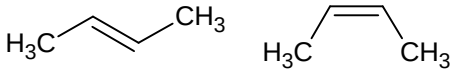
2-Butene and Acetanilide: learning to use WebMO

WebMO is a browser-based Java interface to a number of popular computational chemistry programs. The interface works the same for all such programs; the program we will use is Gaussian.

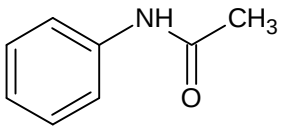
WebMO is provided for academic use in Ohio by the Ohio Supercomputer Center.

To log into WebMO, go to https://webmo.osc.edu. Your username is your last name and first initial (all lower-case), and your password is the last four digits of your student ID number. For example, John Smith (ID # 12345) logs in as "smithj" and his password is "2345".

Your student accounts will be deleted at the end of this semester; if you need to use WebMO for research or other Bluffton-related purposes, please contact Dr. Berger for an account.



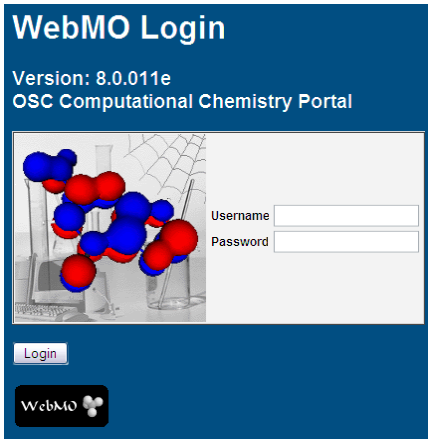
cis and trans 2-butene



acetanilide

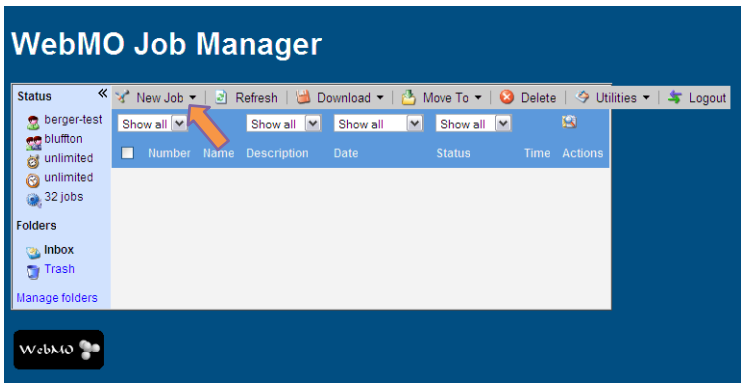
Follow the instructions on the following pages to build the structures and examine their properties.

Building cis- and trans-2-butene



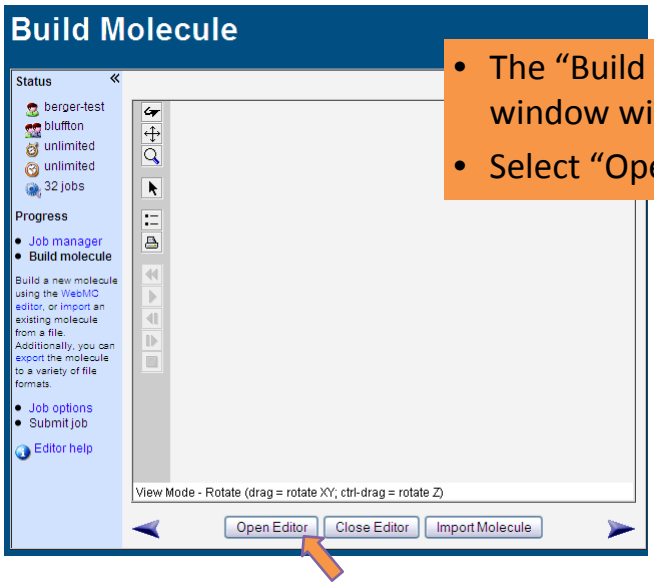
- Go to https://webmo.osc.edu
- Log into WebMO with your username and password

