

How to use Gaussian/GaussView to do this experiment

(Step-by-Step Guide)

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(work together with Jonny Proppe for this practical course)

Outline:

- Part-1. Preparation
- Part-2. Build the molecule by GaussView
- Part-3. Set up calculations
- Part-4. Search the transition states (optional)
- Part-5. Analysis the results from Gaussian

Part-1. Preparation

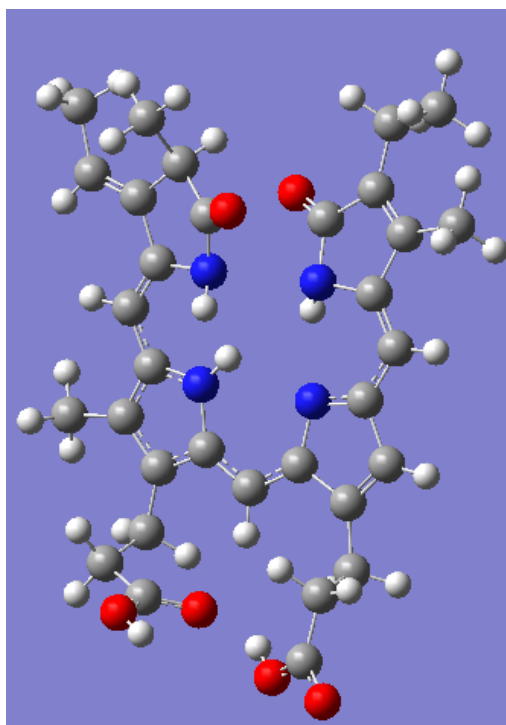
- a. log into the “euler” cluster, open a terminal, type
`ssh -X <nethz>@euler.ethz.ch`
- b. After successfully log in to the “euler” cluster
`vi ~/.bashrc`
add the following line into .bashrc ()
`module load gaussian/09d1`
after that, press “ESC”, type “:wq”, and press “Enter” to save and quit
- c. “source” the .bashrc file, and open the GaussView
`source ~/.bashrc`
`gview &`

Some basic linux commends you may use:

- 1. `mkdir` function creates a new, empty directory with name DIRNAME.
`mkdir DIRNAME`
- 2. `mv` moves or renames files (or directories)
`mv SOURCE DIRECTORY` (move file to directory)
`mv SOURCE SOURCE_WITH_NEW_NAME` (rename file)
- 3. `cp` copies files (or, optionally, directories)
`cp SOURCE DIRECTORY` (copy file to directory)
`cp SOURCE SOURCE_WITH_NEW_NAME` (copy file)
- 4. `scp` copy file between different computers
`scp [[user@]host1:]file1 ... [[user@]host2:]file2`

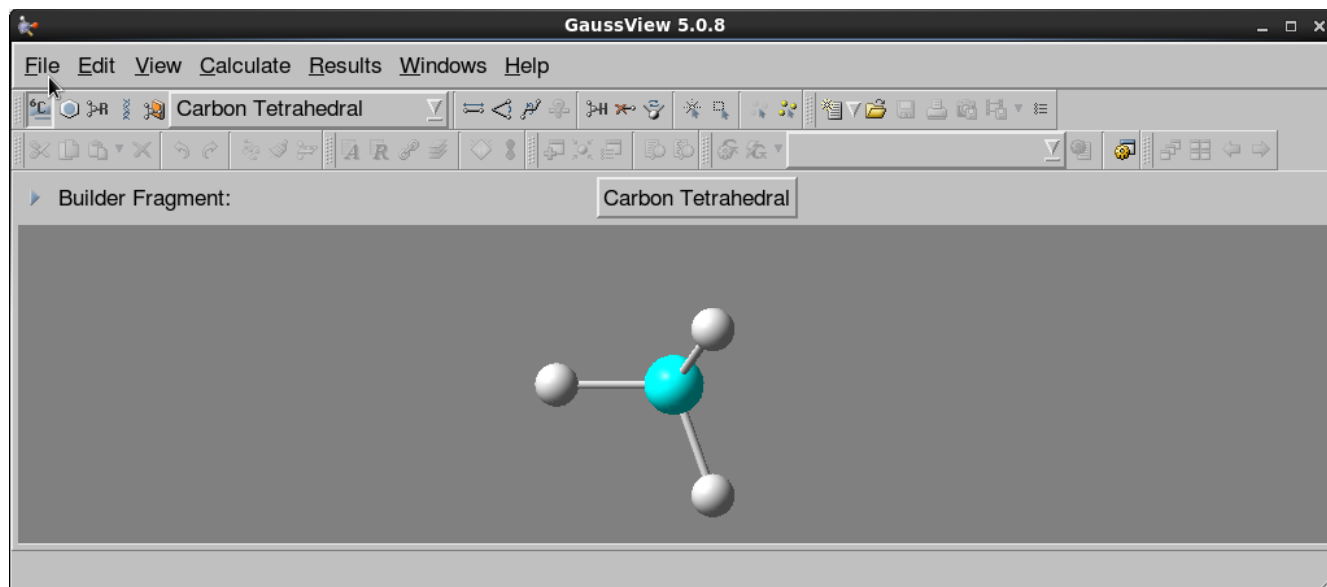
Hints: For detailed information, type “info commend” and press “enter”

