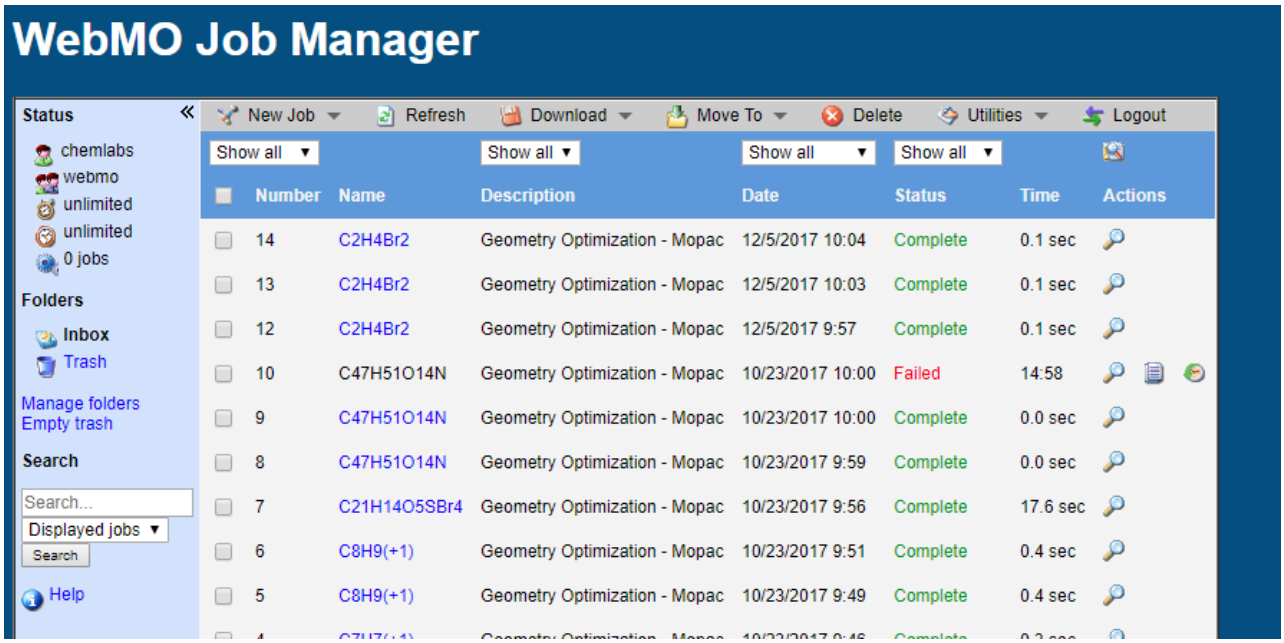
WebMO Basics for Computational Chemistry

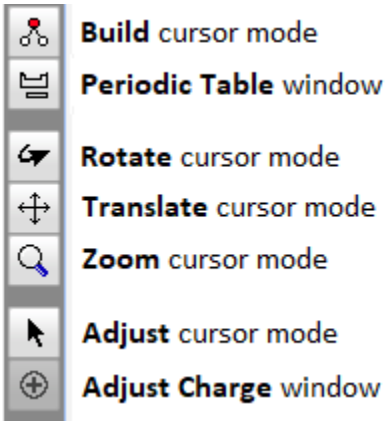
Open a web browser, navigate to **beaker.smith.edu** and click on the WebMO link. Enter the username **chmlabs** and the password **HydrogenElem#1H** to log in.

After logging in, the **Job Manager** window appears. To start a new job, select **New Job** > **Create New Job** from the menu bar at the top.



