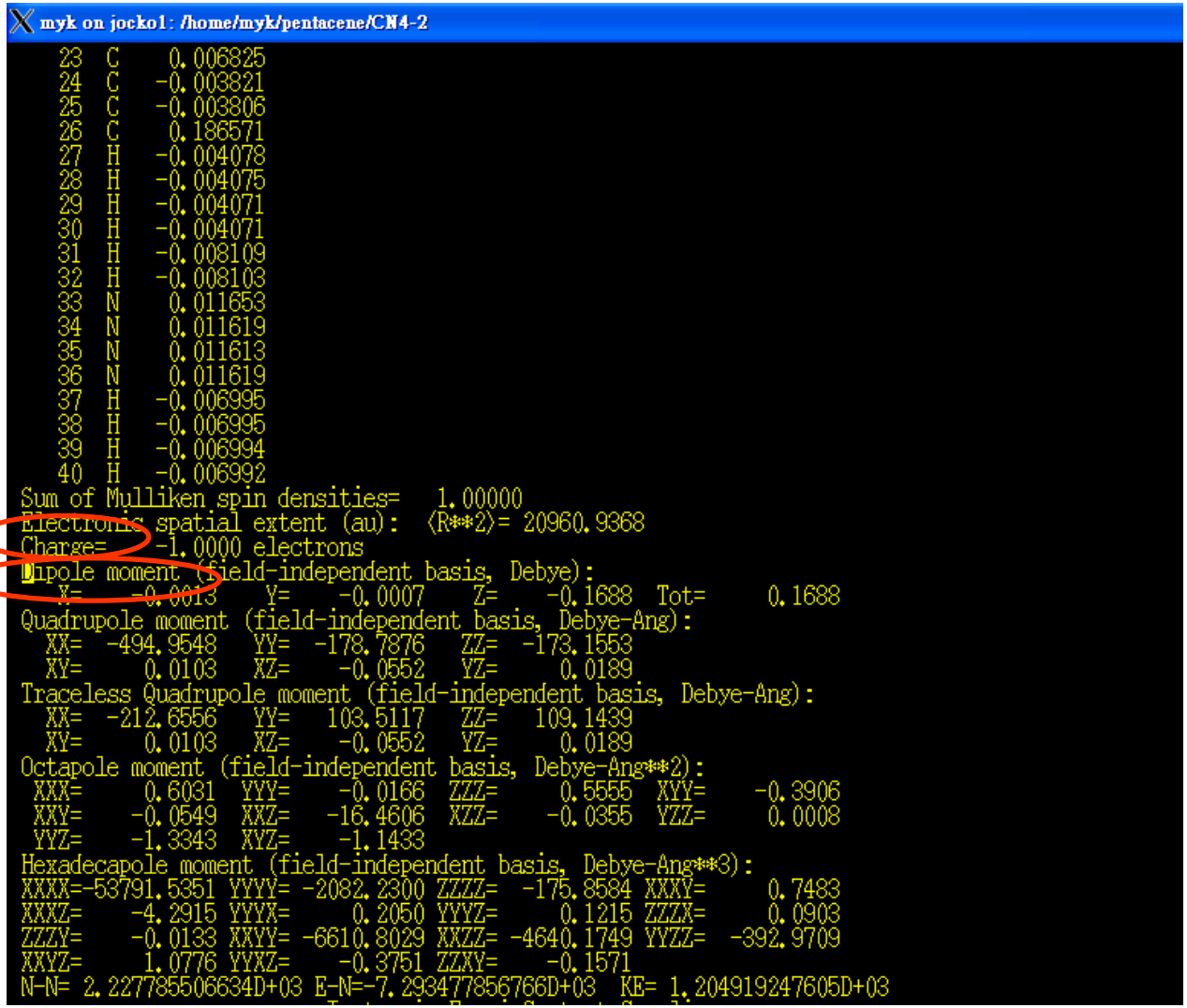
All positive

Press Esc → type :/Frequencies→ Enter



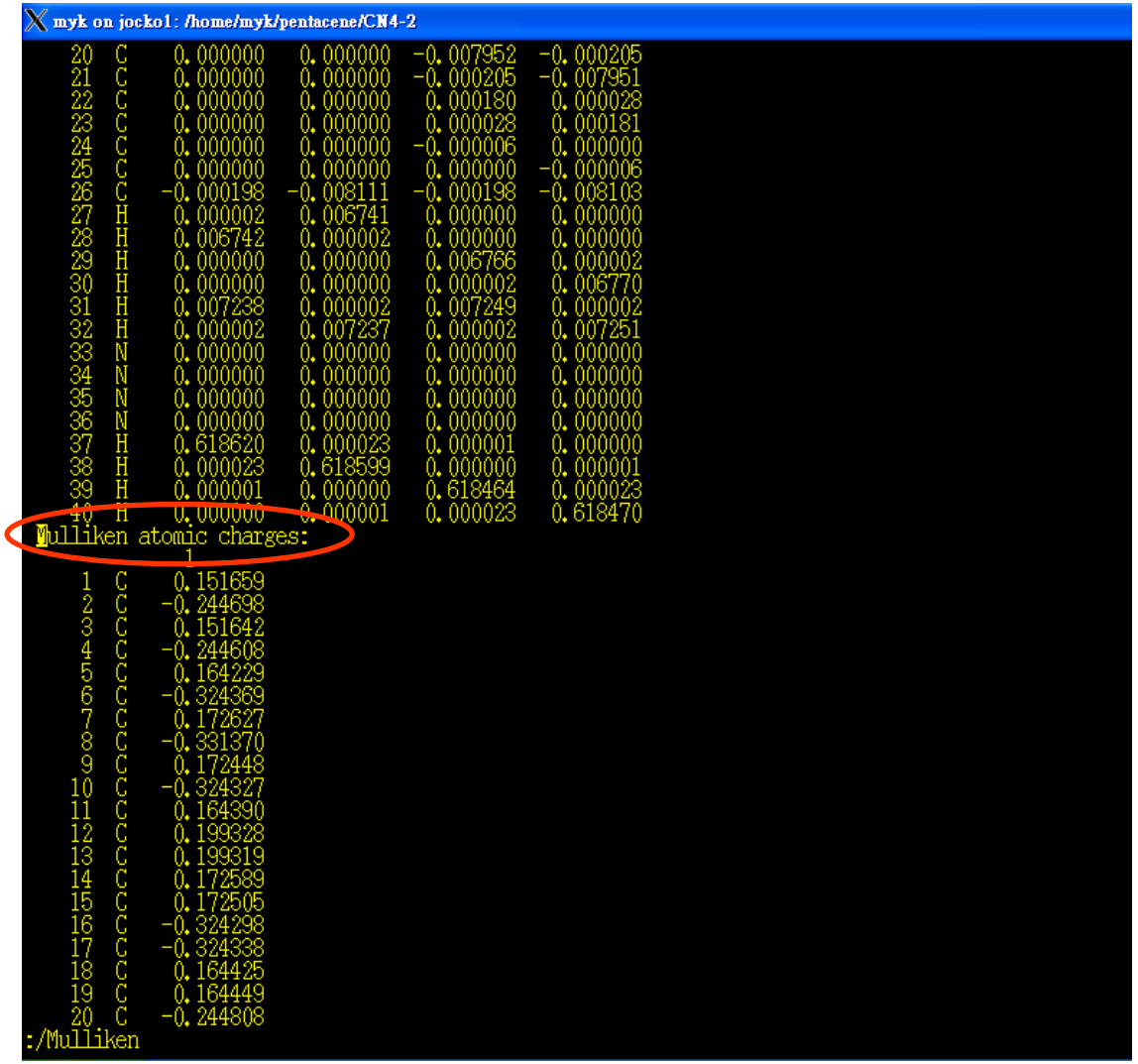
Dipole moment and total charge

