Computational Chemistry warm-up exercise during lab time the first full week of classes

Computational chemistry has grown in importance as computers have become more powerful. In this exercise you will start to explore some capabilities of WebMO as a graphical interface to the program Gaussian 09 which allows you to calculate properties of molecules.

Go to http://pyrite2.truman.edu/~webmo/cgi-bin/webmo/login.cgi by clicking on the link or copy and paste this link in your favorite browser. If one browser does not work, try a different one. Your username is your Truman e-mail address without "@truman.edu" (or Username for TruView). Your password is the last three digits of your Banner ID.
Enter them and either click the "Login" button or press the Enter key on your computer keyboard. The **WebMO Job Manager** screen should appear.

Start a calculation on H_2 by going to the "New Job" tab (it will show "Create new job") and click. If you get a security warning, accept the risk and click on Run. This will take you to the **Build Molecule** screen. Click on the Build tab at the top of the screen and choose H. Then click in the gray space to add that atom. Move the cursor 2-3 cm away and click again to add a second H atom. While holding the left mouse key down, drag the mouse from one atom to the other to draw a bond between the atoms.

When you are done drawing the molecule, click on the blue right arrow in the lower right corner.

(If nothing happens, check to see if the warning  appears on the bottom bar. If so, click on the icon and click "Allow".) This will take you to the **Configure Gaussian Job Options** screen. The program will give your job a name based on the molecule that you drew, and for H_2 you can just accept the job name given. Choose the type of calculation to do from the *Calculation Pulldown* menu; your initial calculation will always be "Geometry Optimization" today, but that is not the default. Keep the theory as "Hartee-Fock" and choose the basis set "Basic: 3-21G." Leave the charge as "0" since your molecule is neutral. Leave the multiplicity as a singlet (this means that there are no unpaired electrons). Verify what you have entered and then start the calculation by clicking the right hand blue arrow head or "Submit job." WebMO returns to **WebMO Job Manager** screen which lists all the jobs you have submitted.

After you have submitted a job it is a good idea to occasionally click on the "Refresh" button on the **WebMO Job Manager** screen to get the most up to date information about your jobs. When your job is finished, its status will be *Complete* and the "View job" icon () will be displayed to the right of the job. Click on the "View job" icon and, if necessary, accept the risk and Run. Note the RHF energy, including sign and units. Compare your value to the value calculated by classmates. You should converge to almost the same value; if there are significant differences, discover the reason and fix the problem.

Go back to the top of the file where the molecule is shown. Click on the 5th button down on the left side of the gray space; it will say Select when the mouse pointer hovers over it. Click on one atom, then press the Shift key and click on the second atom. The bond length should be displayed at the bottom of the picture. Note the value and unit of Ångstrom. Many chemistry programs use the unit of Ångstrom or Å which equals 10^{-10} m because typical bond lengths are around 1 Å.

Now create a new job for the molecule CH_4. Left click on Job Manager and then click on the "New Job" tab which will show "Create new job". In the **Build Molecule** screen you only need to put in a C atom and *Comprehensive Cleanup* will enter the four H atoms in a tetrahedral arrangement. Perform a geometry optimization using HF theory and the basis set 6-31G(d). The molecule is a singlet and has no charge. When the job is complete, go to the *View Job* screen. Scroll down to the section called "Dipole Moment." Click on the "View" icon and scroll back to the top to see the direction of the dipole (i. e., which direction are the electrons pulled in the bond). Explain what you see. Rotate the molecule to see the molecular shape.

Create separate new jobs for the molecules CH_3CH_3 and CH_3F. In the **Build Molecule** screen enter atoms other than hydrogen and connect them with a bond. At the Clean-Up tab choose *Comprehensive - Mechanics* which will add the hydrogen atoms. Perform a geometry optimization on each using HF theory and the basis set 6-31G(d). Both molecules are singlets and have no charge. In the case of CH_3CH_3 is there any difference between using *Clean-Up: Comprehensive* and *Clean-Up: Comprehensive - Mechanics*? When the jobs are complete, go to the *View Job* screen for each molecule. Scroll down to the section called "Dipole Moment." Click on the "View" icon and scroll back to the top to see the direction of the dipole (i. e., which direction are the electrons pulled in the bond). Explain what you see. Again rotate the molecules to see the 3-D shape.

Create a job for ozone. In the **Build Molecule** screen, click on the button Lookup Molecule at the bottom of the screen and type "ozone" in the molecule name box. Perform a geometry optimization using HF theory and the basis set 3-21G. The molecule is a singlet and has no charge. When the job is complete, go to the *View Job* screen. Scroll down to the section called "Dipole Moment." Click on the "View" icon and scroll back to the top to see the direction of the dipole (i. e., which direction are the electrons pulled in the bond). Why does ozone have a dipole moment despite having identical atoms with identical electronegativities?