Building cis- and trans-2-butene



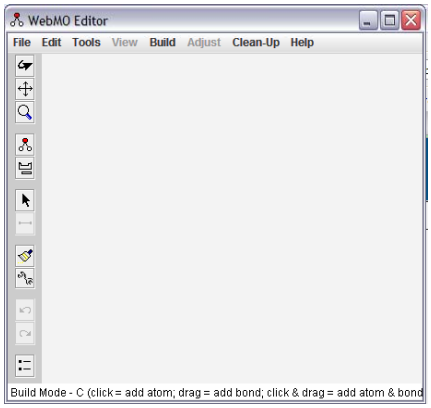
- You will now be in the Job Manager. The first time you log in it will look like this.
- Select “New Job”

Building cis- and trans-2-butene



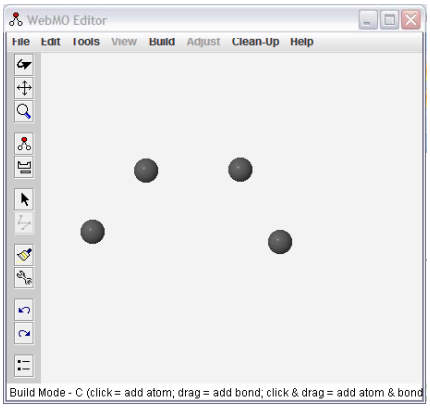
- The "Build Molecule" window will open.
- Select "Open Editor."

Building cis- and trans-2-butene



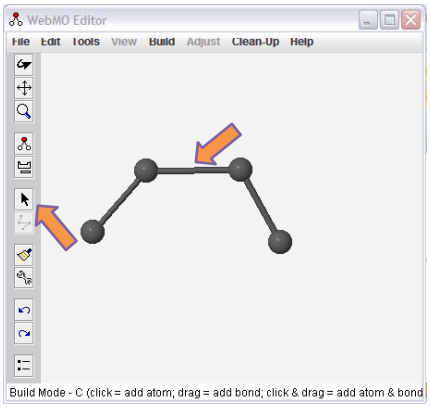
- The Editor is a separate window.
- The Editor defaults to Build Mode – C (building carbon atoms).
- Click in the window four times to place four carbon atoms in a *cis* arrangement.

Building cis- and trans-2-butene



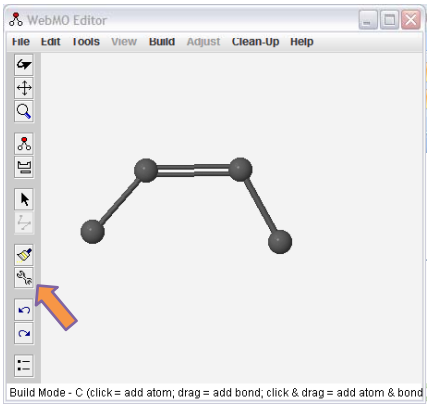
- Now click on the first atom and drag to the second.
- Click on the second and drag to the third.
- Click on the third and drag to the fourth
- You will have placed bonds between the four atoms.

Building cis- and trans-2-butene



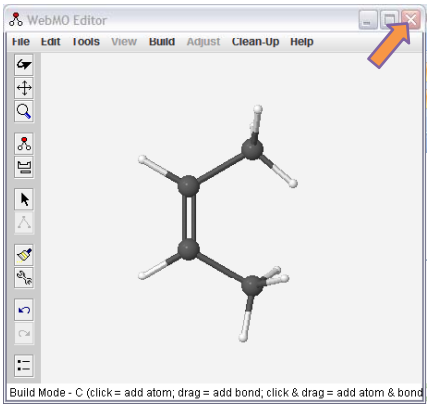
- Click on the “pointer” button (“Adjust”) in the tool menu.
- Right-click on the middle bond, and select “Double” from the menu that appears.