Press Esc → type :/Dipole → Enter



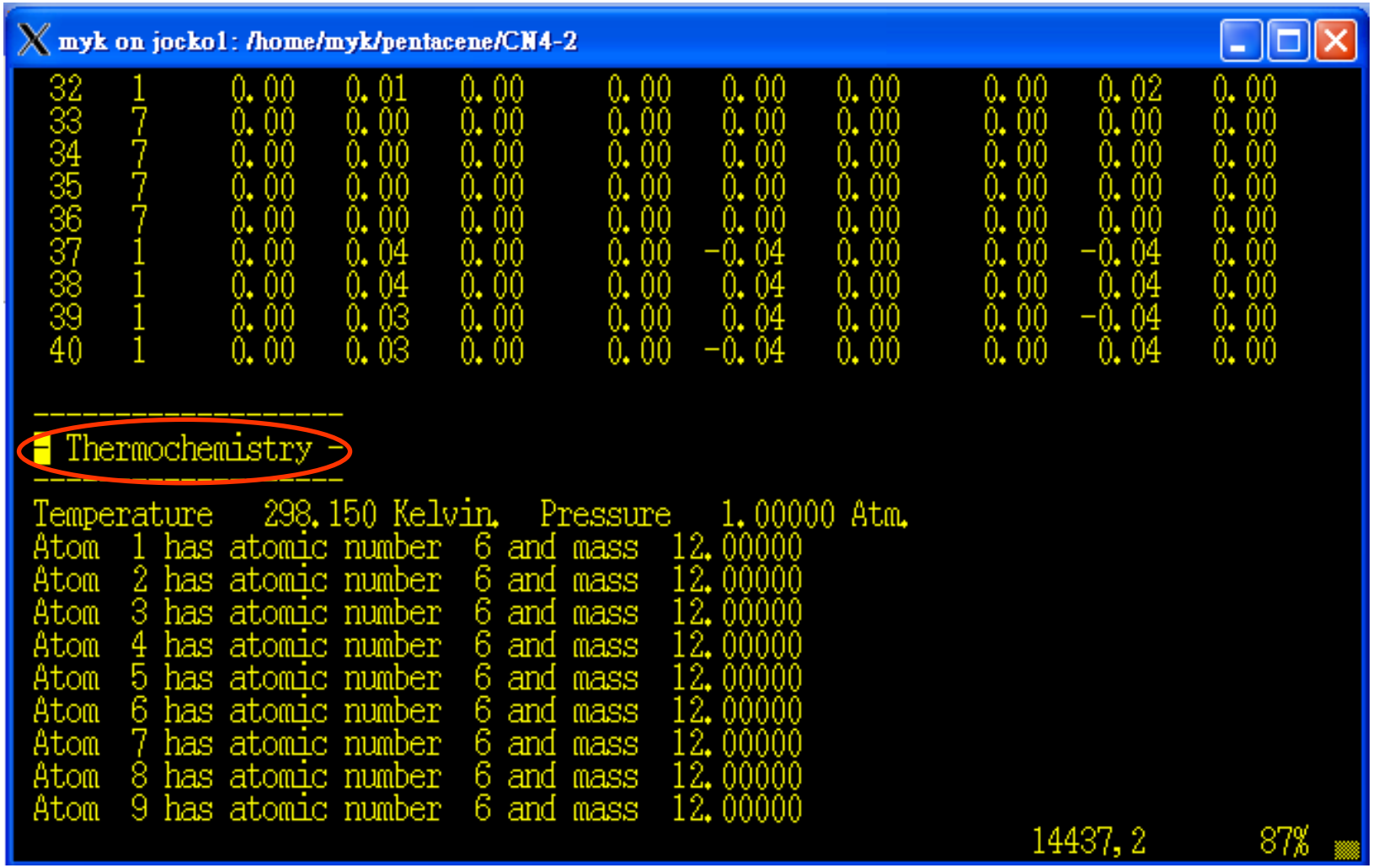
Mulliken charge

Press Esc → type :/Mulliken → Enter



Thermochemistry

Press Esc → type :/Thermo → Enter