Part-2. Build the molecule by GaussView



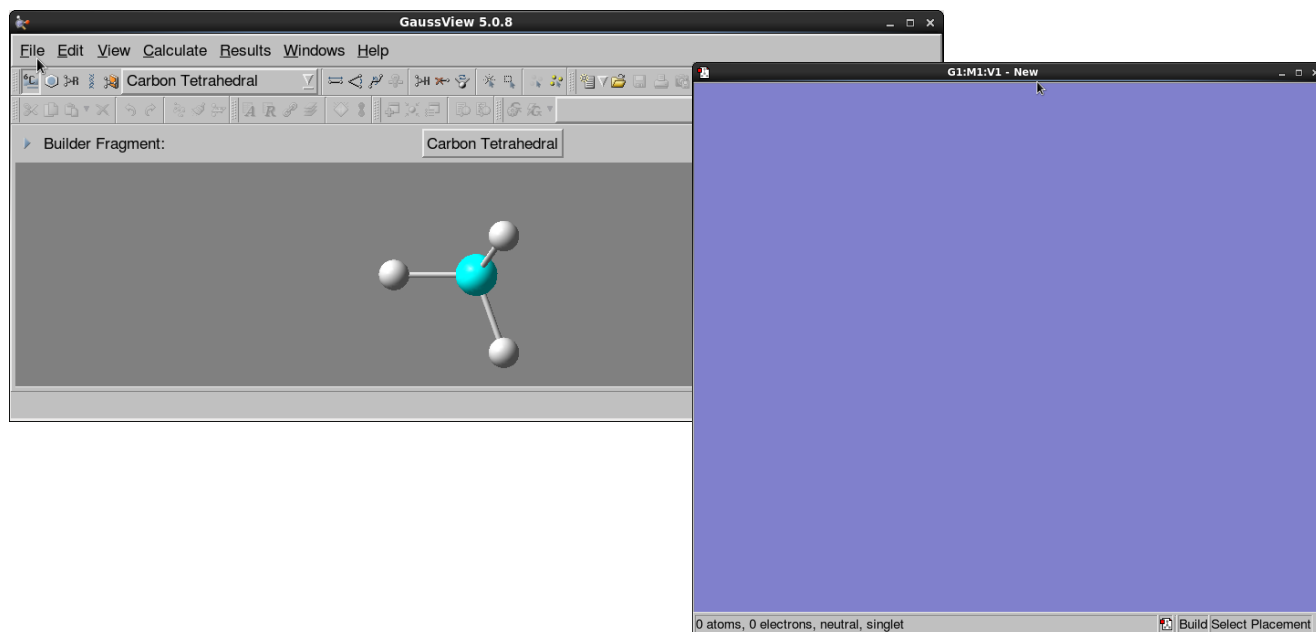
phycocyanobilin in ZZZsss(M) configuration

a. Search “GaussianView”/”GaussView” in applications. Open it. (If use your local machine)



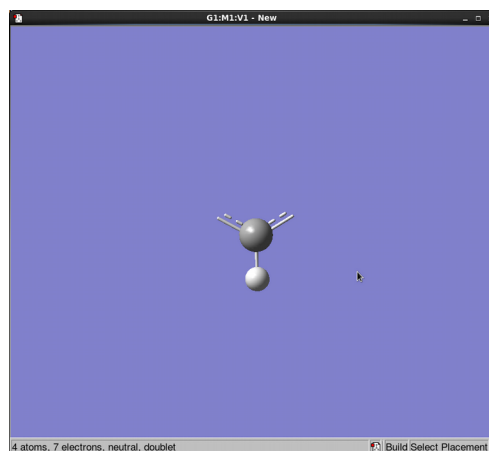
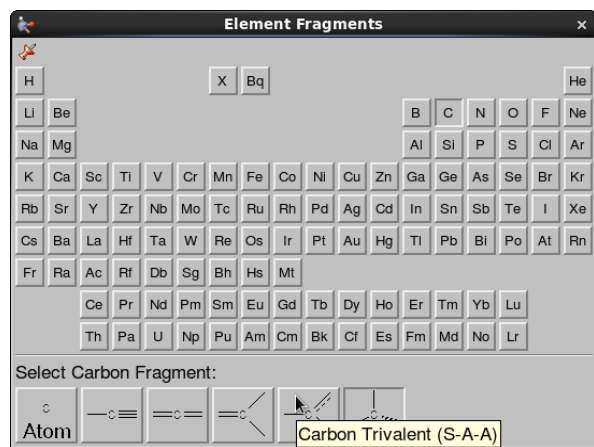
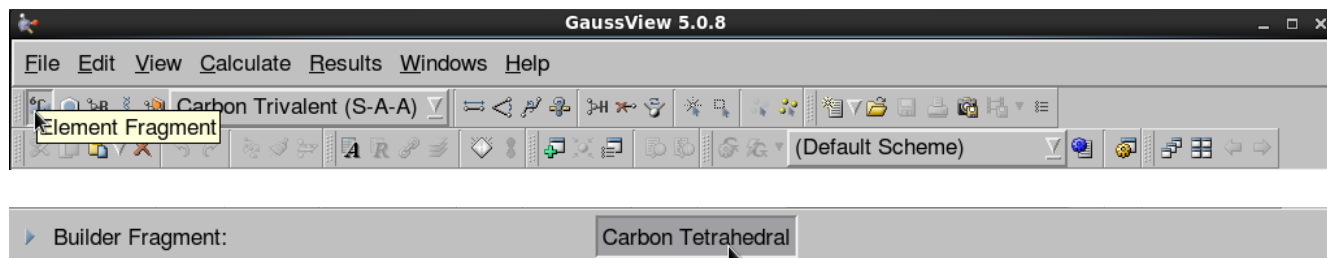
(GaussView Control Panel)

b. Click “File” - “New” - “Create New molecule” (If there is no Building Window)



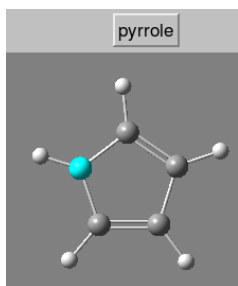
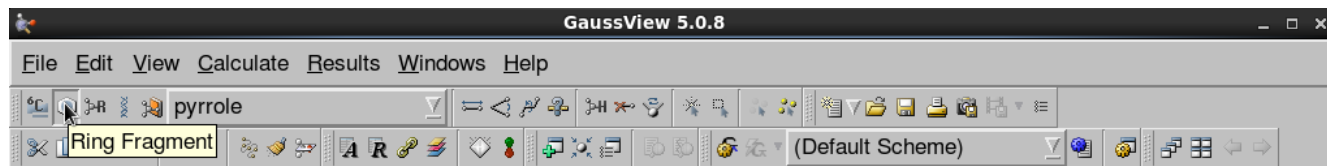
(Building Window)

c. Choose “Element Fragment”, change “Carbon Tetrahedral” to “Carbon Trivalent”, then add it into the Building Window (You could also find the bulider by right-click on the building window)

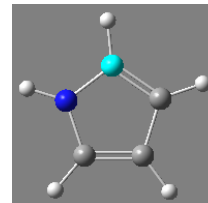


Hints: You can hold on left/right/middle “click”, and at the same time move you mouse, you will find the fragment in the Building Window is responding to your actions.

