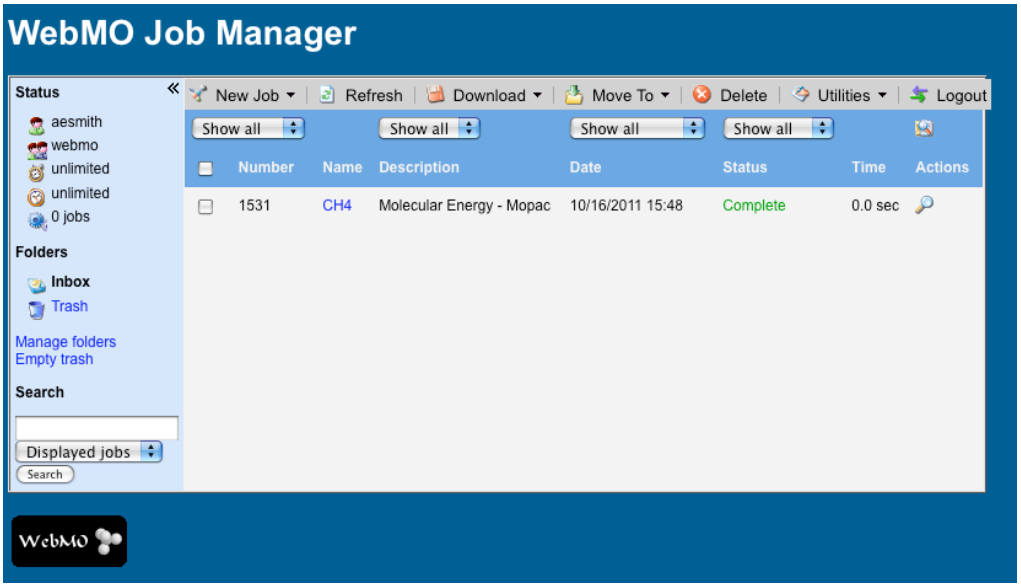
WebMO Tutorial

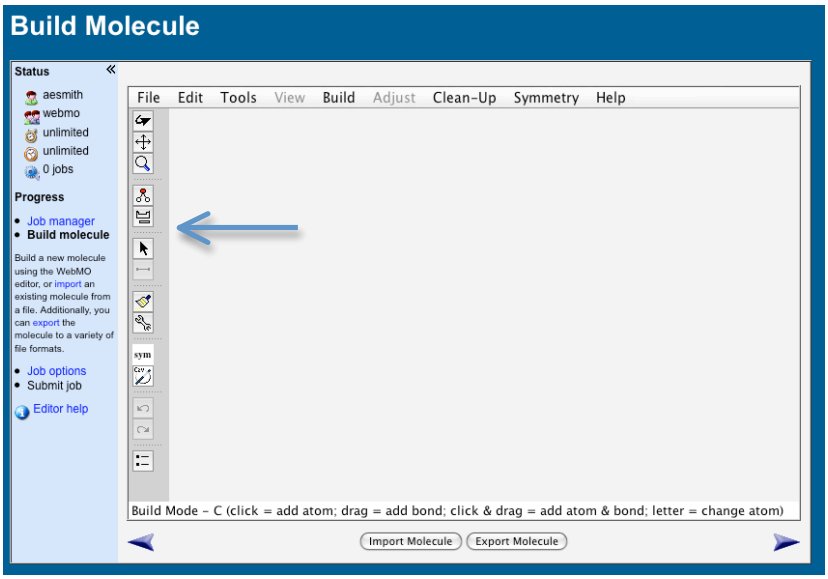
Login to WebMO:

1. Access Web MO by going to: *http://butane.cabrillo.edu/*
2. Click on the Diablo Valley College link.
3. Enter your last name in the Username box using all lower case letters without a first name nor any initials. *(NOTE: See Dr. R. in the event that another Chem 121 student has the same last name as you.)*
4. Use your first name in all lower case letters as your password for your first time login and then change the password to one of your own choosing.