Zero-point energy

Press Page Down

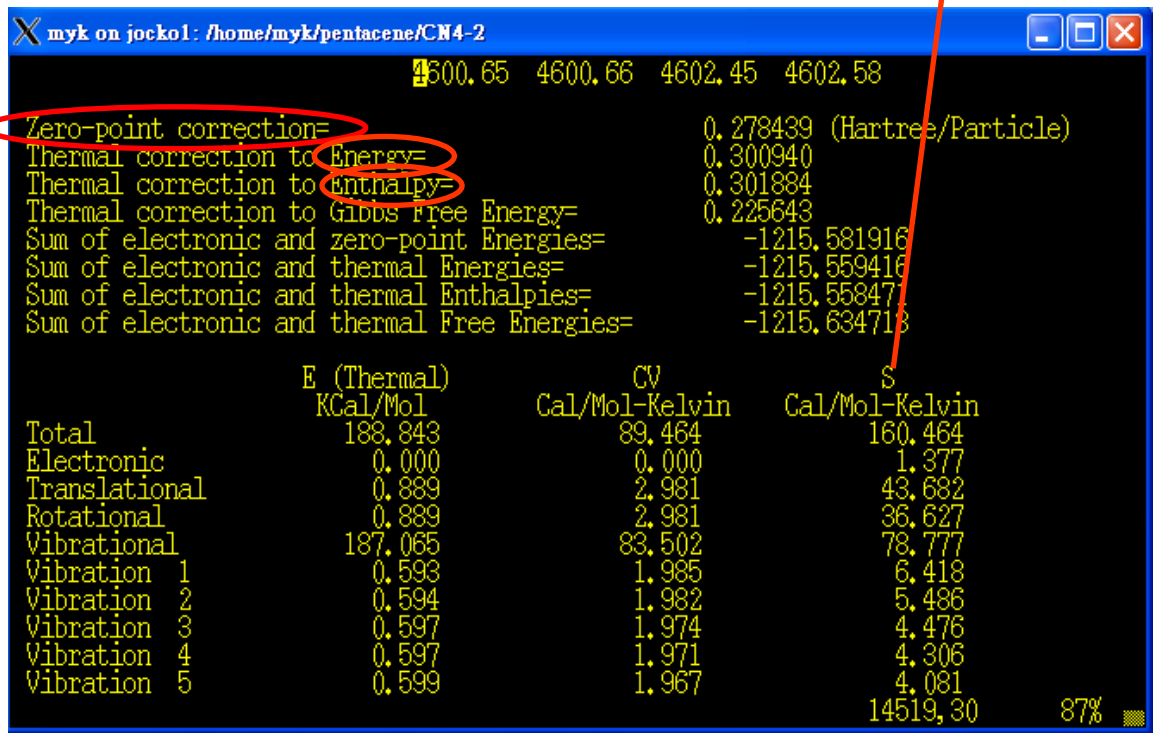
$E_0 = E_{elec} + ZPE$

$E = E_0 + E_{vib} + E_{rot} + E_{transl}$

$H = E + RT$

$G = H - TS$