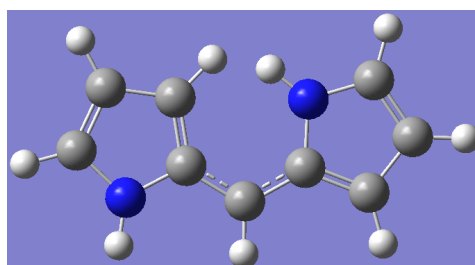
d. Choose “Ring Fragment”, change the Builder Fragment to “pyrrole”, add it to the joint atom of “Carbon Trivalent” by clicking.



also change the joint atom from “N” to “C”



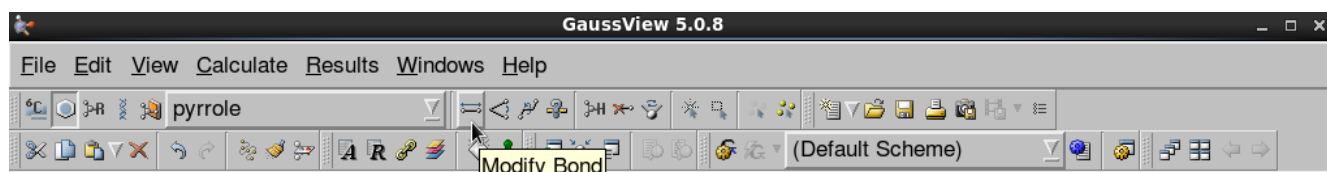
After adding the two “pyrroles”, it probably looks like this, you need to rotate the left “pyrroles”, and delete the “H” which is connecting to the “N” in the right “pyrroles”.



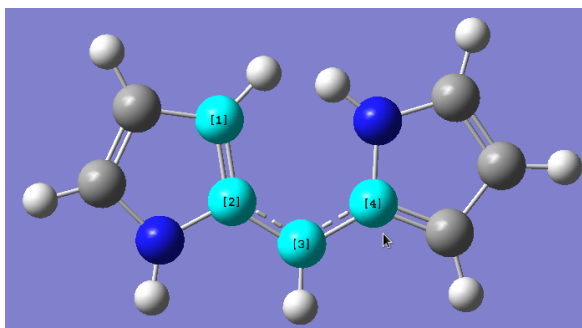
Hints: Any wrong actions can be canceled by “Ctrl” + “z”

e. Modify the molecular structure

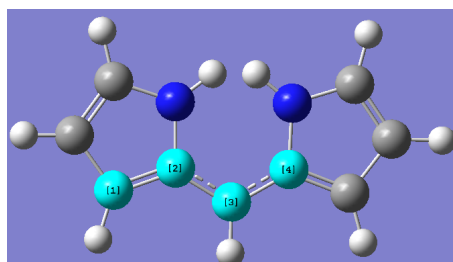
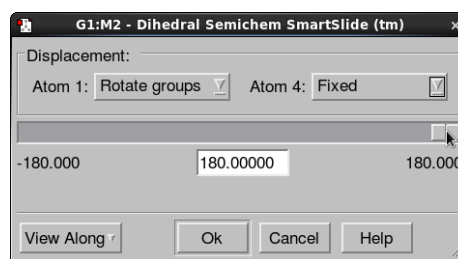
In the control panel, GaussView supplies many tools that can be used to modify the structure, such as “Modify Bond” bellow.



In this example, one can click the “Modify Dihedral”, then sequentially click the 4 atoms in the following figure. On the pop-up “Dihedral Semichem SmartSlide”, set Atom1 as “Rotate group” and Atom 4 as “Fixed”, then change the value to 180°.

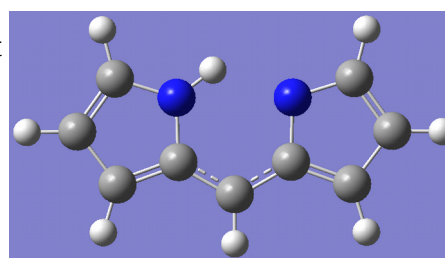


(before)

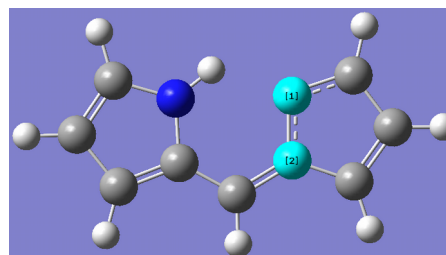
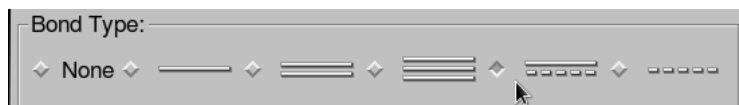


(After)

For the “H” which is connecting to the “N” in the right “pyrroles”, you can first click “Delete Atom” button, then click this “H” atom.

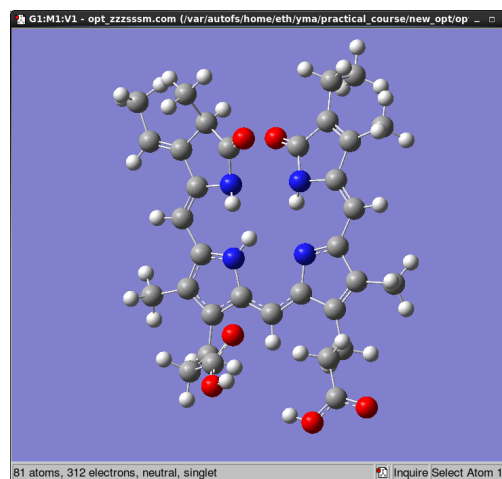


One can also use “Modify Bond” to change the bond type in order to make it looks better. It is optional since the final bond type is depend on the optimized structure.