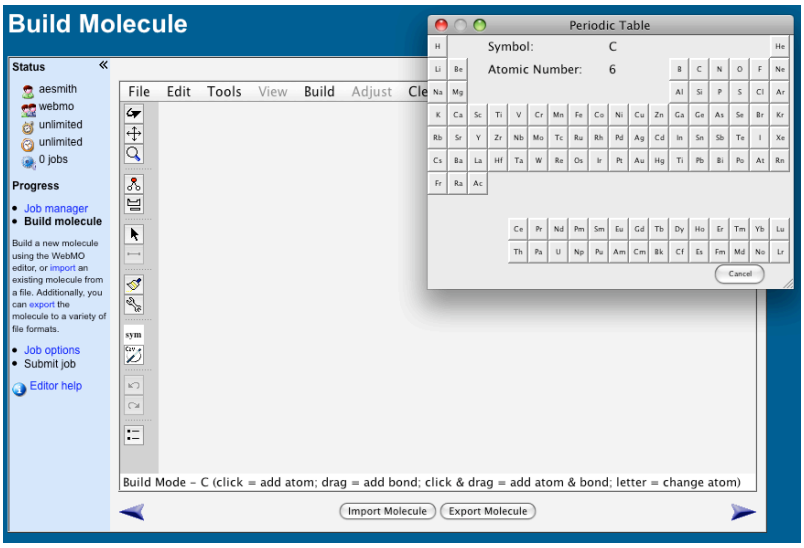
Click on the New Job button and Create New Job link on the WebMO Job Manager page. This will open the WebMO Build Editor in a new window.



This will open the following screen. Click on the icon next to the arrow. It is the periodic table.



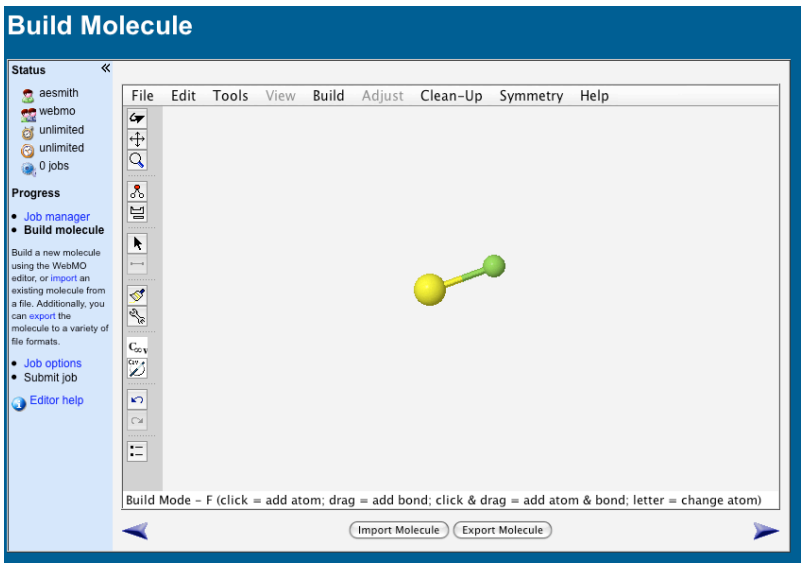
The following inset will appear. (Carbon (C) is the default atom.)



The following example illustrates the steps used to build and model any molecule. *Sulfur tetrafluoride* is used as the example.

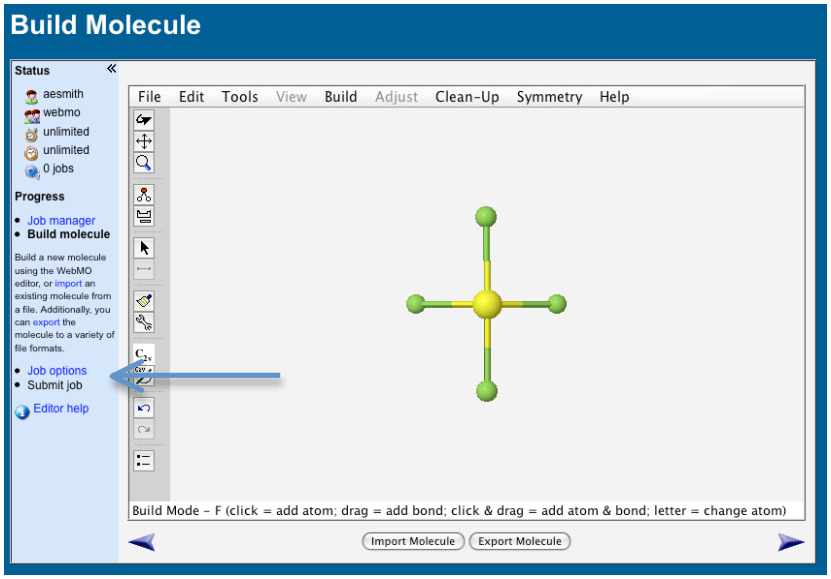
1. Select sulfur from the periodic table and then click on the Build Molecule screen. A yellow colored sphere representing sulfur appears.