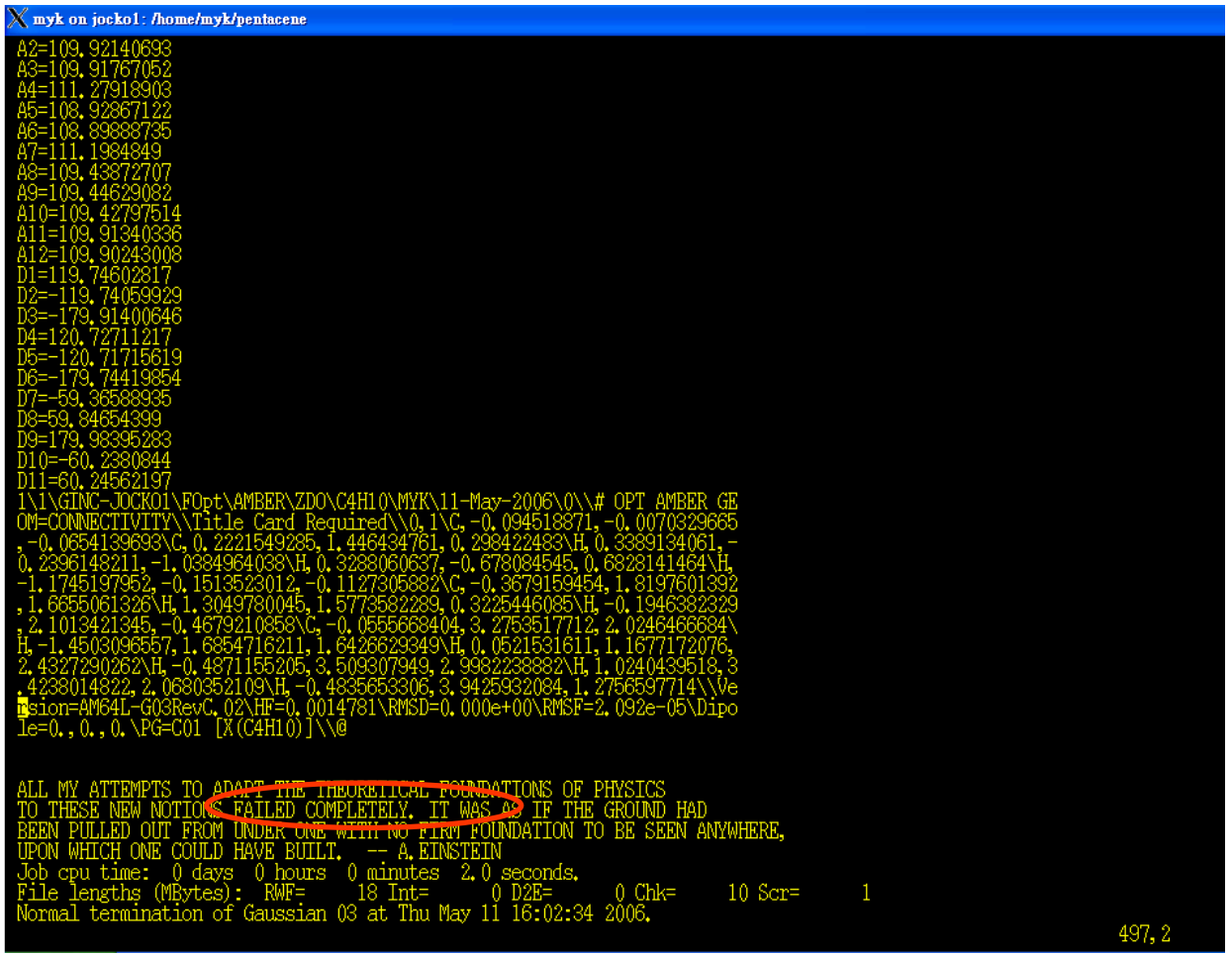
entropy



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

Energy

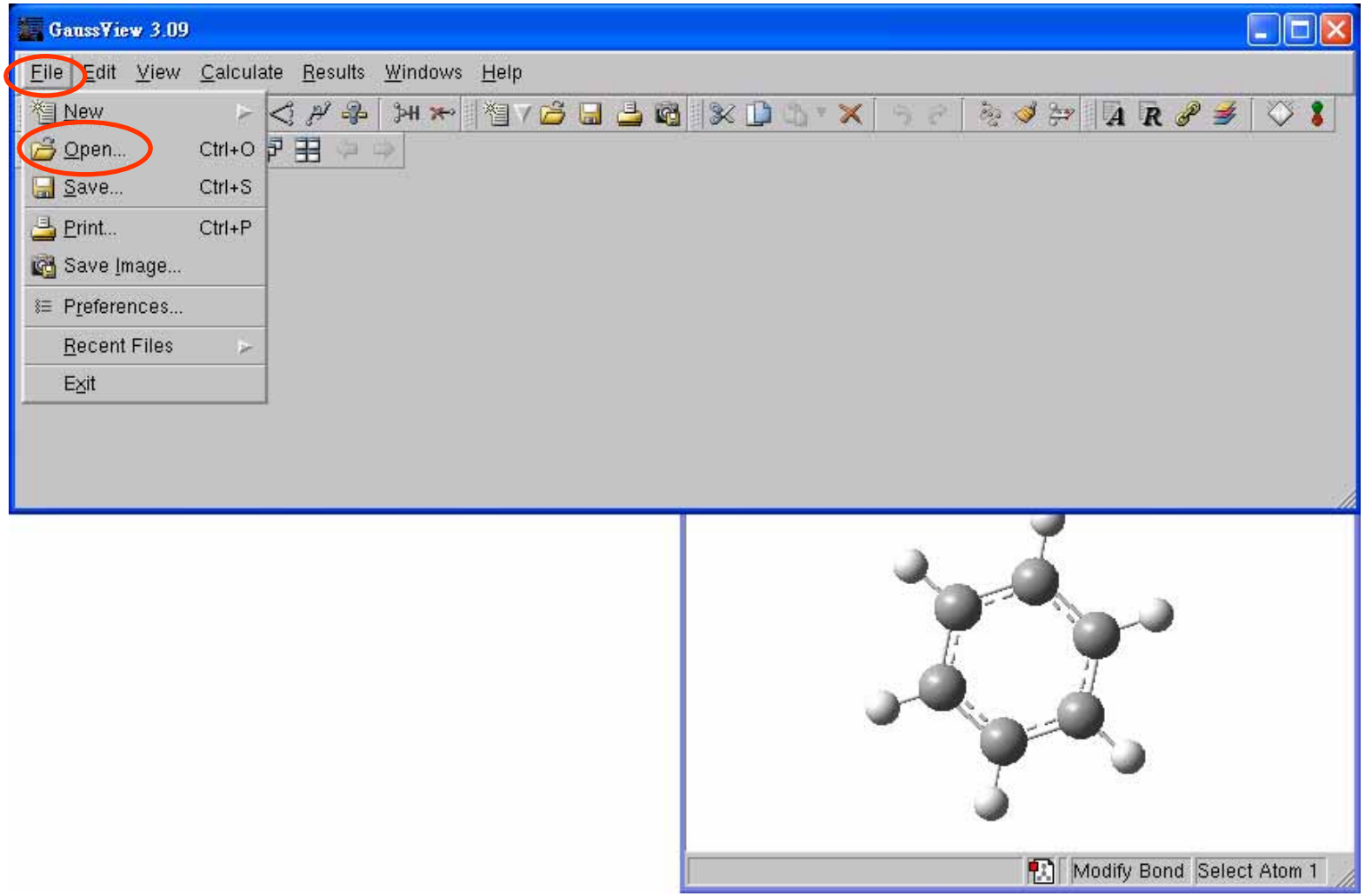
Press Esc → type :/HF= → Enter