<u>To build a new structure:</u>

WebMO has several different cursor modes that can be used to operate the interface. Activating each mode changes the actions that occur when using the mouse, and when using WebMO you will switch between them frequently. These modes are:

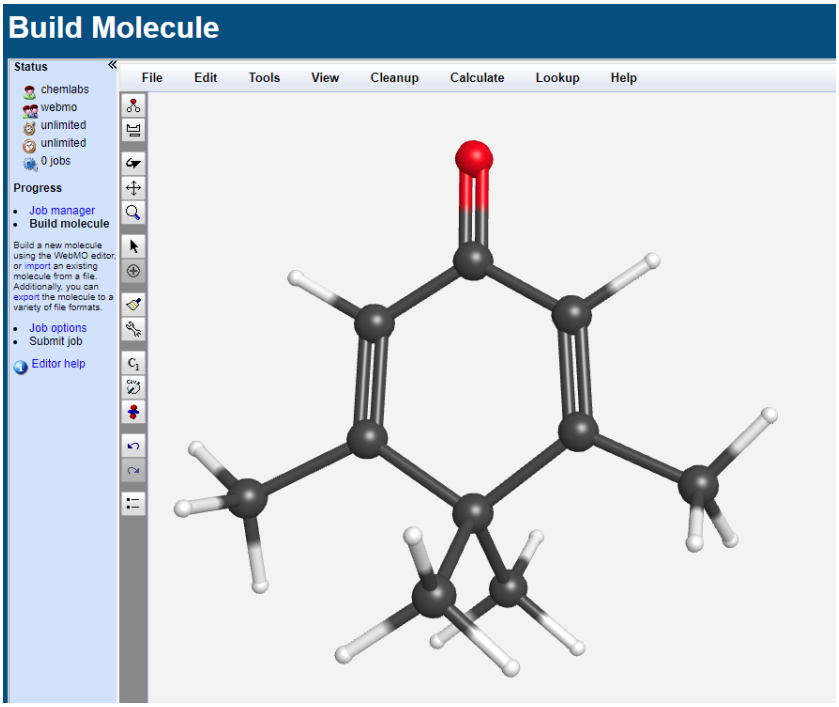


- The **Build** cursor mode will place an atom (carbon by default) when clicked in the workspace. To change which element will be created when clicking, use the **Periodic Table** button.

- Once the first atom is placed, build out the molecule by clicking & holding on an existing atom, then dragging outward to create a newly bonded atom of the chosen type.

- If you wish, you can skip adding all the H atoms manually, and instead click the **Clean Up** icon once the skeleton of the molecule is finished. This will fill in any missing bonding positions with H atoms so that every carbon has 4 bonds, every oxygen has 2 bonds, etc.

- Once the molecule is built, select the **Rotate** control, then click and drag the mouse around to look at your molecule from every angle to make sure the structure is what you intended. The **Translate** (slide) and **Zoom** functions can also be used to help you get additional views if needed.



<u>To modify an existing structure:</u>

- To change an atom to a new type, use the **Periodic Table** button to pick the desired element, then click on the atom you want to change. This also puts the cursor in **Build** mode.

- To delete an atom, use the **Adjust** cursor mode, click to highlight the undesired atom, and then press the delete or backspace key on the keyboard.

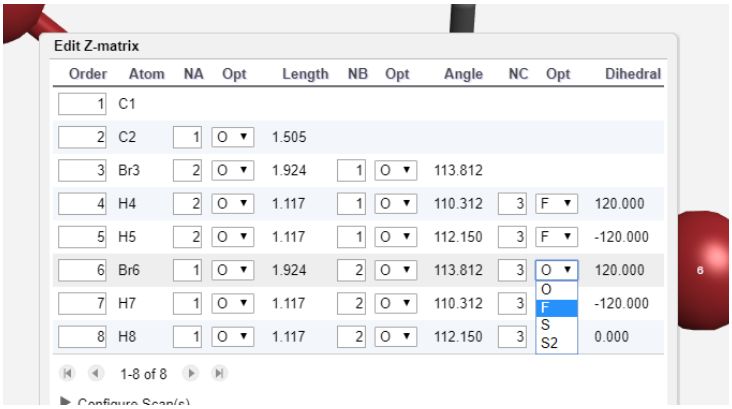
- To change a bond type, right click on the bond while in either the **Build** or **Adjust** cursor modes and select the desired option from the menu that appears.