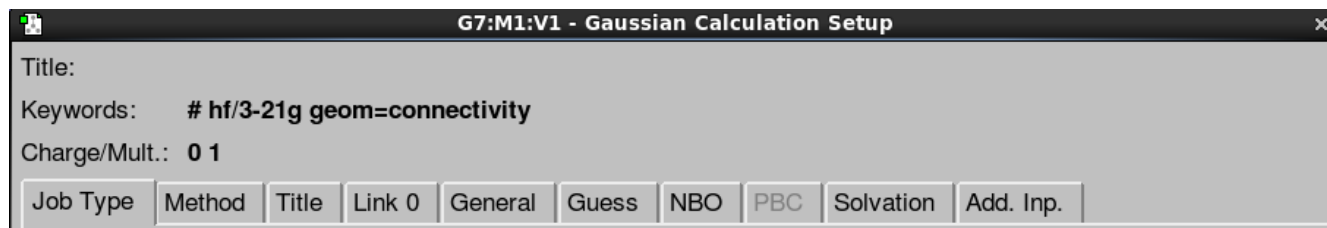
Now, you can repeat the steps “c”, “d”, “e”, until you build up the initial structures of phycocyanobilin (ZZZsssM).

Hints: Many introductions of GaussView can be found in the web, such as Introduction to GaussView 5.0 - YouTube (04:29) <https://www.youtube.com/watch?v=sxKyfwy51h4>



Part-3. Set up calculations

a. Click “Calculate” - “Gaussian Calculation Setup”, a pop-up slide will emerge. Many options will be involved in this experiment.

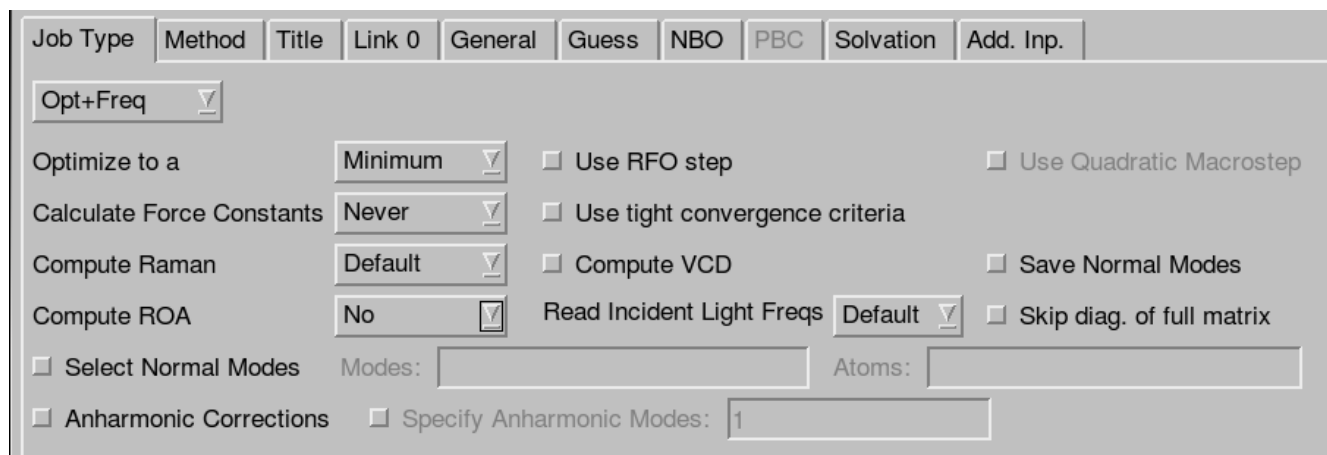


b1. If only the self-consistent file (SCF) calculation is needed.

Set up the “Job Type” as “Energy”. The other options are no need to be set at this moment.

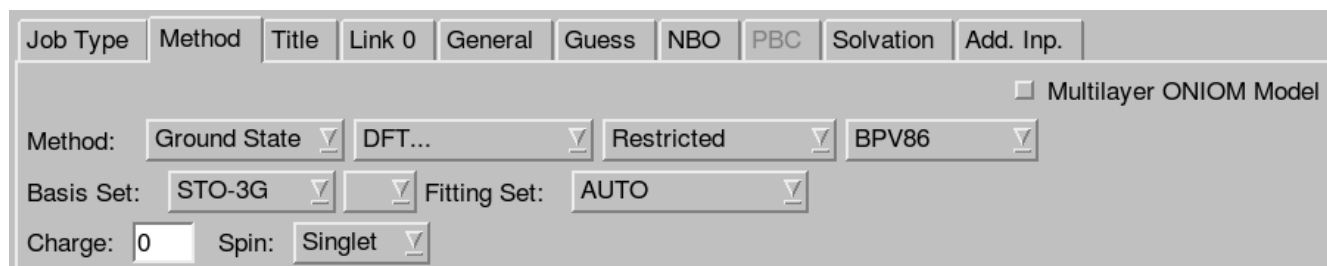
b2. If the optimized geometry is needed.

Set up the “Job Type”, change to “Opt + Freq” (or only “optimization”), and let it Optimize to a “Minimum”, e.g.

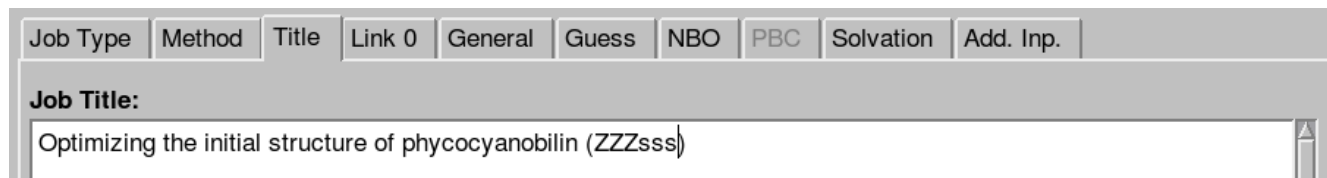


c. Set up “Method”, change Method line to “Ground State” - “DFT...” - “Restricted” - “BPV86”; and Basis Set line to “STO-3G”, Fitting set “AUTO”.