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

Check HOMO

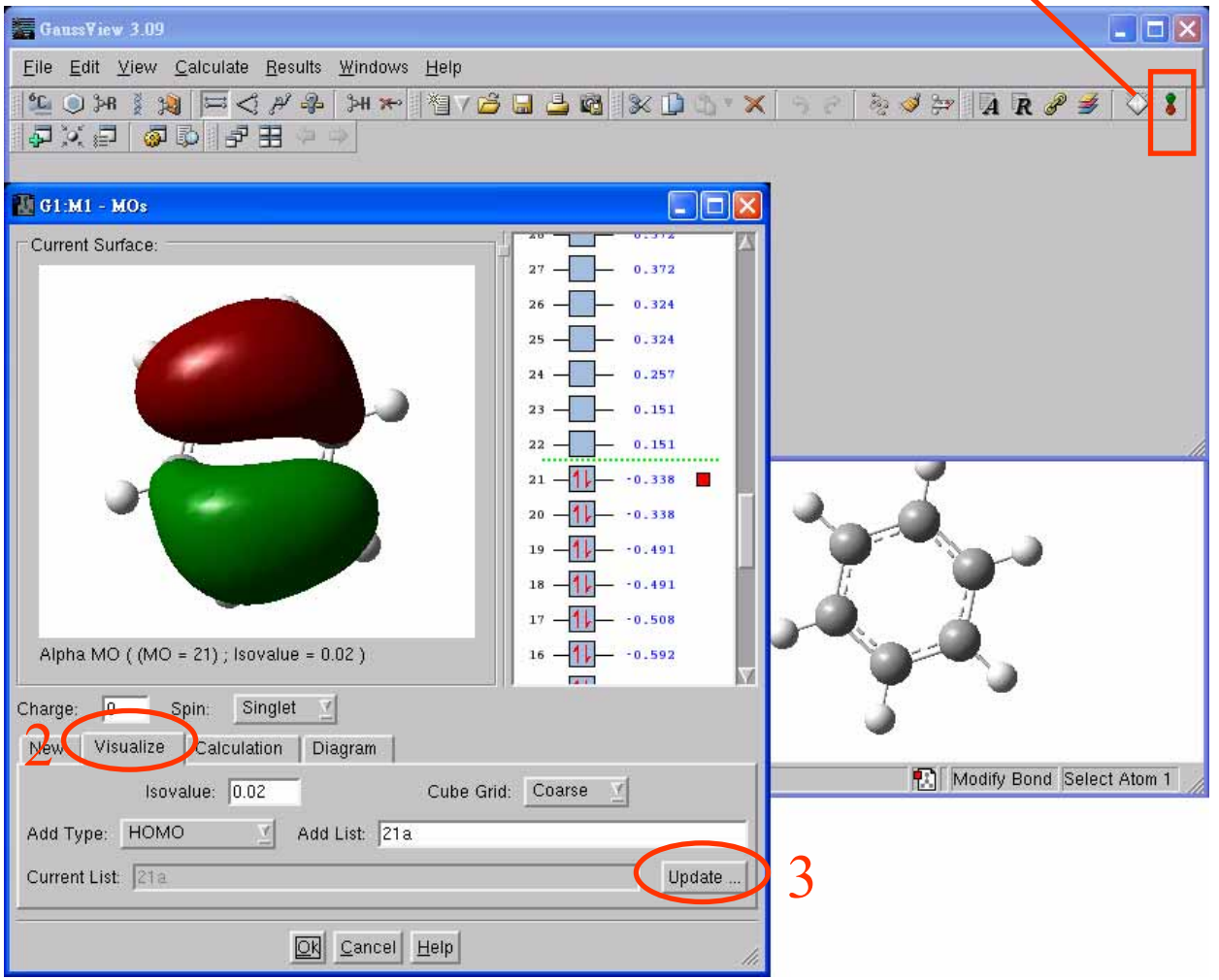
Using GaussView → File → Open *.chk



Check HOMO

Press Molecular Orbital Editor →