Building cis- and trans-2-butene



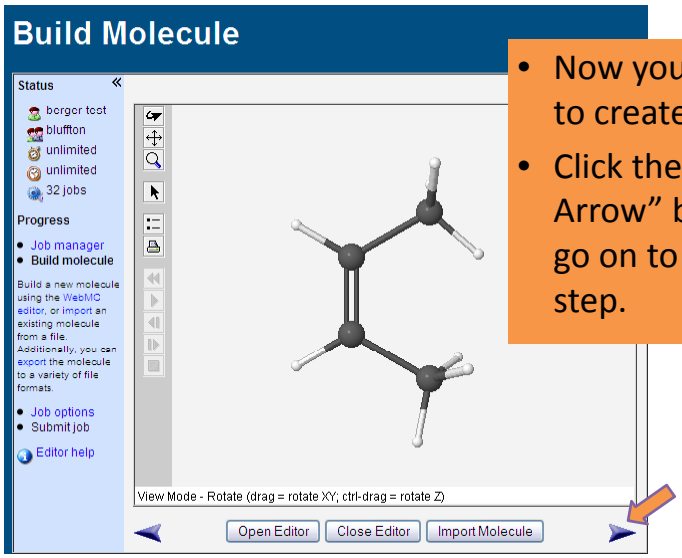
- Click the “Wrench” tool (“Comprehensive Cleanup using Mechanics”).
- The “Broom” tool (“Comprehensive Cleanup”) will also work.

Building cis- and trans-2-butene



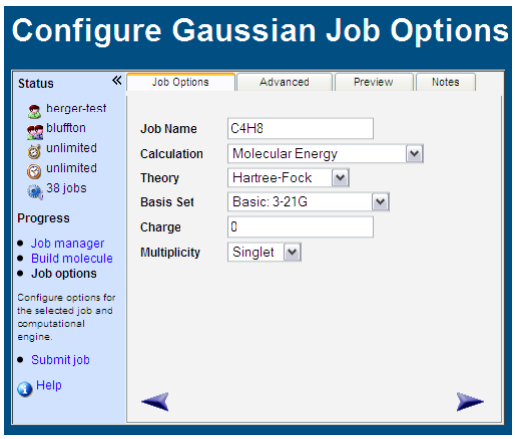
- You have successfully built cis-2-butene.
- Click on the “eXit” button to go back to the Build Molecule window.

Building cis- and trans-2-butene



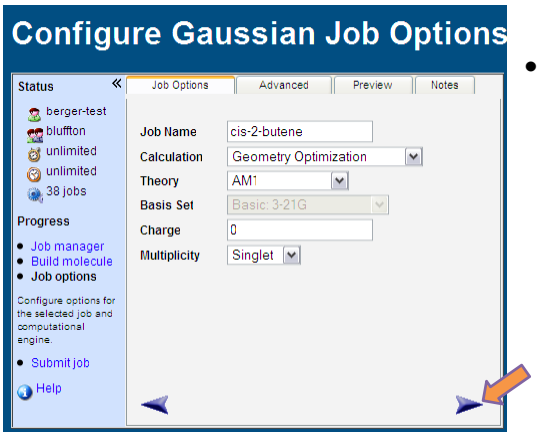
- Now you are ready to create your job.
- Click the "Right Arrow" button to go on to the next step.

Building cis- and trans-2-butene



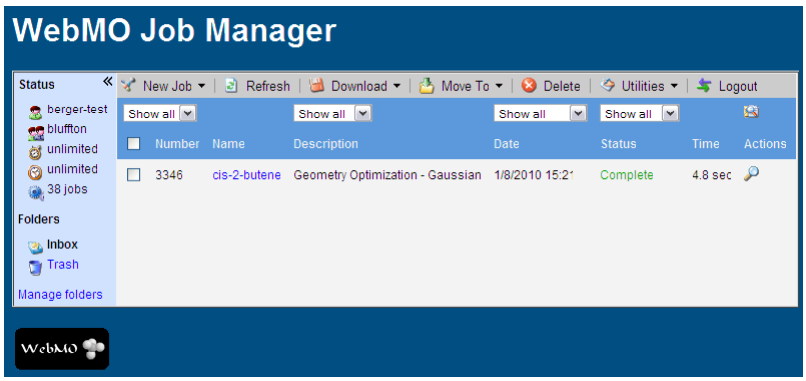
- Name your job "cis-2-butene".
- Change "Calculation" to "Geometry Optimization"
- Change "Theory" to "AM1"

Building cis- and trans-2-butene



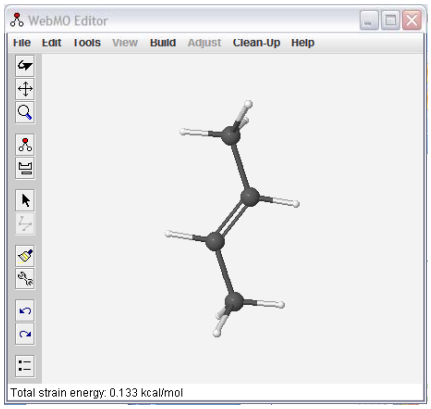
- Click the "Right Arrow" button to submit your calculation to the server.

