Exploring Water Clusters

Go to: http://bobsced.cluster.earlham.edu/cgi-bin/login.cgi and use your assigned credentials to login to the server. *Please use these credentials for the rest of the SC07 conference.*

Part I. WebMO

Exercise 1 Structure of a single H_2O molecule

Click "New Job", then "Open Editor". A small window opens where you build molecules.
Click on the Periodic Table icon (5th down the left side). Choose "O" by clicking on it.
Click once in the center of the workspace. A red oxygen atom appears.
Choose Clean-Up > Add Hydrogens. You should now have water.
Experiment with the Rotate, Translate, and Zoom tools (Top 3 icons on left side).
Click Close Editor in the main WebMO window. Water now appears in the Build Molecule window. This structure contains crude bond lengths and angles. A more accurate structure can be found by carrying out an energy minimization using molecular mechanics, semiempirical methods, or *ab initio* calculations. To reduce the time required for the calculations and to obtain reasonable results, the semi-empirical method PM3 will be used. (This method is available in most molecular modeling programs).
Click the blue "continue" arrow in the lower right side of the Build Molecule window.
Choose Mopac as the computational engine. Click the blue "continue" arrow.
Type in/Choose the following:

Job Name: H20 Single PM3
Calculation: Geometry Optimization
Theory: PM3
Basis Set: Basic: 3-21G (or accept default)
Charge: 0
Multiplicity: Singlet

Click on the blue "continue" arrow. You should now see your job listed.
To kill or stop a job, you would click on the red "X" under Actions on the right side.
Click Refresh (every ~5 seconds) until you see that your job is Complete (under Status).
Click on the hyperlinked name (H2O Single PM3) to open the "View Job" window.
Choose the Select arrow (4th icon down on left).
Click on one of the H atoms in the structure (the other atoms and bonds will "fade").
Shift and Click the O atom (both atoms are now highlighted).

The bond length is displayed just below the molecule. Record the value of the O-H bond length ___________Å (0.959 Å literature). Check the other O-H bond length.

Click on one of the H atoms, then Shift and click the O atom, followed by another H atom. The bond angle is displayed just below the molecule. Record the value of the H-O-H bond angle ___________° (103.9° literature).
Scroll down and review the information under Calculated Quantities.

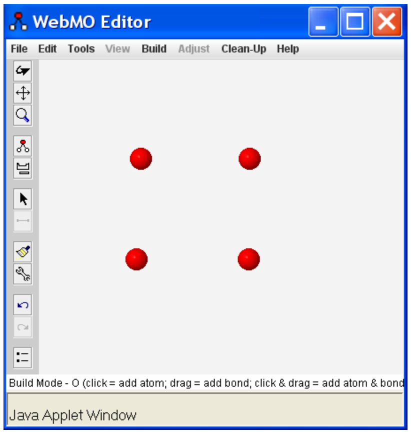
Record the Heat of Formation value __________ kcal mol^{-1} (-57.8 kcal mol^{-1}, literature)
When finished, click the Job Manager link under Actions (to the left of the molecule display).
To continue on to the next exercise, choose New Job > Create New Job.

Exercise 2 Structure of a Water Cluster, $(H_2O)_x$

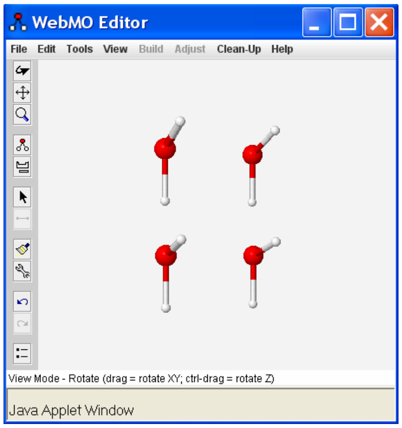
You will each be assigned a value of "x" to model.

Click "New Job", then "Open Editor".
Click on the Periodic Table icon (5th down the left side). Choose "O" by clicking on it.
Click in the workspace "x" times in a systematic, gridlike manner:

Example: *x = 4*



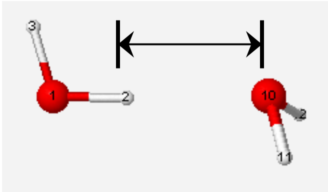
Choose Clean-Up > Add Hydrogens. (NOTE: Depending on the available server, you may have to choose Clean-Up > Comprehensive-Mechanics. Your instructor will let you know). You should now have "x" water molecules. Make sure none of the H atoms are superimposed on the O atoms. If this has occurred, click "File > New" in the WebMO Editor window and draw the O atoms further apart.



Click Close Editor in the main WebMO window.
Click the blue "continue" arrow in the lower right side of the Build Molecule window.
Choose Mopac as the computational engine. Click the blue "continue" arrow.
Type in/Choose the following:

Job Name: H20 x PM3 (where "x" is your assigned cluster size)
Calculation: Geometry Optimization
Theory: PM3
Basis Set: Basic: 3-21G (or accept default)
Charge: 0
Multiplicity: Singlet

Click on the blue "continue" arrow. You should see your job listed.
Click Refresh (every few seconds) until you see that your job is Complete (under Status).
Click on the hyperlinked name (H2O x PM3) to open the "View Job" window.
→ Let's determine the hydrogen bond distance (H on one water to O of nearest neighbor).
Choose the Select arrow (4^{th} icon down on left).
Click on one of the H atoms of one water molecule.
Hold down the Shift key and Click the nearest O atom on a neighboring water molecule:



The bond length is displayed just below the molecule. Record the value of the O···H hydrogen bond length ___________Å (~1.80 Å in ice).

[NOTE: If your initial O atoms were drawn too far apart, there was no attraction registered for the nearest neighbors during the geometry optimization, and your structure may not be hydrogen-bonded].

Scroll to the bottom of the Calculated Quantities area and record the CPU time: __________ sec.
Fill in the table below using your colleagues shared data:

x	CPU time (s)	x	CPU time (s)
1		10	
2		12	
4		14	
6		16	
8		18	

Part II. Molecular Dynamics

Exercise 1 On the Web

Some web sites of interest:

1) Phase diagram of water (cartoon):
http://titanium.fullerton.edu/shock/PHASED.htm

2) Autoionization cartoon with vibrational modes:
http://titanium.fullerton.edu/shock/WATER.htm

3) Ten water molecules, energy minimization:
http://molvis.sdsc.edu/atlas/morphs/water10/water10r.htm

Exercise 2 Molecular Workbench

This is not loaded on your machines, but can be downloaded at:
http://mw.concord.org/modeler/index.html

Exercise 3 Odyssey

The demo version can be downloaded (after registration) at:
http://www.wavefun.com/products/demo_odyssey_univ.html

There are different versions of this software (college, high school, instructor, student, etc.). See:
http://www.wavefun.com/products/odyssey/odyssey.html

Information on GridChem: https://www.gridchem.org/