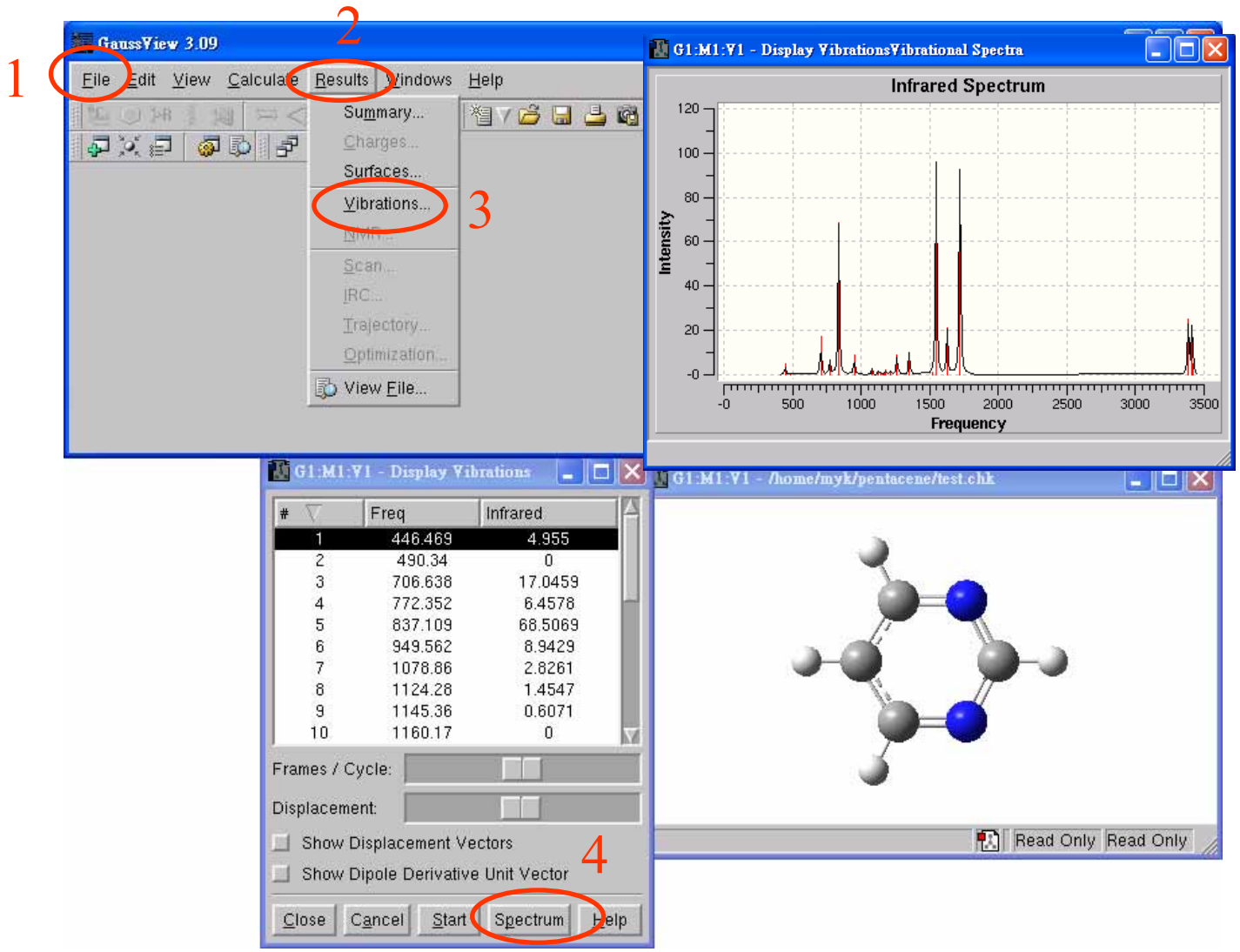
Select Visualize → Press Update



IR Spectrum

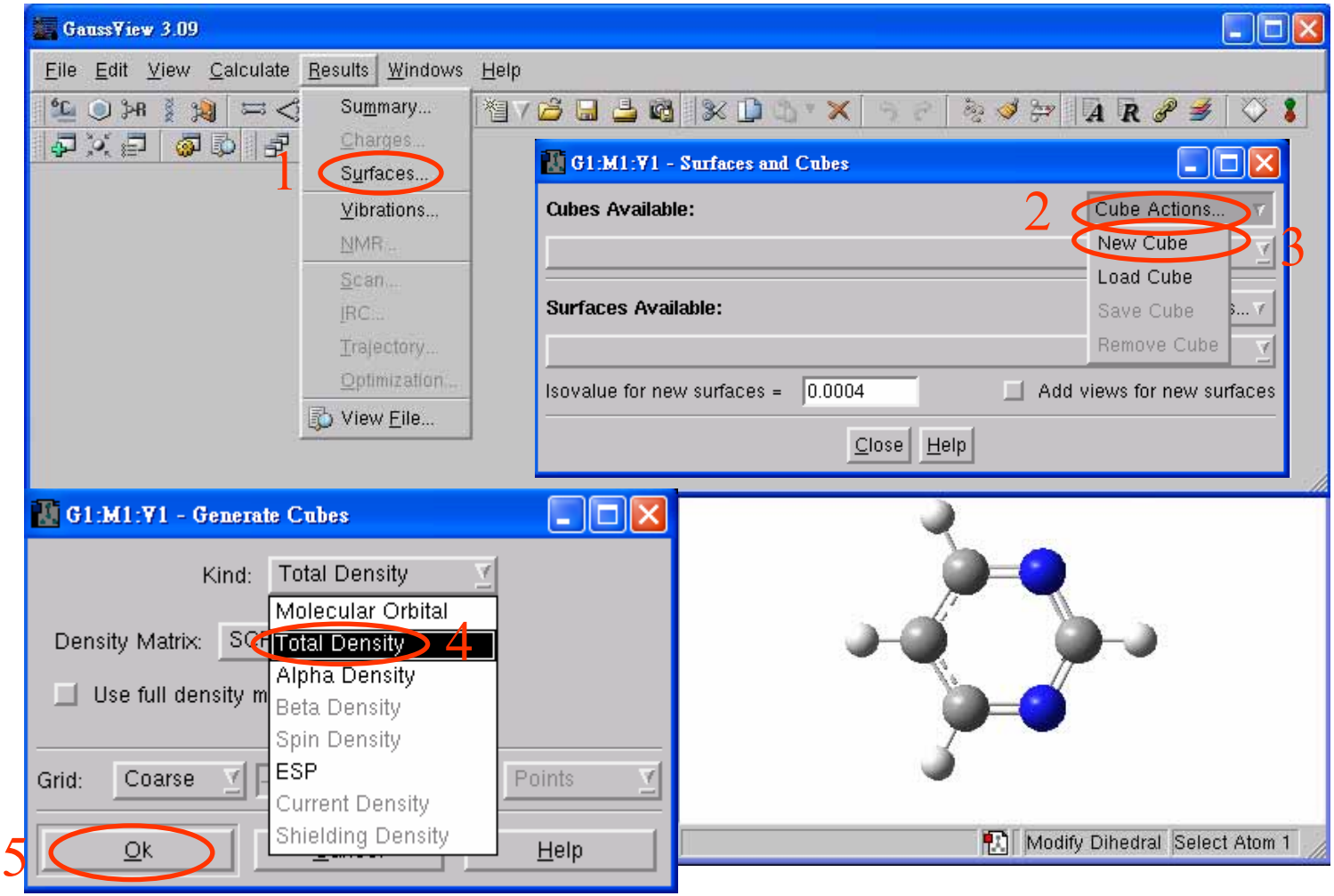
Click File to open *.chk → Click Result →