Building cis- and trans-2-butene



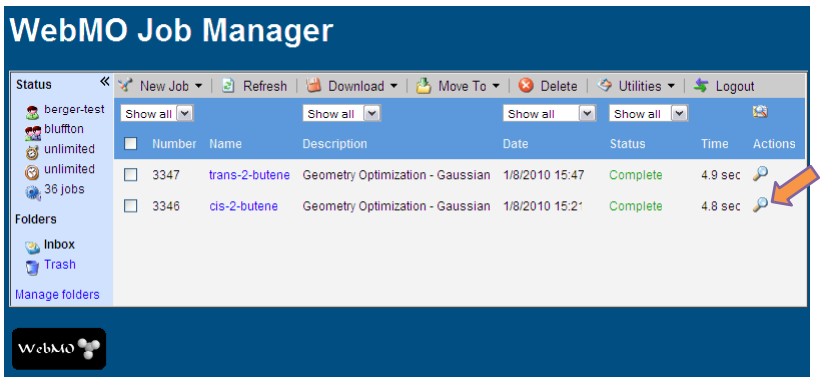
- You will go to the Job Manager. When your job is complete, the Job Manager will update to show that it is complete.

Building cis- and trans-2-butene



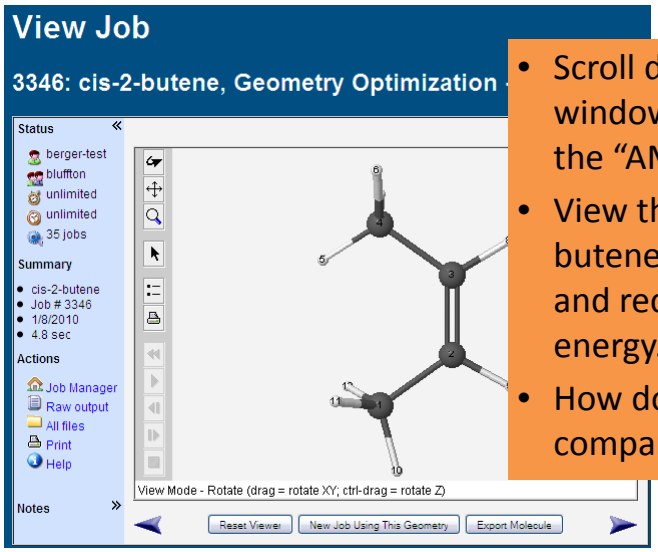
- Repeat these steps to build trans-2-butene.
- Be sure you place your four carbon atoms in a "zig-zag" configuration.
- If you use the "Broom" tool to clean up rather than the "Wrench" tool, you may get cis again. If so, select "Undo" from the Edit menu and try the "Wrench" tool.

Building cis- and trans-2-butene



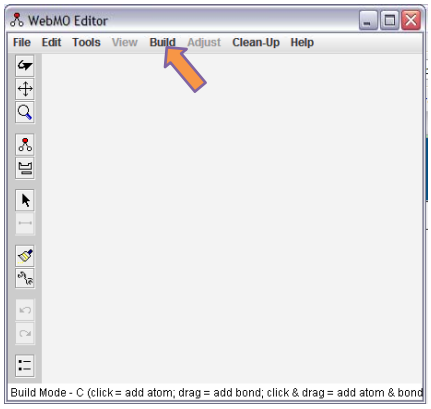
- We will now examine our 2-butene isomers.
- Click on the "View Job" button at the far right, for one of the two jobs.