(Notice: The “BPV86” functional will be changed to “BP86” later)



d. Set up “Title” (as you like)



Job Type Method Title Link 0 General Guess NBO PBC Solvation Add. Inp.

Job Title:
Optimizing the initial structure of phycocyanobilin (ZZZsss)

e. Set up the “Link” by yourself, either “Options” or “Edit” button can be used. Normally 8 GB memory should be enough for this experiment, and 8 processors (at most 24 for each student) can be chosen. Remember that you need to save the check-point file for the later usage.



Job Type Method Title Link 0 General Guess NBO PBC Solvation Add. Inp.

Options Edit

Memory Limit: Specify... 8 GB

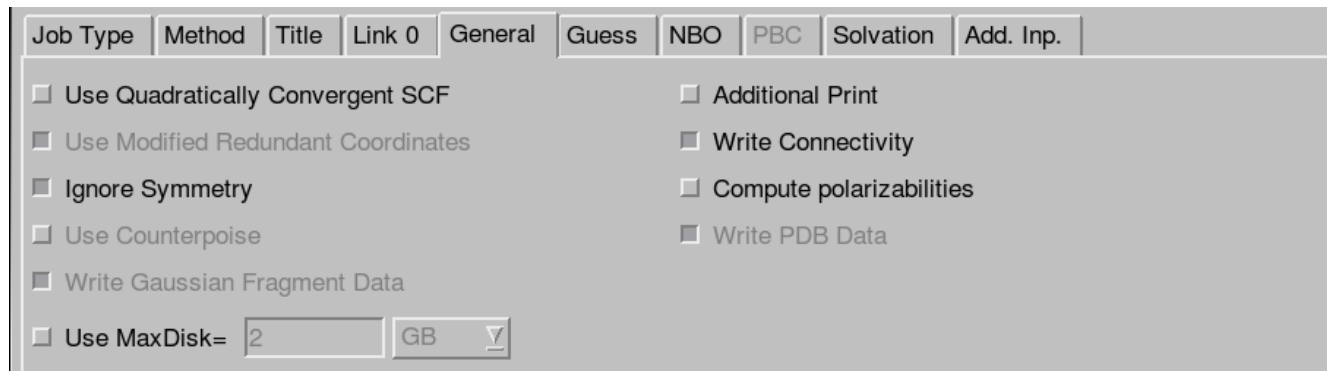
Chkpoint File: Default name {parent file name}.chk

Read-write File: Don't save

Linda Workers: Don't use

Shared Processors: Specify... 24

f. Set up “General”, choose (add) “Ignore Symmetry”, since this molecule is obviously no symmetry.



Job Type Method Title Link 0 General Guess NBO PBC Solvation Add. Inp.

Use Quadratically Convergent SCF Additional Print

Use Modified Redundant Coordinates Write Connectivity

Ignore Symmetry Compute polarizabilities

Use Counterpoise Write PDB Data

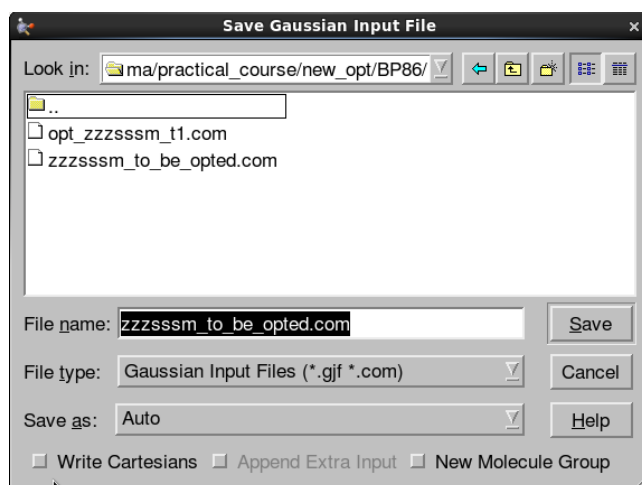
Write Gaussian Fragment Data

Use MaxDisk= 2 GB

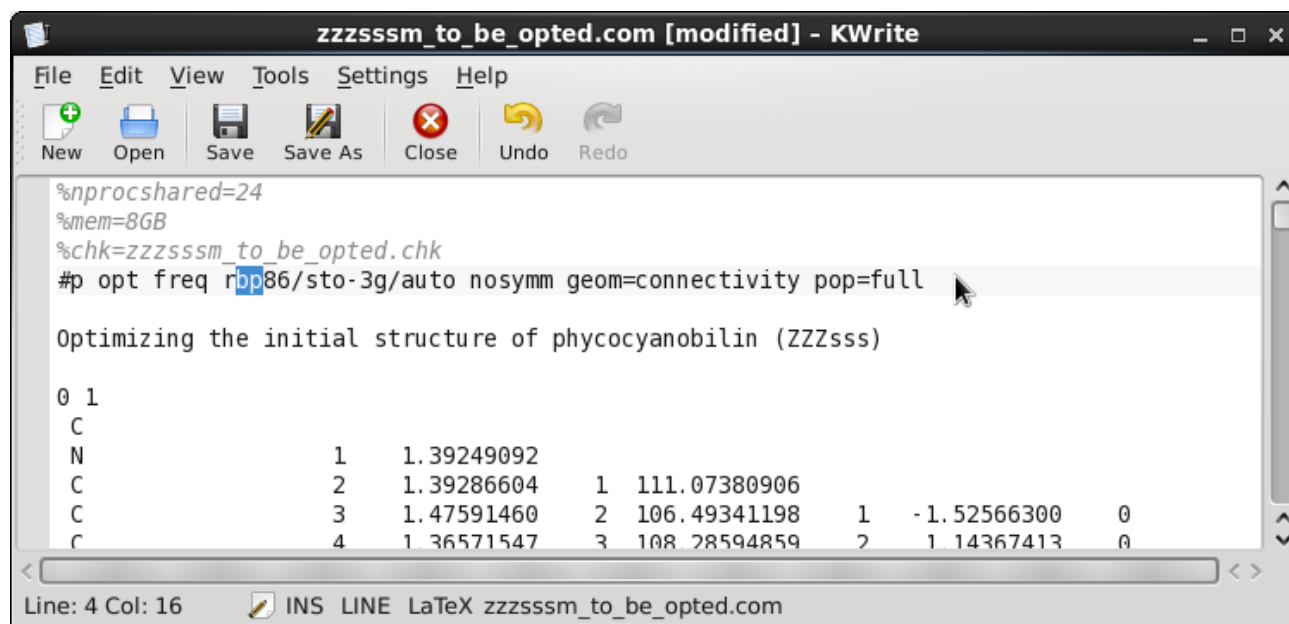
g. The “NBO”, “Guess”, “PBC”, “Solvation” and “Add. Inp.” options are no need to be specified at this moment.

h. After finish all of the set-ups, one can click “Edit”, in the pop-up window, save it as the “Gaussian Input Files”, then one can check and modify this input in Text editor.

