Quantum Chemistry with *Gaussian* using *GaussView*

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This tutorial is designed to introduce preparation and analysis of quantum chemistry calculations using *Gaussian* with *GaussView*. The systems of interest are toluene and p-cresole that can be thought of as mimics of phenylalanine and tyrosine protein side chains.

Estimated time to complete this tutorial is 1.5 hr.

Outline: we will use the SCS computer cluster, triton, to prepare systems and analyze the results using *GaussView* and model using *Gaussian*.

1. Software

Triton: *Gaussian*, *GaussView*. Personal computer: xserver (*Xming* for a Windows machine) or Terminal (for a Mac).
This tutorial can to be completed with iMac computers of the VizLab or with personal computers with Windows or Mac OS. Small modifications might be needed when used on other computers.

2. Starting GaussView

Note: when using a Windows computer, install Xming, http://www.straightrunning.com/XmingNotes/, or other xserver of choice.

Open Terminal window

Connect to Triton (note when working outside of the University network, on need to start a VPN first):

```
> ssh –YC triton.scs.uiuc.edu
```

Make a new directory for this tutorial:

```
> mkdir gaussian-gv-tutorial
```

Go to the newly made directory:

```
> cd gaussian-gv-tutorial
```

Set up your session to use *Gaussian*. You will have to repeat each time you connect to Triton:

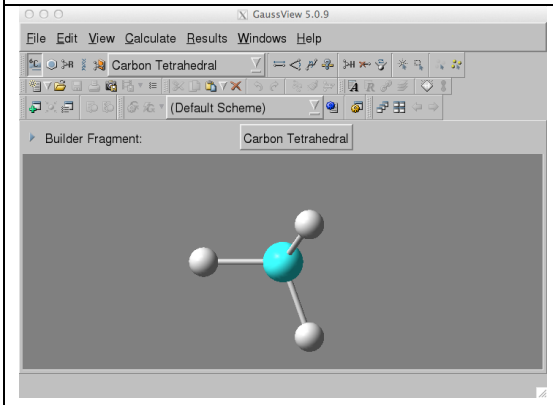
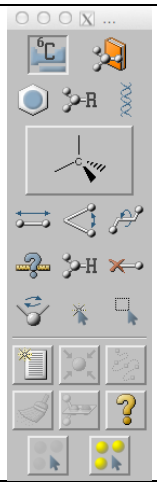
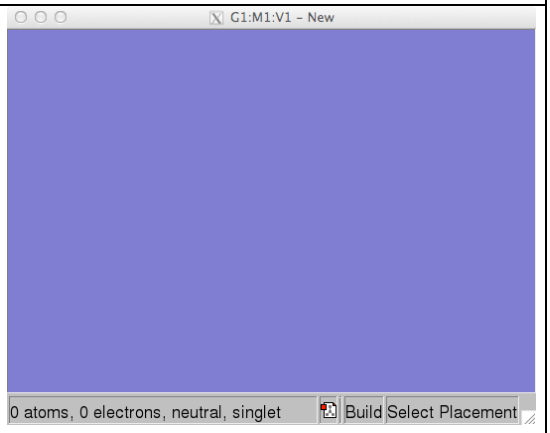
```
> source /share/apps/gaussian/g09_login.csh
```

Lunch *GaussView*:

```
> gv
```

Note: If you are usgin the BASH shell, source `/share/apps/gaussian/g09_login.sh` instead

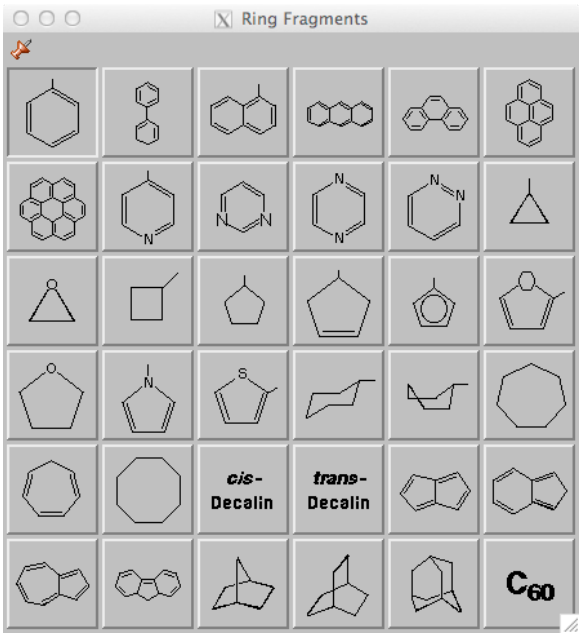
Initially two windows of *GaussView* will be displayed. Open Builder window View->Builder. *GaussView* will remember to keep it open next time.