Building cis- and trans-2-butene



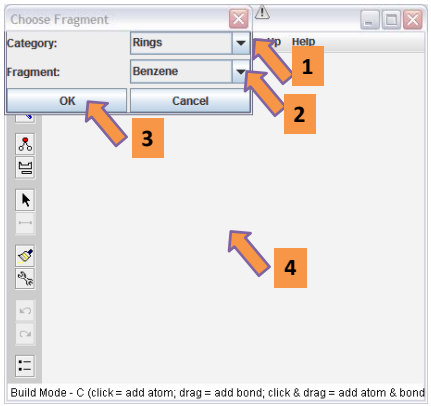
- Scroll down in the window, and record the "AM1 Energy."
- View the other butene calculation and record its energy.
- How do the two compare?

Building acetanilide in WebMO



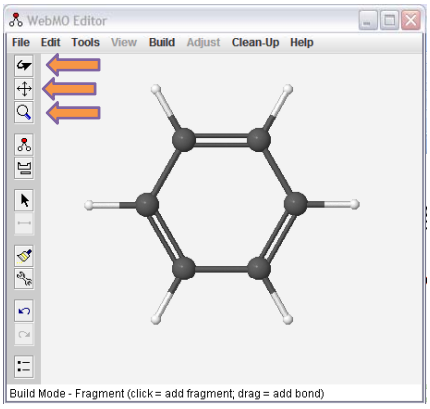
- Using the menu at left, click “Job Manager.”
- Start a new job and open the Editor.
- Within the Editor, select the “Build” menu and choose “Fragment.”

Building acetanilide in WebMO



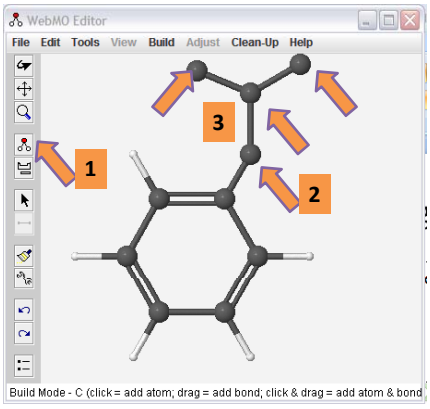
1. Under “Category” select “Rings.”
2. Under “Fragment” select “Benzene.”
3. Click “OK.”
4. Click in the Editor window to place a benzene molecule there.

Building acetanilide in WebMO



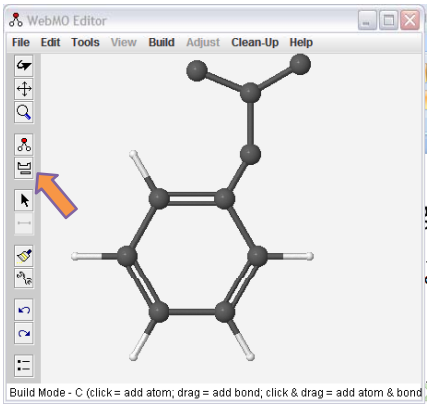
- Acetanilide has an acetamido group attached to benzene.
- Use the "View" tools to adjust the size and position of the molecule so that you have room to build.

Building acetanilide in WebMO



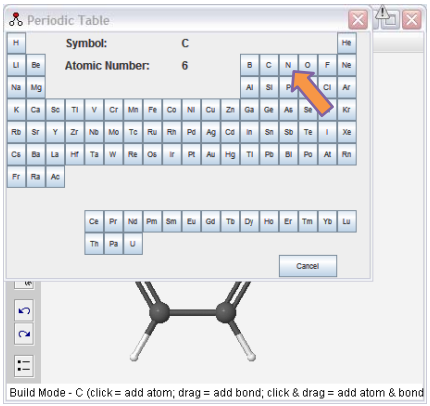
- Click the "Build" button.
- Click on one of the hydrogen atoms to change it to a carbon atom.
- Place three more atoms in the window and connect them as shown.

Building acetanilide in WebMO



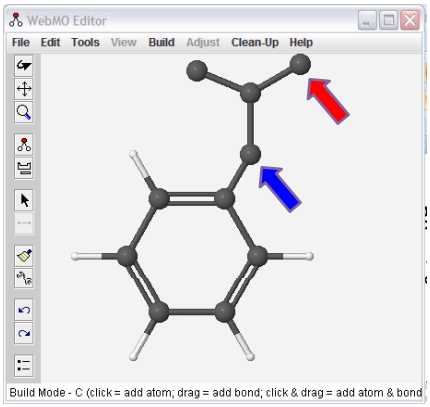
- Click the periodic table button. A dialog window will open.

