How Do I Use WebMO and PSI4?

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1. Connect to WebMO and login using your ID and password provided by the WebMO administrator. (Note: The demo server is https://www.webmo.net/demoserver/cgi-bin/webmo/login.cgi)

2. After login, click on “New Job" and select "Create New Job” which will take you to the molecule editor Java applet.

3. The three most important buttons on the left-hand side of the window are:

   a) Build mode (water molecule icon): Allows you to place atoms of any type into the structure and place bonds of any type (single, double, triple) between them.

   b) Rotate mode (curved up-right arrow icon): Allows you to view the molecule from any angle in three dimensions.

   c) Adjust mode (up-left arrow): Allows you to set geometric parameters to arbitrary values.

4. Select “Build mode” and click anywhere in the window to place a carbon atom. Click a second time a short distance away to create another carbon atom.

5. Create a single bond between the atoms by clicking on one atom and dragging to the other. (Note: You can create double or triple bonds by repeating this action.)

6. Select “Adjust mode” and click once on one of the carbon atoms. Then, while holding down the “shift” key, click on the other atom.

7. Under the “Adjust” pull-down menu, select “Bond length.” This will bring up a new window in which you may set the C-C bond length. Set it to 1.55 (which is in Å by default) and click “OK.”

8. Return to “Build mode.” Under the “Build” pull-down menu, choose “H.”

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9. Click and drag on one of the carbon atoms to add a hydrogen atom. Repeat this until you have added three H atoms so you end up with something that looks like a methyl group.

10. Select “Rotate mode.” Click and drag on the molecule to rotate it so you can see where the hydrogens really are. You will find your methyl group does not really look much like a methyl group.

11. Select “Build mode” again. Under the “Clean-Up” pull-down menu, choose “Add Hydrogens.” This will add three hydrogens to the second carbon atom, in an appropriate methyl-like arrangement.

12. Click on “Clean-Up" and select "Geometry.” This should fix the entire structure to look like ethane. (You can also choose the “Mechanics Optimize” option to use a simple molecular mechanics routine to generate the more reasonable staggered structure of ethane.)

13. Enter “Rotate mode” and rotate the structure so that you can see all the atoms.

14. Return to “Adjust mode” and click on one of the hydrogens. Then while holding the shift key, select the carbon to which that hydrogen is bonded, then the other carbon, and then a hydrogen on the second carbon (in that order).

15. Click on the “Adjust” pull-down menu and select “Dihedral angle.” Enter different values to see how the conformation changes.

16. Click on the right arrowhead at the bottom right-hand side of the window to proceed to the job parameters page.

17. Choose the “PSI4” option for the computational engine and click to right arrowhead at the bottom right.

18. Enter “Ethane SP” in the “Job Name” field, and leave everything else alone.

19. Click on the right arrowhead at the bottom right-hand side of the window to submit the job to the queue.

20. The calculation should require only a few seconds, assuming no other users have calculations that are already running. Use the “Refresh” button to update your job list. Once the task is complete, you may examine a summary of the results by clicking either on the job name or

on the magnifying glass to the right of the jobs CPU time.

Congratulations! You have successfully completed a quantum chemical calculation through the WebMO interface!

Note: The default job is a RHF-Hartree-Fock/6-31G(d) single-point energy computation. Changing the “Calculation,” “Method,” “Basis Set,” or other options in the “Job Options” tab in Step 18 will give different results based on the chosen options included.