INSTRUCTIONS FOR WebMO

WebMO is a World Wide Web-based interface to computational chemistry packages. While WebMO provides an interface for many computational packages (Gamess, Gaussian, MolPro, Mopac, NWChem, QChem, and Tinker) at Temple we have Gaussian and TINKER.

There are two ways to access WebMO. One is to use the departmental site. The departmental WebMO will only work if you are in Beury Hall. The other way is to use the public site (<http://www.webmo.net/demo/index.html>) from anywhere. However that site only allows jobs to be run for 2 min, while using the departmental gives you unlimited time.

The website of WebMO ( <http://www.webmo.net/>) provides tutorials and a User’s guide if you need additional information (http://www.webmo.net/support/index.html). Here are some basic instructions to get you started:

Go to the departmental webpage (http://www.temple.edu/chemistry/)

Click on “Resources”, then “Software Information”, then

“Access WEBMO”

At that point you are on the webpage

<http://moq.chem.temple.edu/~webmo/cgi-bin/webmo/login.cgi>

(An alternative link that runs Gaussian16 can be found here:

<http://naboo.chem.temple.edu/cgi-bin/webmo/login.cgi>)

Login with the username “student” and password “student”.

The following instructions were taken from <http://www.webmo.net/demo/index.html> (with some modifications)

The following instructions will build the formaldehyde molecule, optimize its geometry, and display the results:

1. Log in to the WebMO
2. In the WebMO Job Manager page, click "New Job"
3. In the Build Molecule page, in the WebMO Editor applet:
   1. Note the status line ("Build Mode - C ..."); click in the middle of the applet to insert a carbon atom
   2. In the menu, choose Build: O to make oxygen active; note the status line
   3. Click on the C atom, drag, and let up the mouse button to insert a bond to an oxygen atom
   4. Drag between C and O again to change the single bond to a double bond
   5. In the menu, choose Clean-Up: Comprehensive; note that hydrogens are added, bond lengths are idealized, and bond angles are idealized (WebMO knows organic chemistry!)
4. In the bottom right corner of the Build Molecule page, click the Continue arrow
5. In the Choose Computational Engine page, click TINKER, and then click the Continue arrow
6. In the Configure TINKER Job Options page:
   1. ◦ Select Calculation: Geometry Optimization
   2. ◦ Click the Continue arrow to submit your job; note that your job appears in the WebMO Job Manager page
7. In the WebMO Job Manager page, click "Refresh" to update the page; note that the job Status is Complete
8. Click the job title "CH2O" to arrive at the View Results page; scroll down to look at your Calculated Quantities