Building acetanilide in WebMO



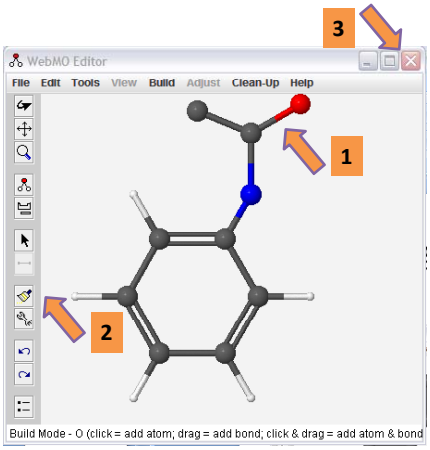
- Click “N” for nitrogen.

Building acetanilide in WebMO



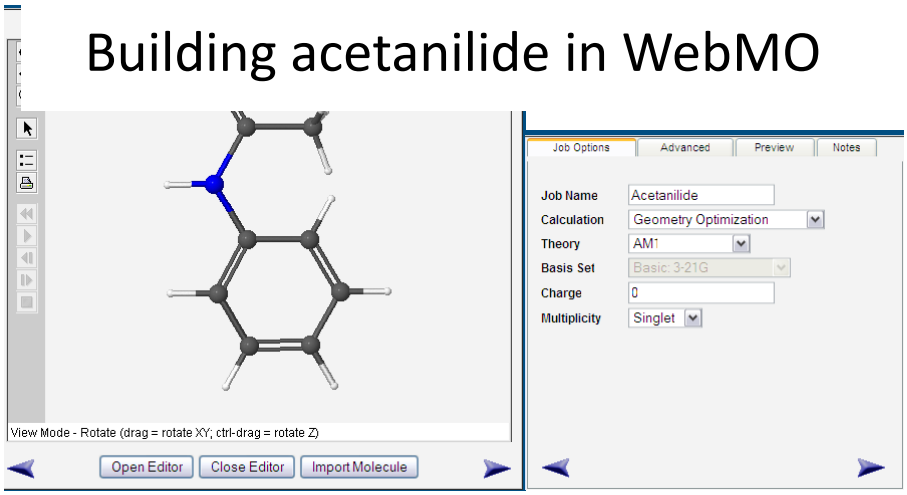
- Click the carbon atom indicated by the blue arrow, to change it to nitrogen.
- Now, using the periodic table button, change to oxygen and convert the carbon atom indicated by the red arrow.

Building acetanilide in WebMO



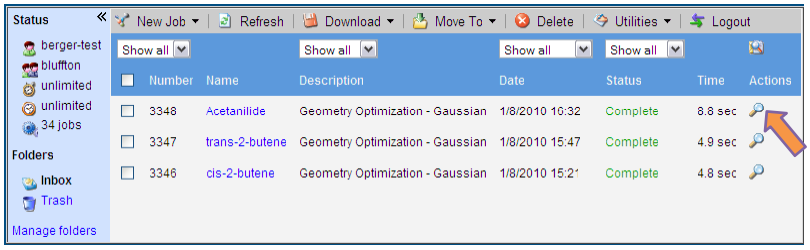
1. Right-click to change the bond indicated to a double bond.
2. Click the Broom button ("Comprehensive Cleanup").
3. Close the Editor window.

Building acetanilide in WebMO



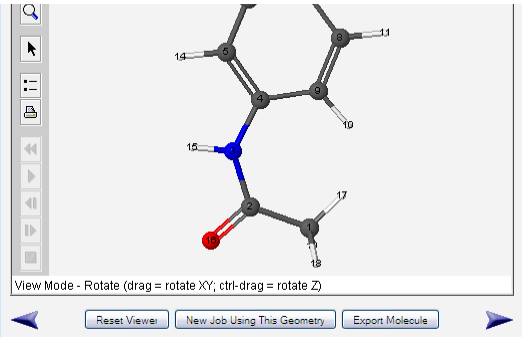
- Click the right-arrow button, and name the job "Acetanilide." Use the same parameters as before (as above).
- Click the right-arrow button again to submit the job.

