Exercise Set 1.

1.)

a. Use the WebMO Molecule Builder to construct a formaldehyde (CH$_2$O) molecule. Perform a Comprehensive Clean-up using idealized Geometry. Take a moment to explore the Builder by rotating, translating, zooming, etc.

b. Continue with the formaldehyde structure you built in part a. Setup to run a Molecular Energy calculation using Hartree-Fock theory and the STO-3G Basis set. Set the Job Name as: E_S1_1
   Do not submit the job just yet. Go to the “Preview” tab and click the Generate button. An overview of the Gaussian input file format is given at: [http://www.gaussian.com/g_tech/g_ur/m_input.htm](http://www.gaussian.com/g_tech/g_ur/m_input.htm)
   Take a few minutes to review this page and then see if you can identify the basic parts in your generated input script.

c. Continue with the Molecular Energy calculation of formaldehyde. When you continue a pop-up box will appear which have something to the effect of: “This will submit the original (un-edited) input file. Continue?”
   Click OK to continue. Your simulation will be submitted to the queue and soon run.

d. When your Molecular Energy calculation is complete go to the View Job window (click the magnifying glass to the right of the job run time). Your formaldehyde molecule should be displayed. Scroll down the page to the Calculated Quantities. Notice the Symmetry (C$_{2v}$). If you are familiar with determining point groups take a moment to determine if this is what you would expect. Next check the RHF Energy. This quantity is the molecular energy that your job was set-up to calculate. Notice the units are in Hartree. Look up conversions and determine what the molecular energy is in both eV and kCal/mol.

e. Display the Dipole Moment. Does it point in the direction you would expect?
   Next display the partial charges and take a moment to examine them. Does the distribution of partial charge match with the trends of electronegativity and subsequent bond polarization?
   Once you are done return to the job manager.

2.)

a. Create a new job. In the Builder build a molecule of benzene and do a Comprehensive Clean-up using idealized Geometry.

b. Continue with the new benzene. Run a Molecular Orbitals calculation using Hartree-Fock theory and the 3-21G basis set. Name the job: E_S1_2

Once the job is complete, go to the View Job window. Scroll down to the calculated quantities. In the Molecular Orbitals section find the HOMO and LUMO orbitals (Hint: Look at the value of the occupancy). Are there any degeneracies in the HOMO and LUMO orbitals? Is this what you would expect if you were to draw an MO diagram for benzene?
d. Display the HOMO and LUMO orbital iso-surfaces (Click the magnifying glass). Display any degenerate orbitals. You should now have multiple tabs in the MO Viewer window. Take a moment to examine each orbital visually. How many nodes does the HOMO have? How many nodes does the LUMO have?

3. 

a. Create a new job. Build the molecule acetaldehyde (CH\textsubscript{3}CHO) and run a NMR calculation using Hartree-Fock theory and the 6-21G basis set. Give the job as: E\_S1\_3

b. Once the simulation is complete, view the $^1$H and $^{13}$C NMR spectra. Do they correspond to what you might expect?

c. Look up the experimental $^1$H and $^{13}$C NMR spectra for acetaldehyde relative to TMS (http://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi) and compare the chemical shifts with the calculated values. Do they agree? If they are different, how significantly and what are some possible explanations for the difference?