(Notice: no need to choose “Write Cartesians”, since the internal coordinates should work better in this experiment)



i. In the Text editor, we need change the functional to “BP86”, and also add “pop=full” to active detailed output.



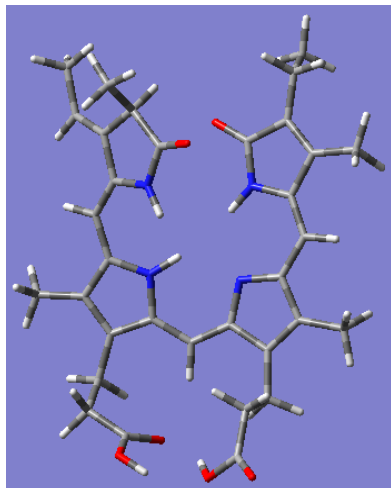
Please notice:

- 1) Typical time for each optimization job is about 15~30min. When there is a job running you can prepare the other configurations.
- 2) If you plan to do the transition state search (e.g. QST3 in the next part), the order of atoms in the three configurations must be the same. It means it is wise to build the base structure (e.g. ZZZsss), then modify some bond/angle/dihedral to get the other structure.
- 3) **DO NOT** submit you job directly. Use “`bsub -n ncpus -W 8:00 nohup g09 your_input_file.com`”, e.g.

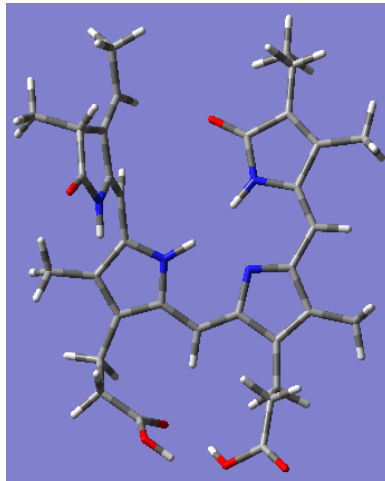
`bsub -n 8 -W 8:00 nohup g09 SCF_ZZZsssM.com`

Part-4. Search the transition states using QST3 in Gaussian (optional)

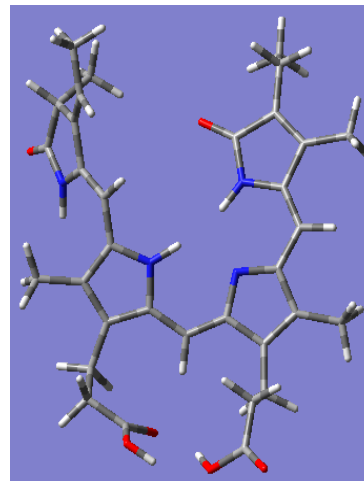
Assuming that we already get all of the optimized structures, and we want to search the transition state (TS) between ZZZsss and ZZZass, in this case, a guess structure of TS need to be given when using QST3.



ZZZsss



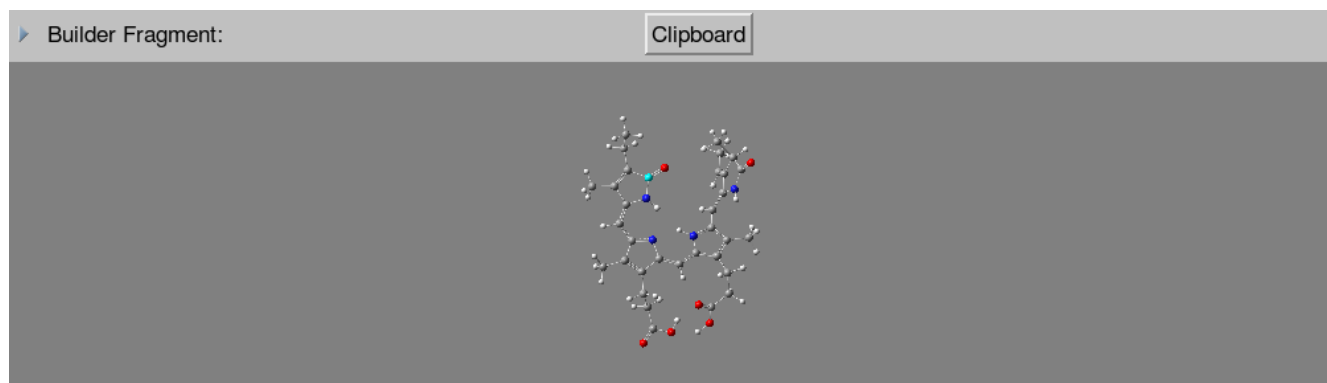
guess TS?