Main window	Builder	New molecule window
		

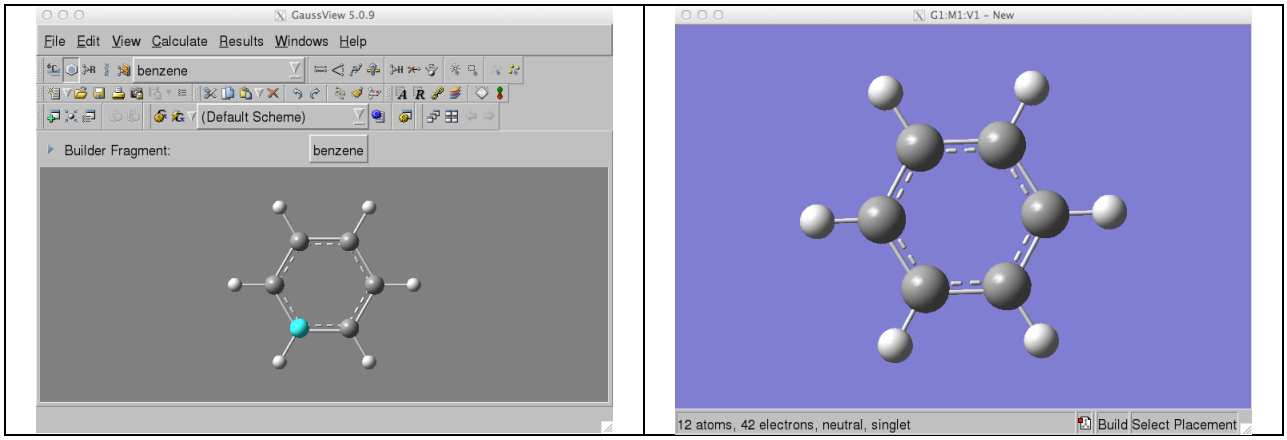
3. Build a molecule of toulene

3.1 Start new molecule from the Main window: File->New->Create Molecule Group

3.2 In the Builder window click the ring button - the Ring Fragments window will appear:

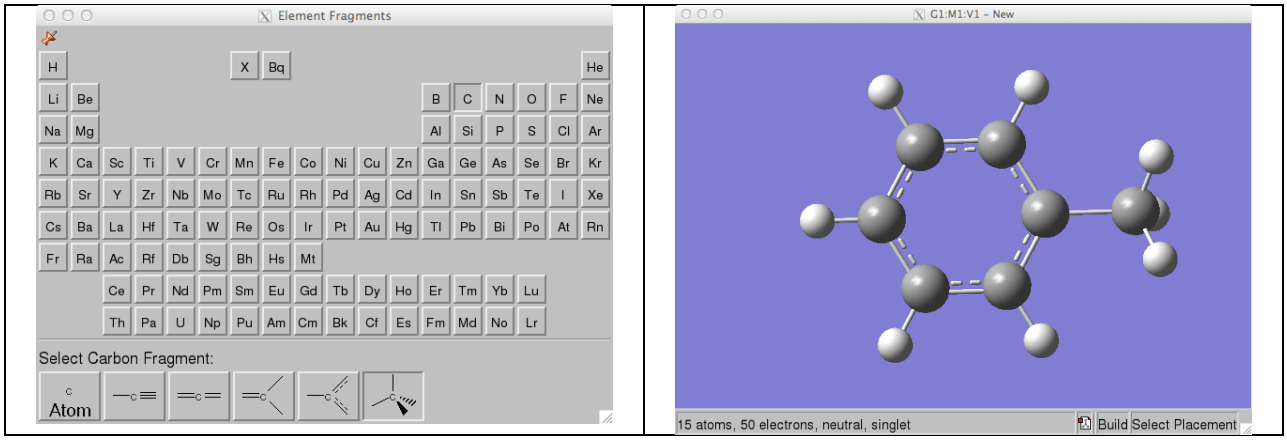


Select benzene and it appears in the Main window. Note the Builder Fragment button also displays “benzene.” Click anywhere in the New window and benzene will be added:



3.3 Click on the Element button on the Builder panel and Element Fragments palette will be shown. Select Carbon Tetrahedral and click on of the hydrogen atom to make toluene.