2. Click on the periodic table icon again and select fluorine. Point the mouse cursor at the center of the yellow sulfur atom and while holding the mouse button down draw the cursor away from the center and release. The molecule now has one S-F bond.



3. Add three more S-F bonds. Select Clean-Up /Comprehensive Idealized from the menu at the top of the screen.

The screen should look like this:



4. Click on the icon Job options next to the arrow. Select / Enter the following parameters:

Job Name *For* any molecule provide the IUPAC name, followed by an underscore and an identifier of your choice, such as in this case **Sulfur tetrafluoride_1.**

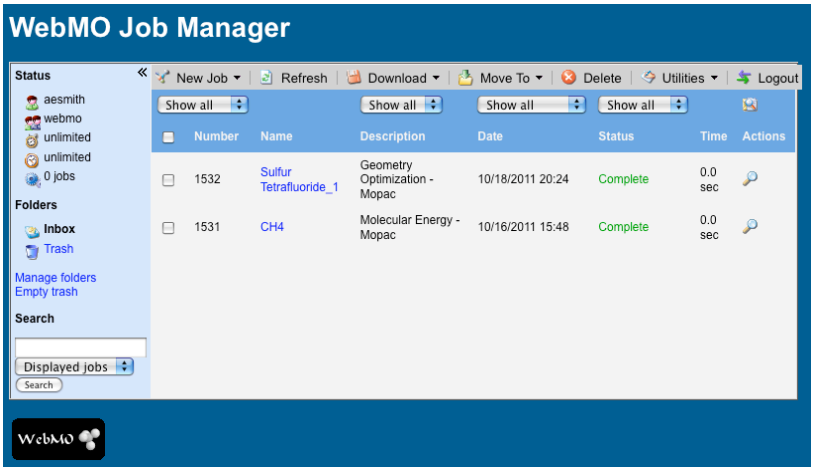
Calculation Select Geometry Optimization from the *Calculation* drop-down menu. This will calculate the minimum energy conformation for your molecule.

Theory Select AM1 from the *Theory* drop-down menu.

Charge 0.

Multiplicity Singlet.

Submit job. Wait ~20 sec. If still "running", click reload page. Your job's status should now say *Complete* in green.



5. Click on the File Name link to view the molecule and results of the calculation.

Several types of information are available from the completed job page.

The Job number and name are at the top of the page. Job numbers are in order of all of the jobs run on the server, each job has a unique number.

The symmetry point group to which the molecule belongs is displayed

The calculated Heat of Formation for the molecule is displayed in kcal/mol

The calculated Dipole Moment of the molecule is displayed in Debye and can be visualized by clicking the adjacent 'View' button.

The calculated partial charge on each element of the molecule is given in table format. The partial charges can be visualized by clicking the adjacent !View button.

The calculated bond orders (strength of bonding interaction) are displayed. Values less than one indicate no existing bond. Values approximately one indicate a single bond interaction between the two atoms. Values approximately two and three indicate a double or triple bond interaction, respectively.

It is possible to rotate, translate, and enlarge or decrease (zoom) the size of the model in the window using the tool bar in the upper left hand corner. The white bar (information bar) directly below the gray model window conveys information regarding each tool name as the curser rolls over the tool. Once the tool is selected by clicking once on the icon, the information bar provides instructions on the use of each tool.

Crossed Arrows — Translate	Default tool, used to rotate the molecule by clicking and holding the mouse button down while moving the mouse.
Curved Arrow — Rotate	Used to move the molecule to a different position on the screen.
Magnifying Glass — Zoom	Used to enlarge or decrease the size of the molecule in the window
Straight Arrow — Selection	This tool has many uses. Clicking once on an atom will provide the hybridization of the atom in the information bar. Clicking beside the molecule (not on an atom) will remove the selection. Two atoms can be selected at the same time to provide a bond length (or simple distance between two non-bonded atoms). To select two atoms, click on the first atom to select it, then holding the shift key select the second atom. Bond angles and dihedral angles can be obtained by select three and four atoms, respectively.

Click on the Job Manager button to return to the Job Manager screen.