ZZZass

I. When using GaussView

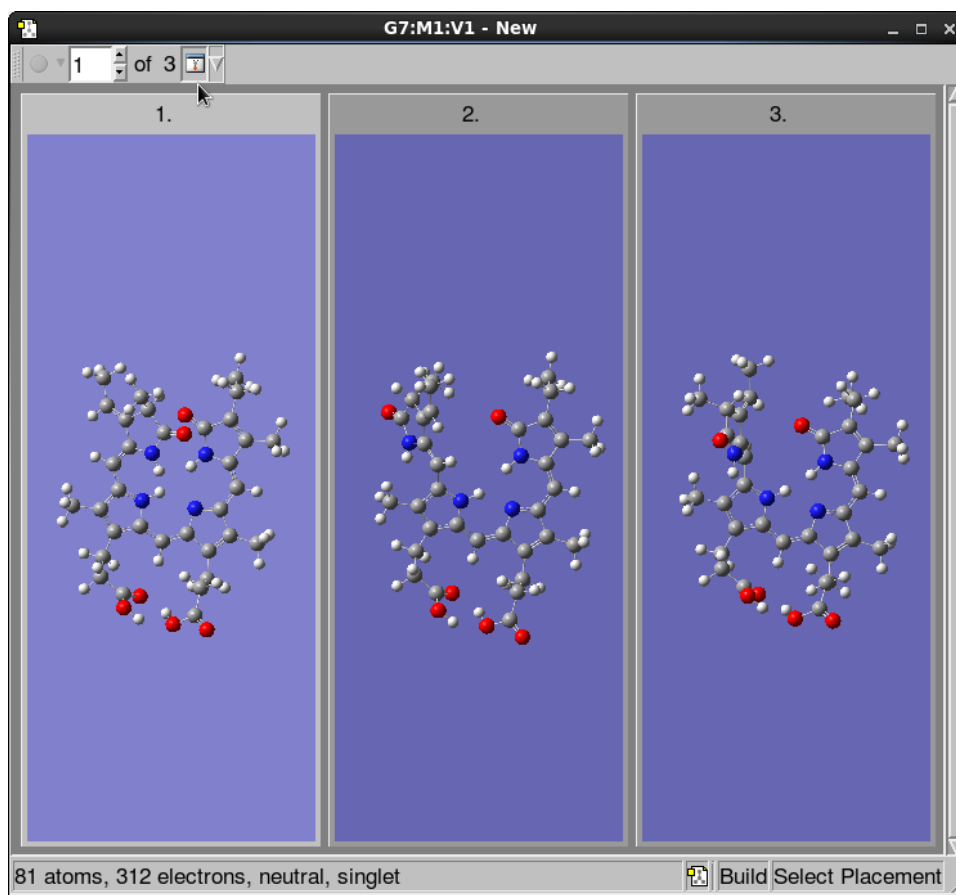
a. Open the optimized structure of ZZZsss (e.g. .log or .fchk file), click “Edit” - “Copy”, then you can find now the molecule is in the working “Control Panel”.



b. Open a new building window, click “Edit” - “Paste” - “Add to Molecule Group”

c. Open the optimized structure of ZZZassM (e.g. .log or .chk file), copy and also add it into the building window that opened in b.

d. Build a guess TS structure (it can be obtained by modifying some bond/angle/dihedral in this case), copy and also add it into the building window that opened in b. If you click the “list view”, you will see



e. Set up the Calculations. An example is shown bellow:

The screenshot shows the "G1:M1:V1 - Gaussian Calculation Setup" dialog box. The "Title" field is "Title Card Required". The "Keywords" field contains "# opt=(calcfc,qst3) freq sto-3g nosymm geom=connectivity rbp86". The "Charge/Mult." is "0 1". The "Job Type" is "Opt+Freq". The "Optimize to a" dropdown is set to "TS (QST3)". There are several checkboxes: "Use RFO step" (unchecked), "Use Quadratic Macrostep" (unchecked), "Use tight convergence criteria" (unchecked), "Compute VCD" (unchecked), "Save Normal Modes" (unchecked), "Skip diag. of full matrix" (unchecked), "Select Normal Modes" (unchecked), and "Anharmonic Corrections" (unchecked). The "Specify Anharmonic Modes" field is set to "1". The "Geometry to use for TS Guess" is set to "3". The "Additional Keywords" field contains "rbp86". The "Scheme" is "(Unnamed Scheme)". At the bottom, there are buttons for "Submit...", "Quick Launch", "Cancel", "Edit...", "Retain", "Defaults", and "Help".

Hint: You could also use QST2, then the guess structure is not needed because the averaged structure will be used as the guess structure.

II. When using Text editor

This is quite straightforward, just modify the Gaussian input file

```
%nproc=8
%mem=8GB
%chk=TS_zzzsss_to_zzzass.chk
#p opt=(calcfc,qst3) freq rbp86/sto-3g/auto nosymm geom=connectivity
```

Reactant (ZZZsss)

charge spin
[copy the structure]

Product

charge spin
[copy the structure]

TS-guess (must in the last)

charge spin
[give the structure]
(Don't forget these is a blank line in the end)

When the job finish, you need to check the log file. One imaginary frequency should be found for a Transition state. e.g.

	1	2	3
	A	A	A
Frequencies --	-45.3774	11.3251	17.8614

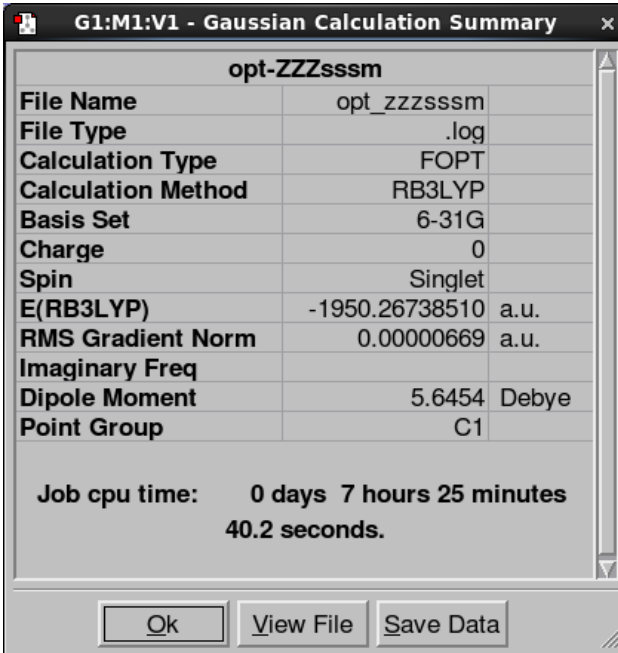
After get the transition states from QST3

- * Better use opt=(TS,tight) to do a further optimization of the TS structure from QST3
- * Frequencies analysis should be followed in order to check whether it is a true TS state.
- * The calculation of reaction path should be followed by integrating the intrinsic reaction coordinate (IRC)

For the advanced usages of “opt”, “freq”, and “IRC”
http://www.gaussian.com/g_tech/g_ur/k_opt.htm
http://www.gaussian.com/g_tech/g_ur/k_freq.htm
http://www.gaussian.com/g_tech/g_ur/k_irc.htm

Part-5. Analysis the results from Gaussian

For the **general information** of the your finished job, one can use GaussView to open a **.chk** file, then click “Results” - “Summary”. The detailed **text output** could also be opened by “View file”.