3.4 Use Minimization routine to quickly improve geometry: click the Clean button (the broom icon). *GaussView* will run a classical mechanics minimization of the prepared structure. The calculation will be completed very fast. Save your work as toluene.com



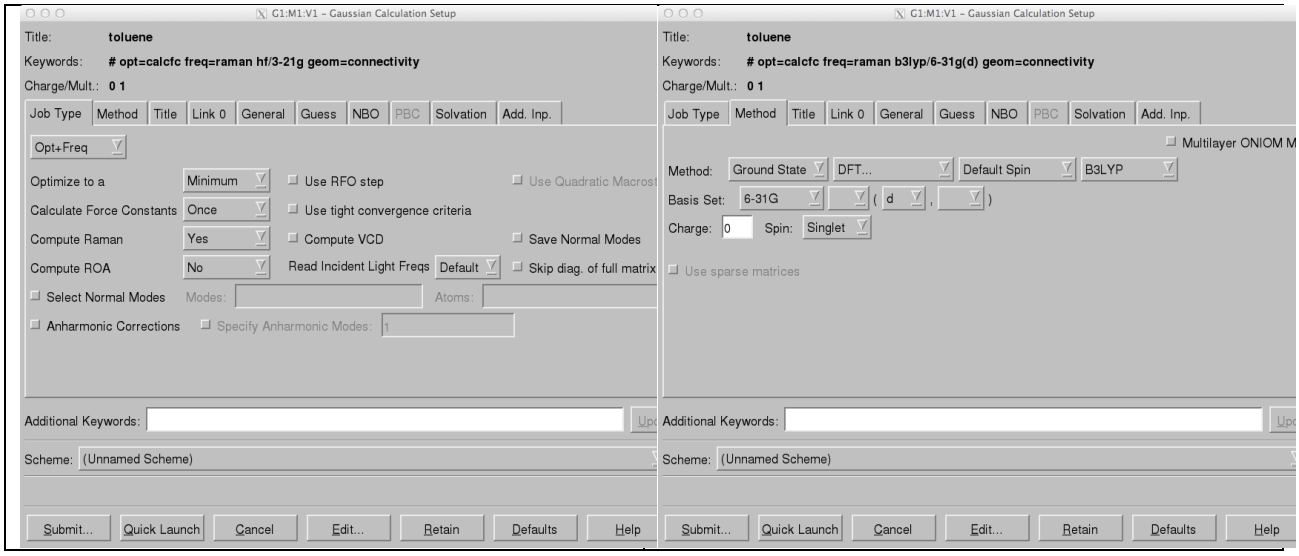
4. Calculation setup

Open Calculation setup window: Calculate-> Gaussian Calculation Setup. The Gaussian Calculation Setup window will appear.

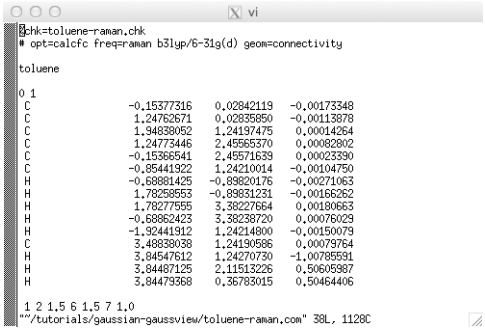
Overview. We will need to make selection in the following tabs: 1) Title, 2) Job Type – Opt+Freq/Minimum/Compute Raman, 3) Method- Ground State/DFT/B3LYP/6-31G(d) and 4) Link 0 – memory and number of CPUs.

Please note below the selections on the Job Type and Methods tabs.

Note: the keywords selected are reprinted on the top of the Calculation Setup window, for example the basis set was changed from 3-21g to 6-31g(d). The title “toluene” was entered on the Title tab. Under the Link 0 tab set memory to 8 GB and number of processors to 8.



Save file: File->Save. Name: toluene-raman.com.



Hint: It is always a good idea to visually inspect prepared file. One can click Edit button to display the current file. The text editor that is available on triton is *vi*.

Please see the last part of our Unix tutorial for a very brief introduction to vi: http://computing.scs.illinois.edu/tutorials/unix-primer-0

5. Calculation submission

We will not use submission from *GaussView* but will use the bash Linux script, submit-g09, to submit a *Gaussian* job. If you like to have more details on the exact content of the script, open it in vi: vi /usr/local/bin/submit-g09. Please remember to quit vi, without saving the changes using “:q!” in the editing mode.