- To change the hybridization and/or charge of an atom, right click on the atom while in either the **Build** or **Adjust** cursor modes and select the desired option from the menu that appears.

- To change a bond length, use the **Adjust** cursor mode and select the two atoms involved. Select **Adjust** > **Bond Length** from the menu bar at the top and enter the new value.

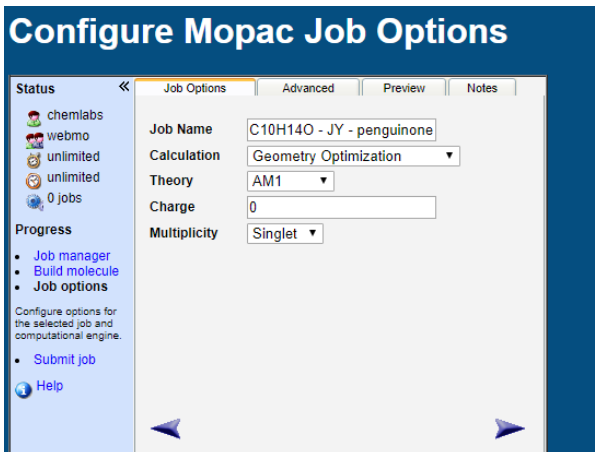
- To change a bond angle or dihedral angle, follow a similar procedure as for a bond length, except select 3 atoms for a bond angle or 4 atoms for a dihedral angle. The atoms must be selected in the order in which they are directly bonded.

- If you choose a particularly unstable configuration (say, a dihedral angle that puts the molecule in an eclipsed conformer) you may want to **freeze** one or more bond lengths, bond angles, or dihedral angles. To do this, go to the **Tools** menu and select **Edit Z-matrix**. This brings up a menu with the raw molecular connectivity table. For any parameters you want to freeze, (e.g. all the dihedral angles in the rightmost column) change the **O** option to an **F**, then click **OK**.



To perform a calculation:

Now that you have built your molecule, you are ready to do calculations on it. First, click the blue arrow at the bottom right of the job creation window. This brings up the **Configure Job Options** page (in our case, Mopac is the mathematical engine performing the calculations behind the scenes of the WebMO interface.)



- In the **Job Name** field, give your job a descriptive name that will be obvious in the Job Manager page among your classmates' jobs - it is a good idea to include your name/initials.

- In the **Calculation** field, select **Geometry Optimization** to have WebMO find the most stable structure close to the one you provided. (The other options can be used to perform other types of calculations in more advanced situations. For example, if your species is not that stable and you want to run the calculation for it *without* optimizing the structure into a very different one, select **Molecular Energy**.)

- In the **Theory** field, choose **AM1**. This level of theory is *semi-empirical*, which uses some initial guesses from real experimental data to speed up the theoretical calculation. AM1 is a good compromise level of theory that is accurate enough for our purposes while still being fast to calculate.

- In the **Charge** field, enter 0 unless your structure is an ion, in which case enter the appropriate value (remember to include the negative sign for anions!)

- In the **Multiplicity** field, leave the option as **Singlet** (the other options are for exotic situations with unpaired electrons.)

- Click the blue forward arrow at the bottom right to submit the job. You will be taken back to the Job Manager window, where you can monitor the progress of the calculation. After a few seconds, the job should read **Complete** – at that point, click the magnifying glass to examine the job output. If the job reads **Failed** at the end instead, you can try modifying it (look for badly placed or overlapping atoms or bonds), or just start over with a new job.

<u>To analyze the output:</u>

- Use the **Rotate** cursor mode to look at your molecule from various angles and make sure it is still in the configuration you intended.

- To find the heat of formation ΔH_f of your structure, scroll down and read the "AM1 Heat of Formation" in the **Calculated Quantities** area.

- To measure a bond length, use the **Adjust** cursor mode, select the two atoms involved, and read the value from the bottom line of text on the workspace. To measure a bond angle or dihedral angle, use the same method but select three or four atoms, respectively.