<u>V. Eclipsed Ethane Coordinate Scan</u>

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. To draw an eclipsed *ethane* molecule: Start by drawing the two carbons of the ethane molecule. 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 Comprehensive Clean-Up (the broom icon) to add the hydrogens. Do not click on comprehensive-mechanics (the wrench icon) as this will place the molecule into a staggered conformation.

6. To run a Coordinate Scan on the dihedral angle:

*   Use the selection tool (the straight arrow) to select one of the eclipsed H-C-C-H that form a 0° dihedral angle by shift clicking on each atom in turn.
*   With all four atoms selected click on the <u>Adjust menu</u> and select <u>Dihedral Angle.</u>
*   Verify that the selected dihedral angle actually is 0° in the widow that pop's up. If the angle is specified as other than 0°, go ahead and change it in the window to 0° and hit <u>OK.</u>
*   With all four atoms still selected click on the <u>Adjust menu</u> and select <u>Scan Coordinate</u>. Once Scan Coordinate is selected you should get a pop-up window titled Scan Coordinate
*   In the Scan Coordinate window you will be presented with the following options:

	Start	Stop	# Steps
Scan			

Type   Optimized

The <u>Start</u> and <u>Stop</u> are the starting and ending angles, in degrees, for the dihedral angle scan, and the <u># Steps</u> is the number of divisions the calculation will be divided into.

*   You may not enter the same data point twice, doing so will cause the job to fail. This means that the first data point must differ from the starting geometry. Because our geometry specifies a dihedral angle of 0.000^o, enter 0.01 for the starting angle and 360 for the finish. Enter 100 for the number of steps. The boxes should look like:

	Start	Stop	# Steps
Scan	0.01	360	100

*   The <u>Type</u> pull-down menu is for selecting the type of calculation that will be performed. Optimized tells the computer that for each dihedral angle step the dihedral angle will be fixed and the rest of the structure optimized to produce the lowest energy with the specified fixed dihedral angle. Rigid indicates that the entire molecule will be fixed at the specified dihedral angle and that the structure will not be optimized, but rather a single point energy determination will be made at that geometry. Leave the pull-down menu set at Optimized.
*   Click OK to close the Scan Coordinate Window.

7. Click on the <u>Job Options</u> 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 ethane_scan. Use any identifier you find useful, as long as the molecule name begins with the IUPAC name and an underscore.
Calculation	**Select <u>Coordinate Scan</u> from the *Calculation* drop-down menu**. This will calculate the heat of formation for the molecule at each of the specified dihedral angles through your specified range.
Theory	Select <u>AM1</u> 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 <u>Submit Job</u> 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 bottom-left corner of the screen.

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

11. The heat of formation and dipole moment listed below the molecule window are for the specific geometry displayed by the model, which is the last geometry calculated. In other words: the values listed are for the last specified geometry. To view the results of the Coordinate Scan you must scroll down to the Coordinate Scan table at the bottom of the page. Click on the View link to see a graph of the calculated energies. The graph is interactive reporting the energy verse angle data values corresponding to the location of the mouse cursor. Note the highest energy occurs when the hydrogens are eclipsed: a dihedral angle of 0°, 120°, or 360°. The lowest energy values occur when the hydrogens are staggered: at dihedral angles of 60°, 180°, or 300°. It is possible to zoom in on a point of interest (e.g., the lowest energy point).

VI. Eclipsed 1,2 Dichloroethane Coordinate Scan

1. Login to WebMO.

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

3. To draw an eclipsed *1,2-dichloroethane* molecule: Start by drawing the two carbons of the ethane molecule. 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 Comprehensive Clean-Up (the broom icon) to add the hydrogens. Do not click on comprehensive-mechanics (the wrench icon) as this will place the molecule into a staggered conformation.

5. Click on the Periodic Table tool and select Chlorine. Now click on the hydrogen atom that you would like to change to a Chlorine. The hydrogen will be replaced with a Chlorine atom. Click on the eclipsed hydrogen on the adjacent carbon and change it to a chlorine as well.

6. To run a Coordinate Scan on the dihedral angle:

- Use the selection tool to select one of the eclipsed Cl-C-C-Cl that form a 0° dihedral angle by shift clicking on each atom in turn.
- With all four atoms selected click on the <u>Adjust menu</u> and select <u>Dihedral Angle.</u>
- Verify that the selected dihedral angle actually is 0° in the widow that pop's up. If the angle is specified as other than 0°, go ahead and change it in the window to 0° and hit <u>OK.</u>
- With all four atoms still selected click on the <u>Adjust menu</u> and select <u>Scan Coordinate</u>. Once Scan Coordinate is selected you should get a pop-up window titled Scan Coordinate
- In the Scan Coordinate window you will be presented with the following options:

	Start	Stop	# Steps
Scan			

Type   Optimized

The <u>Start</u> and <u>Stop</u> are the starting and ending angles, in degrees, for the dihedral angle scan, and the <u># Steps</u> is the number of divisions the calculation will be divided into.

- You may not enter the same data point twice, doing so will cause the job to fail. This means that the first data point must differ from the starting geometry. Because our geometry specifies a dihedral angle of 0.000^o, enter 0.01 for the starting angle and 360 for the finish. Enter 100 for the number of steps. The boxes should look like:

	Start	Stop	# Steps
Scan	0.01	360	100

- The <u>Type</u> pull-down menu is for selecting the type of calculation that will be performed. Optimized tells the computer that for each dihedral angle step the dihedral angle will be fixed and the rest of the structure optimized to produce the lowest energy with the specified fixed dihedral angle. Rigid indicates that the entire molecule will be fixed at the specified dihedral angle and that the structure will not be optimized, but rather a single point energy determination will be made at that geometry. Leave the pull-down menu set at Optimized.
- Click OK to close the Scan Coordinate Window.

7. Close the editor window. You should now see your *1,2-dichloroethane* molecule on the Build Molecule page, if you don't see the model try clicking the Close Editor button just below the model window. Once you can see the model click on the Job Options link.

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 1,2-dichloroethane_scan. Use any identifier you find useful, as long as the molecule name begins with the IUPAC name and an underscore.

Calculation   **Select Coordinate Scan from the *Calculation* drop-down menu**. This will calculate the heat of formation for the molecule at each of the specified dihedral angles through your specified range.

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.

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 bottom-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. The heat of formation and dipole moment listed below the molecule window are for the specific geometry displayed by the model, which is the last geometry calculated. In other words: the values listed are for the last specified geometry. To view the results of the Coordinate Scan you must scroll down to the Coordinate Scan table at the bottom of the page. Click on the View link to see a graph of the calculated energies. The graph is interactive reporting the energy verse angle data values corresponding to the location of the mouse cursor. Note the highest energy occurs when the chlorines are eclipsed: a dihedral angle of 0°, or 360°. The lowest energy values occur when the Chlorines are staggered: at a dihedral angle of 180°. There are also local energy minima when the chlorines are gauche to one another: dihedral angles of 60°, and 300°. It is possible to zoom in on a point of interest (e.g., the lowest energy point).