Check the status of queues on Triton to select a queue, which has available processors:

```
> qstat –g c
```

Submit job on 8 processors (specified in the .com file) to the queue named “ib1”:

```
> submit-g09 –q ib1 toluene-raman.com
```

Check the status of your job in the queue:

```
> qstat –u mylogin
```

Here are possible outputs: qw – your job is waiting to be ran; r the job is running. No output means your job is completed.

Look in the end of the log file to see whether the job is completed:

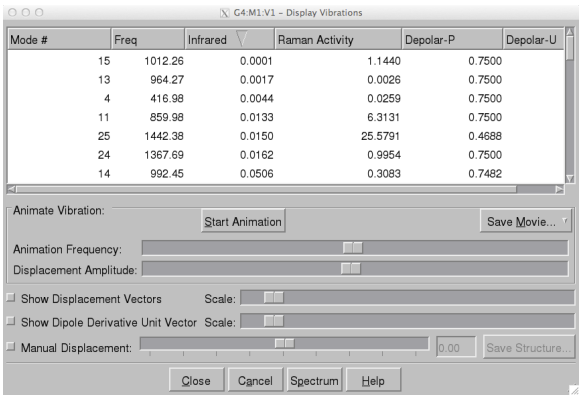
`> tail *log` (or you can use `>vi *log`)

Hint: to delete a job type: `qdel JOB#`

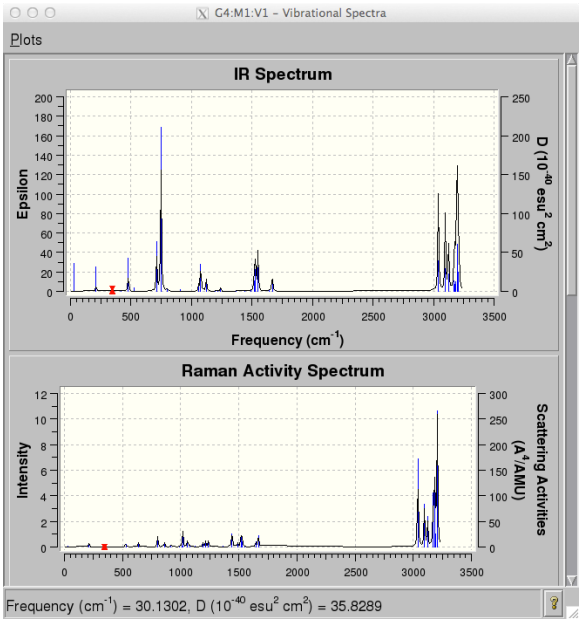
Note: the job will take ~4 min.

6. Visualize the results in *GaussView*

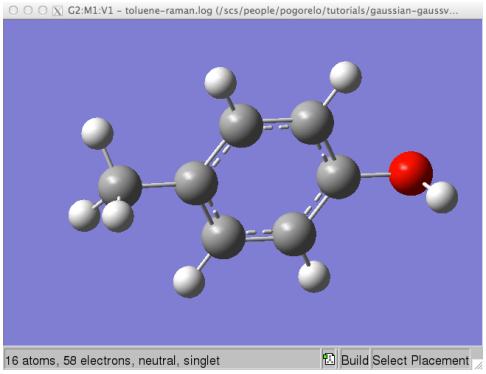
Load the output file, toluene-raman.log. Open Display Vibrations menu from the Main window: Results-> Vibrations:



Try visualizing animations of various modes. To see the spectra click the Spectrum button:



Right click on a graph provides a menu for saving the data.



If time permits build p-cresol: select oxygen in the Element Fragment and modify the hydrogen atom opposite to the methyl group. Repeat steps 3-5 and compare the results. Will the hydroxyl group influence the Raman and IR spectra? How the presence of the hydroxyl group modifies the chemistry of phenylalanine vs. tyrosine?

7. Summary

This tutorial covered basics of using *GaussView*: building molecules, preparing and performing geometry optimization and frequency calculations in gas phase.

8. Contact

If you found errors/typos or have suggestions or comments on material in this tutorial please contact us at the SCS Computer Center. We are looking forward to hearing from you. http://computing.scs.illinois.edu

9. Bibliography

1. J. B. Foresmann and A. Frisch, Exploring chemistry with electronic structure methods, 2nd Ed., 1996.

10. Acknowledgments

We are grateful to Mr. Michael Hallock for writing submission scripts for *Gaussian* and for carefully reading and testing this tutorial.