Select Vibration → Click Spectrum



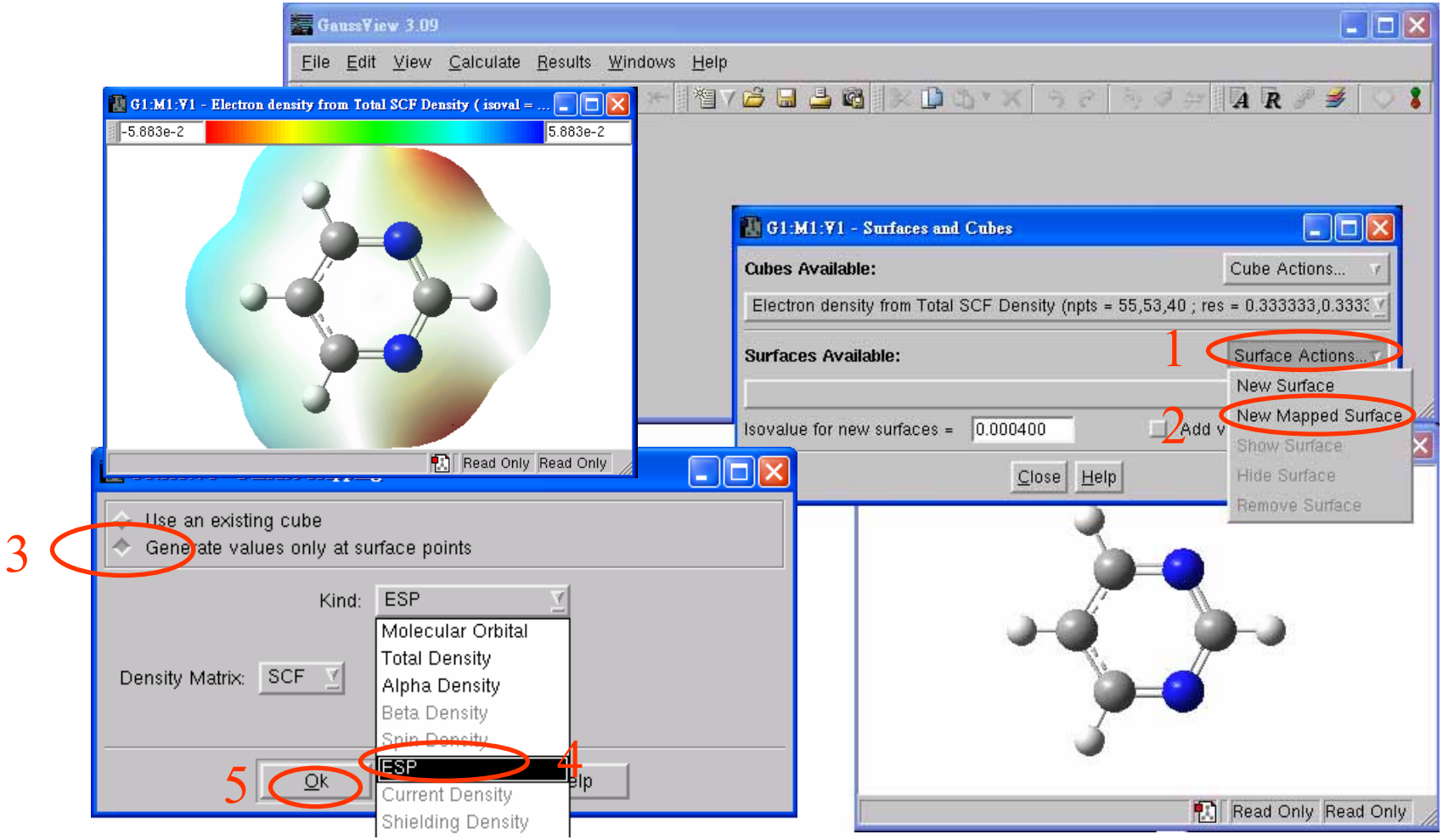
Total density

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

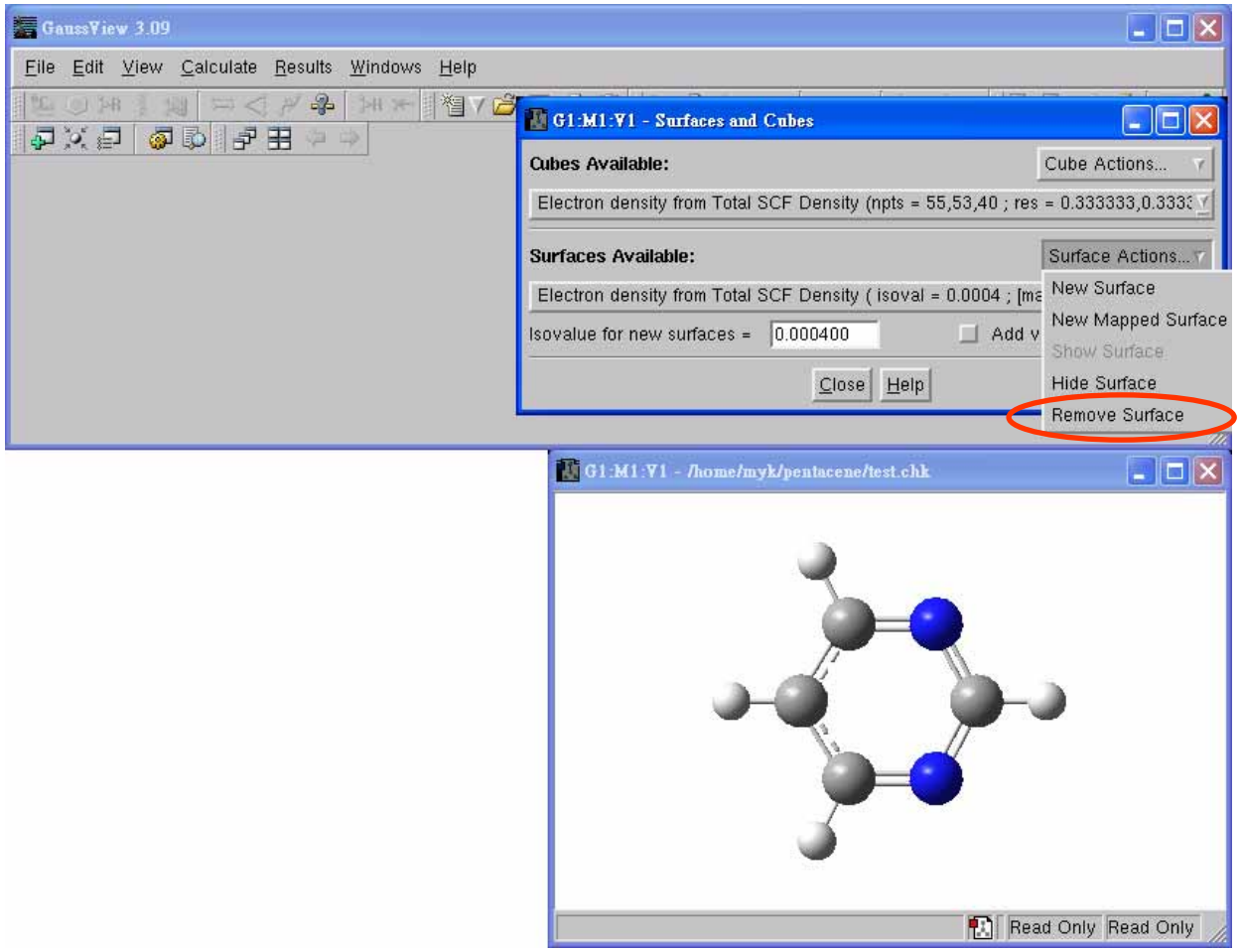


Mapping the MEP

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

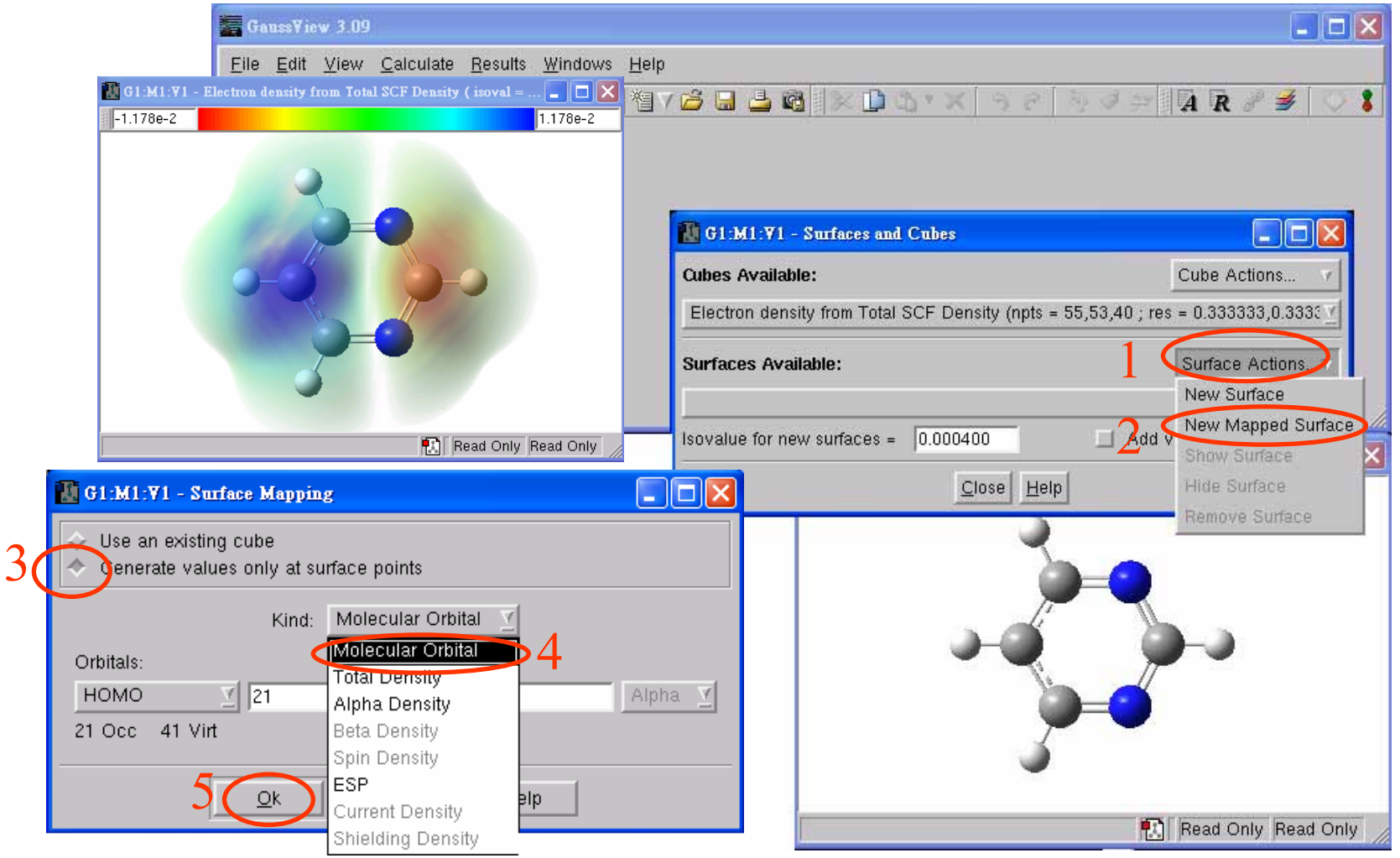


Remove MEP Mapping



HOMO Mapping

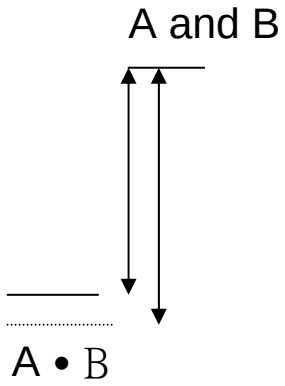
Click Surface Actions → Select New Mapped Surface → Select Molecular Orbital → Click OK



Basis Set Superposition Error (BSSE)

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

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



Counterpoise correction for BSSE

$$\Delta E^{CP}_{\text{BIND}} = E_{\text{HF}}^{a\cup b}(\text{A}\bullet\text{B})_{\text{A}\bullet\text{B}} - E_{\text{HF}}^{a}(\text{A})_{\text{A}} - E_{\text{HF}}^{b}(\text{B})_{\text{B}}$$
$$+ [E_{\text{HF}}^{a}(\text{A})_{\text{A}\bullet\text{B}} - E_{\text{HF}}^{a\cup b}(\text{A})_{\text{A}\bullet\text{B}}] + [E_{\text{HF}}^{b}(\text{B})_{\text{A}\bullet\text{B}} - E_{\text{HF}}^{a\cup b}(\text{B})_{\text{A}\bullet\text{B}}]$$

BSSE correction for A BSSE correction for B

How to Setup Counterpoise Correction in G03

Counterpoise Calculation Results