G1:M1:V1 - Gaussian Calculation Summary

opt-ZZZsssm

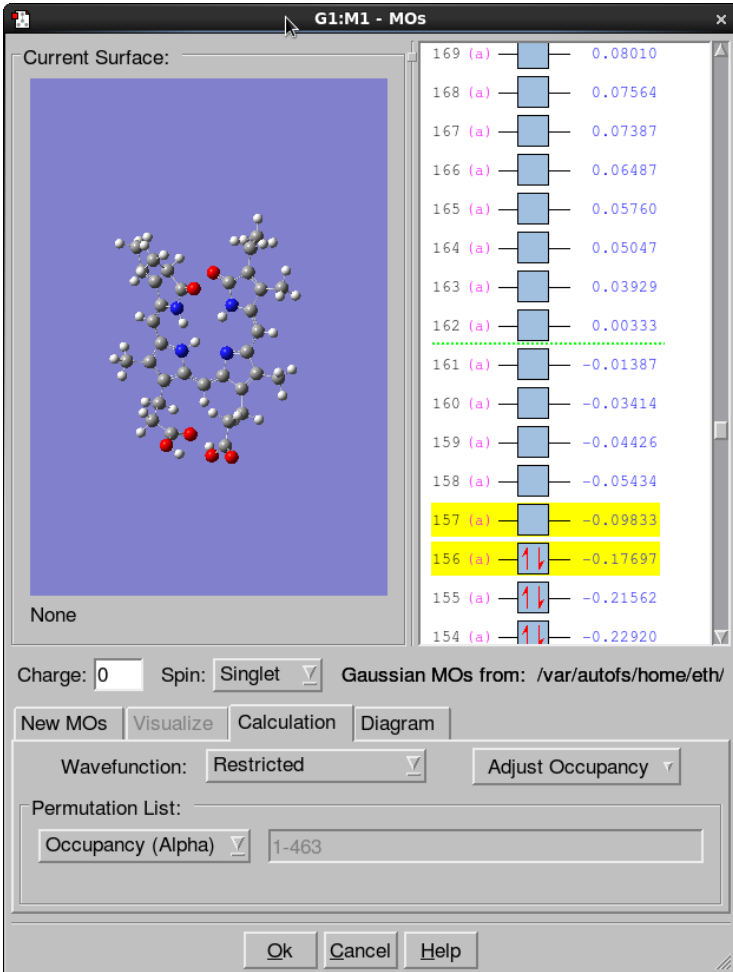
File Name	opt_zzzsssm	
File Type	.log	
Calculation Type	FOPT	
Calculation Method	RB3LYP	
Basis Set	6-31G	
Charge	0	
Spin	Singlet	
E(RB3LYP)	-1950.26738510	a.u.
RMS Gradient Norm	0.00000669	a.u.
Imaginary Freq		
Dipole Moment	5.6454	Debye
Point Group	C1	

Job cpu time: 0 days 7 hours 25 minutes 40.2 seconds.

Ok View File Save Data

For the **electron configuration** as well as the **orbital energies**, they can be shown by clicking “Edit” - “MOs”.

For example, in this case the HOMO is NO. 156 orbital with orbital energy -0.17697 A.U., the LUMO is NO. 157 orbital with orbital energy -0.09833 A.U..



G1:M1 - MOs

Current Surface: None

169 (a)	0.08010
168 (a)	0.07564
167 (a)	0.07387
166 (a)	0.06487
165 (a)	0.05760
164 (a)	0.05047
163 (a)	0.03929
162 (a)	0.00333
161 (a)	-0.01387
160 (a)	-0.03414
159 (a)	-0.04426
158 (a)	-0.05434
157 (a)	-0.09833
156 (a)	-0.17697
155 (a)	-0.21562
154 (a)	-0.22920

Charge: 0 Spin: Singlet Gaussian MOs from: /var/autofs/home/eth/

New MOs Visualize Calculation Diagram

Wavefunction: Restricted Adjust Occupancy

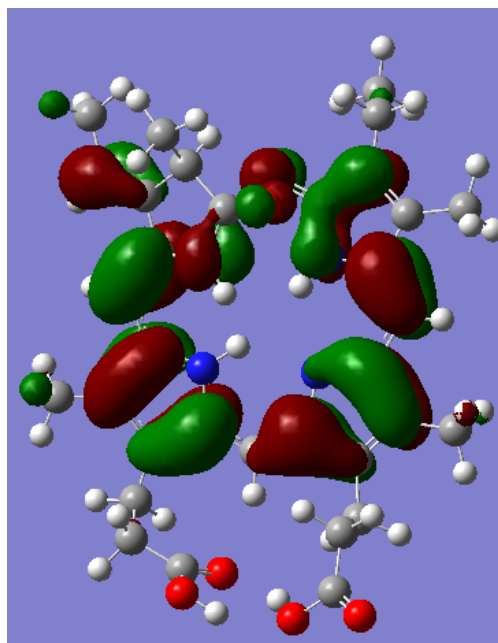
Permutation List:

Occupancy (Alpha) 1-463

Ok Cancel Help

For the **Atomic charges and Dipole Moment**, one can use GaussView to open a .chk/.fchk file, then they can be shown by click “Results” - “Charge Distribution”.

For the “**electron density**”/ “**spin density**”/ “**molecular orbitals**” etc., use GaussView by clicking “Results” - “Surfaces/Contours”. In the pop-up slide, one can use the “Cube Actions” to generate the cube file, “Surface Actions” - “New Surface” button to show the HOMO orbital.



HOMO orbital (NO. 156)