WebMO Tutorials

I. Methane (CH_4)

1. Login to WebMO.

2. At the top of the WebMO Job Manager Page, click on the New Job button. This will bring up the Build Molecule page.

3. Click once in the Editor window. This will draw a single carbon atom.

4. Click once on the Clean-Up menu at the top of the screen to open it, and choose Comprehensive - Mechanics. This will add four hydrogen atoms to your carbon atom, with sp^3 geometry, and you will have a complete methane molecule. Clicking once on the wrench icon at the left of the editor window will do the same thing.

5. Click on the Job Options link to the left of the model window or the arrow to the right on the bottom of the screen.

6. On the Configure Mopac Job Options page,

Job Name Give your molecule its standard IUPAC name, followed by an underscore and an identifier of your choice, such as methane_practice. Use any identifier you like, as long as the molecule name begins with the IUPAC name and an underscore.

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 Leave the charge at 0.

Multiplicity Leave the multiplicity at Singlet.

Leave *Preview Input File* unchecked. Do not select Advanced Options.

Click on the Submit Job link to the left of the window or click the right arrow at the bottom of the screen.

7. This will return you to the Job Manager Page, where you will see your job listed. In the status column you will see *Running* in red. Click on the Refresh button at the top-left corner of the screen.

8. Your job's status should now say *Complete* in green. Click on the View link to the right of the job's status to see the results of the calculation.

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

Job Number & Name 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.

Calculate Geometry The molecule is displayed with the optimized geometry

Keywords (Route) The keywords the computational engine used to optimize the molecule are displayed

Symmetry The symmetry point group to which the molecule belongs is displayed

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

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

Partial Charges 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* magnifying glass button.

Bond Orders 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.

Other Information 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.

Curved Arrow – Rotate	Default tool, used to rotate the molecule by clicking and holding the mouse button down while moving the mouse.
Crossed Arrows – Translate	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.

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

II. Ethanol (CH_3CH_2OH)

1. Login to WebMO (if you haven't already).

2. At the top of the WebMO Job Manager Page, click on the Create New Job button. This will bring up the Build Molecule page.

3. Click once near the center of the Editor window, this will set a single carbon atom. Click on the Carbon atom and hold the mouse button down. Now drag the mouse horizontally away from the first carbon in the direction where you would like to place the second carbon, all the while holding down the mouse button. Release the mouse button when the curser resides where you would like to place the second carbon atom. Do not put the atoms too close together, or too far apart (about two to three atom diameters is about right) as this can cause problems during the calculations. Also do not rotate the molecule while building unless absolutely necessary, this often makes building more difficult.

4. Click on the Build menu at the top of the screen and select O. Alternately, click on the periodic table icon at the left of the window and select oxygen from the table.

5. Click once, and hold the mouse button down, on the carbon atom to which you would like to attach the oxygen atom. Now drag the curser away from the carbon atom, approximating a good bond angle of 109.5^o. Release the mouse button to place the oxygen atom, placing it two to three atom diameters away from the carbon.

6. Click once on the Clean-Up menu at the top of the screen to open it, and choose Comprehensive - Mechanics. This will add hydrogen atoms, and you will have a complete ethanol molecule. Clicking once on the wrench icon at the left of the editor window will do the same thing.

7. If you want to see the molecule from another angle, click on the curved arrow icon at the top-left corner of the editor window, and you will be able to click and drag to rotate the molecule. It is best not to do this until you are finished building the molecule.

8. Click on the Job Options link to the left of the model window or the arrow to the right on the bottom of the screen.

9. On the Configure Mopac Job Options page,

Job Name Give your molecule its standard IUPAC name, followed by an underscore and an identifier of your choice, such as ethanol_practice. Use any identifier you find useful, as long as the molecule name begins with the IUPAC name and an underscore.

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 Leave the charge at 0.

Multiplicity Leave the multiplicity at Singlet.

Leave *Preview Input File* unchecked. Do not select Advanced Options.

Click on the Submit Job link to the left of the window or click the right arrow at the bottom of the screen.

10. This will return you to the Job Manager Page, where you will see your job listed. In the status column you will see *Running* in red. Click on the Refresh button at the bottom-left corner of the screen.

11. Your job's status should now say *Complete* in green. Click on the View link to the right of the job's status to see the results of the calculation.

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

III. *Trans*-2-butene ($CH_3CHCHCH_3$)

1. Login to WebMO (if you haven't already).

2. At the top of the WebMO Job Manager Page, click on the Create New Job button. This will bring up the Build Molecule page.