Building acetanilide in WebMO



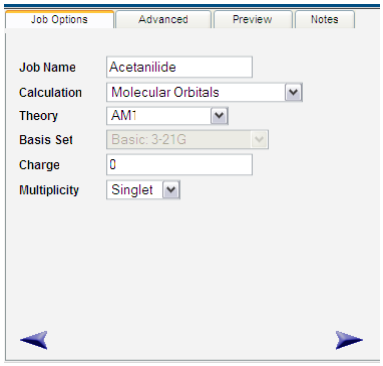
- When the job is finished, the Job Manager will show it as "Complete."
- Click "View Job" for your acetanilide structure.

Building acetanilide in WebMO



- We will now examine the molecular orbitals and electrostatic potential map (charge map) of acetanlide.
- Click "New Job Using This Geometry." Click the right-arrow button to reach the "Configure Guassian" window.

Building acetanilide in WebMO



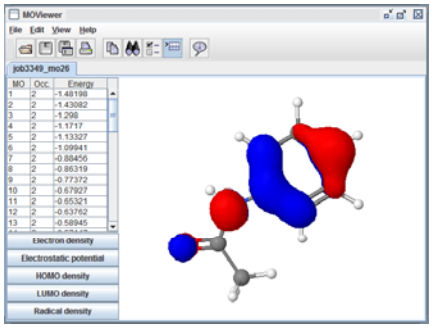
- Set up the parameters as shown at left:
  - Acetanilide
  - Molecular Orbitals
  - AM1
  - 0
  - Singlet
- Click the right arrow to submit the job.

Building acetanilide in WebMO

15	A'	2	-0.55989 Hartree
16	A'	2	0.53945 Hartree
17	A'	2	-0.52765 Hartree
18	A'	2	-0.51872 Hartree
19	A'	2	-0.50411 Hartree
20	A'	2	-0.48055 Hartree
21	A'	2	-0.46267 Hartree
22	A'	2	-0.44191 Hartree
23	A'	2	-0.42710 Hartree
24	A'	2	-0.41020 Hartree
25	A'	2	-0.36720 Hartree
26	A'	2	-0.32707 Hartree
27	A'	0	0.00340 Hartree
28	A'	0	0.01060 Hartree
29	A'	0	0.05066 Hartree

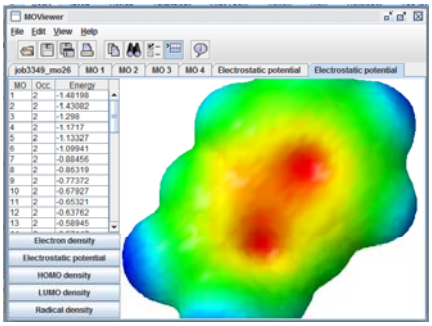
- When the job is completed, click “View job”.
- Scroll down to molecular orbital 26, and select “View”.
- A new window will open. Be patient while it loads.

Building acetanilide in WebMO



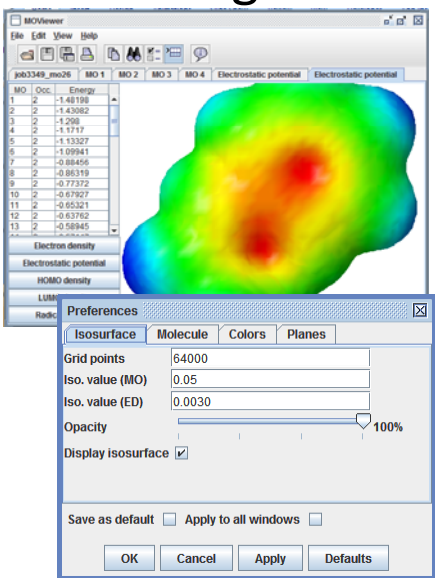
- The selected Molecular Orbital is shown in the window.
- You can view other orbitals by click on them in the menu at the left.

Building acetanilide in WebMO



- To see the electrostatic potential surface, click the labeled bar.
- If you have a three-button mouse, drag the middle button to resize.
- If you have a scroller mouse, use the scroller to resize.

Building acetanilide in WebMO



- To make the surface more transparent, select “Edit MOViewer Preferences.”
- Change “Opacity” to 66% or less.
- Click “Apply” or “OK.”
- Exit the window when you are done.