Assignment A00: *GaussView* & *G09W* Basics

We will be using *GaussView* as the graphical user interface (GUI) to run the Windows version *Gaussian*09, *G09W*. *Gaussview* allows for (a) the building of molecules, (b) the setup of *Gaussian* jobs, and (c) the display of the output from *Gaussian* jobs.

GaussView Basics: http://www.gaussian.com/g_tech/gv5ref/basics.htm

GaussView Reference: http://www.gaussian.com/g_tech/gv5ref/gv5ref_toc.htm

It is the goal of this exercise to (a) build a simple molecule, (b) setup an entry-level Hartree-Fock computation of this molecule (optimize the structure and compute frequencies) and save and submit the GJF file to run using *G09W*, (c) edit the GJF file with a text editor and recognize the sections in the GJF file, (d) display key results contained in the output files (LOG and CHK files), and (e) edit the LOG file with a text editor and recognize the sections in the LOG file.

(a) Building Molecules. Launch *GaussView*. See the main *GaussView* **control panel**, containing the menu bar, a variety of toolbars, and the Current Fragment window. The **active View window** contains the molecule being built. Using the items in the "Builder" menu, build a simple donor-acceptor substituted (hetero)arene of your choice. One example would be 4-nitroaniline. Select ring fragment "benzene" and click in active View window. Select the nitro group in the "R-Group Fragment" and click on a benzene-H. Selected "N" in "Element Fragments" and click on the para-H in nitroaniline. Alter bond lengths, angles and dihedrals as needed. Using menu "View", explore "Display Format" and focus on "Molecule" options. Explore mouse functions to change orientation, size, and position of the displayed molecule.

(b) Setup Structure Optimizations and Frequency Computation at RHF/6-31G* Level. With initial structure displayed in the **active View window**, select menu "Calculate". The "Gaussian Calculation Setup" window opens. Under "Job Type", select "Opt+Freq". Under "Method", select the 6-31G* basis set (6-31G, no "+" functions, "d" for polarization functions on elements of period 2 and higher, no polarization functions on H). Under "Title", add a job

title. Under "Link 0", select memory limit 256 MW (= 2048 MB = 2 GB, word = 8 byte, byte = 8 bit), specify "2" shared processors. Click "submit". When asked, save your GJF file on the desktop with the extension "gjf" (i.e., PNA.gjf). Then submit. *G09W* window opens while job runs (a few minutes). When *G09W* is done, close the *G09W* window. You now have three files on your desktop: GJF input file, LOG and CHK output files.

(c) Content of the GJF File. If you drop the GJF file onto the control panel, *GaussView* will open an active View window and display the initial structure. To view the content of the GJF file, under the "Results" window click on "View File". Recognize the sections in the GJF file: Instructions about hardware, information about directories, command line to control the job, title line, charge and multiplicity, geometry specification, connectivity information. You can change the content of the GJF file and save the altered file.

Another way to view and change the content of the GJF file: Simply open the file with "Notepad", "Wordpad", or as text file with "Word".

(d) Display Key Results (LOG & CHK Files). Drop the LOG file onto the control panel, *GaussView* will open an active View window and display the optimized structure. Under "Results", select "Summary" and find total energy, dipole moment, etc. Under "Results", select "Vibrations" and find vibrational frequencies, IR and Raman intensities, etc. Select "Spectrum" and view computed IR and Raman spectra. Select "Start Animation" and explore normal modes.

Now delete the active View window and open the LOG file again but this time "open it from within the application" as follows: Under "File" menu, select "Open", then browse for your LOG file, and mark "Read Intermediate Geometries" before clicking on "open". This process will read not only the final optimized structure from the LOG file, but *GaussView* will read the initial structure, all intermediate structures and the final structures, and you can look at each one. Under "Results", the option "Optimization" is now available; click it and find graphs that show the total energy and the RMS Gradient for each step.

CHK files are binary files and cannot be opened with text editors. We will learn later on how to create formatted checkpoint files, the FCHK or FCH files, and those contain ASCI characters and can be read. Drop the CHK file onto the control panel, *GaussView* will open an active View window and display the optimized structure. Under "Results", the option "Charge Distribution" is now available; click it and explore. Under "Results", the option "Surfaces/Contours" is now and we will explore these options later in the course. Under "Results", clicking on the option "View File" converts the binary CHK file into an ASCI FCH file and displays the FCH file. We will deal with the content of an FCH file later.

(e) Content of LOG File. LOG files are large, very large, or extremely large. Never print a LOG file! Learn how to read and navigate a LOG file online. You can open the LOG file as a text file in various ways: From *GaussView* by clicking "View File" in the "Results" menu. Or simply open the file with "Notepad", "Wordpad", or as text file with "Word".

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GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
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Note the "Grad" lines in the LOG files. These lines separate the various sections. Without going too much into details, recognize the input echo section and the "Initial Parameters" Table. For the initial structure, every intermediate structure, and the final structure, there will be one section which contains the following items: Structure in Input Orientation, Distance Matrix, Stoichiometry and Symmetry, Structure in Standard Orientation, Basis Set Information, Total Energy and Virial Ratio, Population Analysis, Dipole Moments etc., Forces Analysis, and Structure Convergence Check. There will be an "Optimized Parameters" Table once the optimized structure has been located.

Requesting an optimization and a frequency computation basically requests two jobs which are run in sequence. The results of the first job (the structure optimization) are written to the CHK file and the second job (the frequency computation) finds its input in the CHK file and then writes more to the CHK. The following lines exemplify where the structure optimization ends and the frequency computation starts.

```
AN AIRPLANE IS A COLLECTION OF SPARE PARTS
FLYING IN CLOSE FORMATION.
Job cpu time:       0 days  0 hours  2 minutes  2.0 seconds.
File lengths (MBytes):  RWF=     14 Int=      0 D2E=      0 Chk=      3 Scr=      1
Normal termination of Gaussian 09 at Wed Aug 17 09:57:20 2016.
Link1:  Proceeding to internal job step number  2.
--------------------------------------------------------------
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RHF/6-31G(d) Freq
--------------------------------------------------------------
1/10=4,29=7,30=1,38=1,40=1/1,3;
```

For the frequency computation of the final, optimized structure, there will be sections that contain: Structure read from CHK file, Structure in Input Orientation, Distance Matrix, Stoichiometry and Symmetry, Structure in Standard Orientation, Basis Set Information, Total Energy and Virial Ratio, Population Analysis, Dipole Moments etc., Results of Vibrational Analysis (Frequency etc. for each normal mode, Thermochemistry), Forces Analysis, Structure Convergence Check, and an "Optimized Parameters" Table.

Submission & Deadlines: This is an un-scored exercise and requires no submission.