3. Start by drawing the two center carbons of the carbon-carbon double bond. Click once near the center of the Editor window, this will set a single carbon atom. Click on the Carbon atom and hold the mouse button down. Now drag the mouse *horizontally* away from the first carbon in the direction where you would like to place the second carbon, all the while holding down the mouse button. Release the mouse button when the curser resides where you would like to place the second carbon atom. Do not put the atoms too close together, or too far apart (about two to three atom diameters is about right) as this can cause problems during the calculations. Also do not rotate the molecule while building unless absolutely necessary, this often makes building more difficult. To make the double bond, click once on the first carbon atom and hold the mouse button down while dragging to the second carbon atom. Release the mouse button while the curser is over the second carbon atom. The two atoms should now be connected by a double bond.

4. Proceed by placing the third and fourth carbon atoms at appropriate distances and angles (one above the plane of the double bond, and the other below) from the carbon-carbon double bond.

5. Click once on the Clean-Up menu at the top of the screen to open it, and choose Comprehensive - Mechanics. This will add hydrogen atoms, and you will have a complete trans-2-butene molecule. Clicking once on the wrench icon at the left of the editor window will do the same thing.

6. If you want to see the molecule from another angle, click on the arrow icon at the top-left corner of the editor window, and you will be able to click and drag to rotate the molecule. It is best not to do this until you are finished building the molecule.

7. Click on the Job Options link to the left of the model window or the arrow to the right on the bottom of the screen.

8. On the Configure Mopac Job Options page,

Job Name Give your molecule its standard IUPAC name, followed by an underscore and an identifier of your choice, such as *trans*-2-butene_practice. Use any identifier you find useful, as long as the molecule name begins with the IUPAC name and an underscore.

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 Leave the charge at 0.

Multiplicity Leave the multiplicity at Singlet.

Leave *Preview Input File* unchecked. Do not select Advanced Options.

Click on the Submit Job link to the left of the window or click the right arrow at the bottom of the screen.

9. This will return you to the Job Manager Page, where you will see your job listed. In the status column you will see *Running* in red. Click on the Refresh button at the top-left corner of the screen.

10. Your job's status should now say *Complete* in green. Click on the View link to the right of the job's status to see the results of the calculation.

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

IV. *Cis*-2-butene ($CH_3CHCHCH_3$) *This one's built differently*!

1. Login to WebMO (if you haven't already).

2. At the top of the WebMO Job Manager Page, click on the Create New Job button. This will bring up the Build Molecule page.

3. Start by drawing the two center carbons of the carbon-carbon double bond. Click once near the center of the Editor window, this will set a single carbon atom. Click on the Carbon atom and hold the mouse button down. Now drag the mouse *horizontally* away from the first carbon in the direction where you would like to place the second carbon, all the while holding down the mouse button. Release the mouse button when the curser resides where you would like to place the second carbon atom. Do not put the atoms too close together, or too far apart (about two to three atom diameters is about right) as this can cause problems during the calculations. Also do not rotate the molecule while building unless absolutely necessary, this often makes building more difficult. To make the double bond, click once on the first carbon atom and hold the mouse button down while dragging to the second carbon atom. Release the mouse button while the curser is over the second carbon atom. The two atoms should now be connected by a double bond.

4. Proceed by placing the third and fourth carbon atoms at appropriate distances and angles (both above the plane of the double bond, one on the left and the other on the right, so that they are on the same side) from the carbon-carbon double bond.

5. Here's where it gets tricky. **Do not select Comprehensive Clean-up**, In order for the completed molecule to have the cis conformation, you need to do the follow two additional steps:

- Select H from the Build menu and add a single hydrogen atom to each of the terminal carbons. Place the hydrogen atoms two to three atom diameters away from the carbons and with good approximate bond angles (109.5^o).

- Click once on the Clean-Up menu at the top of the screen to open it, and **choose Add Hydrogens**. This will add the rest of the hydrogen atoms, and you will have a complete cis-2-butene molecule. Now you can use **Comprehensive Clean-Up** and the molecule should retain the *cis*- geometry.

6. If you want to see the molecule from another angle, click on the arrow icon at the top-left corner of the editor window, and you will be able to click and drag to rotate the molecule. It is best not to do this until you are finished building the molecule, especially when you are trying to build a molecule in a single plane like this one.

7. Click on the Job Options link to the left of the window or click the right arrow at the bottom of the screen.

8. On the Configure Mopac Job Options page,

Job Name Give your molecule its standard IUPAC name, followed by an underscore and an identifier of your choice, such as *cis*-2-butene_practice. Use any identifier you find useful, as long as the molecule name begins with the IUPAC name and an underscore.

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 Leave the charge at 0.

Multiplicity Leave the multiplicity at Singlet.

Leave *Preview Input File* unchecked. Do not select Advanced Options.

Click on the Submit Job link or click on the arrow to the right at the bottom of the screen.

9. This will return you to the Job Manager Page, where you will see your job listed. In the status column you will see *Running* in red. Click on the Refresh button at the top-left corner of the screen.

10. Your job's status should now say *Complete* in green. Click on the View link to the right of the job's status to see the results of the calculation.

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