Lab #4: Single Point Energies and Geometry Optimizations

Exercise 1 – Potential Energy Surface of Bond Stretching in Dinitrogen.

Build a molecule of N_2 (triple bond!).

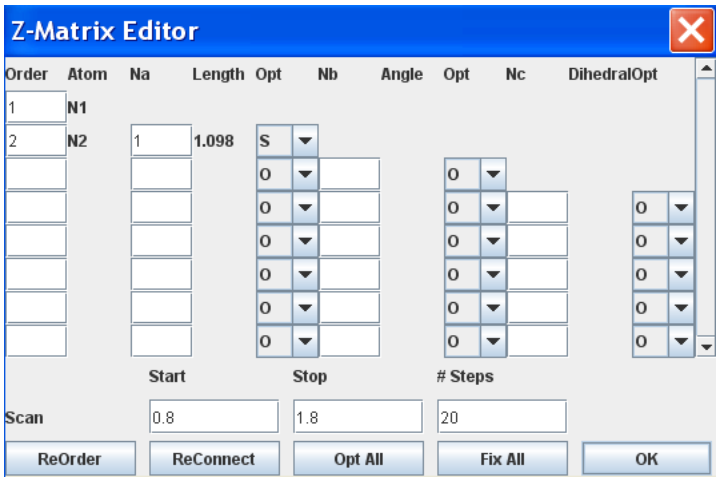
Perform a geometry optimization using PM3 (Job Name: N2PM3) using Gaussian or Mopac.

Click on New Job Using This Geometry > Open Editor.

Choose the Adjust tool (Arrow, 6th down) and click on one N atom. Hold down the shift key and click on the other N atom. Record the bond length: _____ Å (literature, 1.098Å).

Choose Tools > Z-matrix.

To the right of the bond length, select "S" from the pull down menu, then type in the values for Start, Stop, and # Steps shown below. We will calculate the energy of the molecule every 0.05 Å between the limits we have set.



Click OK, then Close Editor. Click the blue continue arrow. Choose the same engine used above.

Choose/Type in the following:

- Job Name: N2Scan
- Calculation: Coordinate Scan
- Theory: PM3
- Basis Set: Basic: 3-21G (or accept default)
- Charge: 0
- Multiplicity: Singlet

Click the blue continue arrow. When the job is complete, open the file and scroll down to the Coordinate Scan data. Click on the magnifying glass in the title bar.

On the graph that appears, use your mouse and place the cursor on the lowest energy point. Look at the coordinate values above the graph.

Exercise 2 – Potential Energy Surface of Bond Angle Bending in Water.

Build a molecule of H_2O.

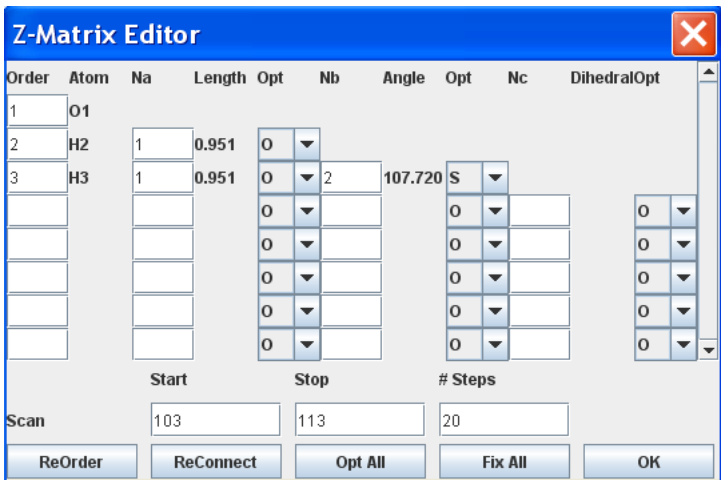
Perform a geometry optimization using PM3 (Job Name: H2OPM3) using Gaussian or Mopac.

Click on New Job Using This Geometry > Open Editor.

Choose the Adjust tool (Arrow, 6th down) and click on one H atom. Hold down the shift key and click on the O atom, and then the remaining H atom. Record the bond angle: _____ Å (literature, 103.9 °).

Choose Tools > Z-matrix.

To the right of the bond angle, select "S" from the pull down menu, then type in the values for Start, Stop, and # Steps shown below. We will calculate the energy of the molecule every 0.5 ° between the limits we have set.



Click OK, then Close Editor. Click the blue continue arrow. Choose the same engine used above.

Choose/Type in the following:

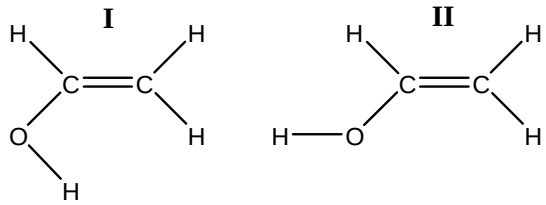
Job Name: H2OScan
Calculation: Coordinate Scan
Theory: PM3
Basis Set: Basic: 3-21G (or accept default)
Charge: 0
Multiplicity: Singlet

Click the blue continue arrow. When the job is complete, open the file and scroll down to the Coordinate Scan data. Click on the magnifying glass in the title bar.

On the graph that appears, use your mouse and place the cursor on the lowest energy point. Look at the coordinate values above the graph.

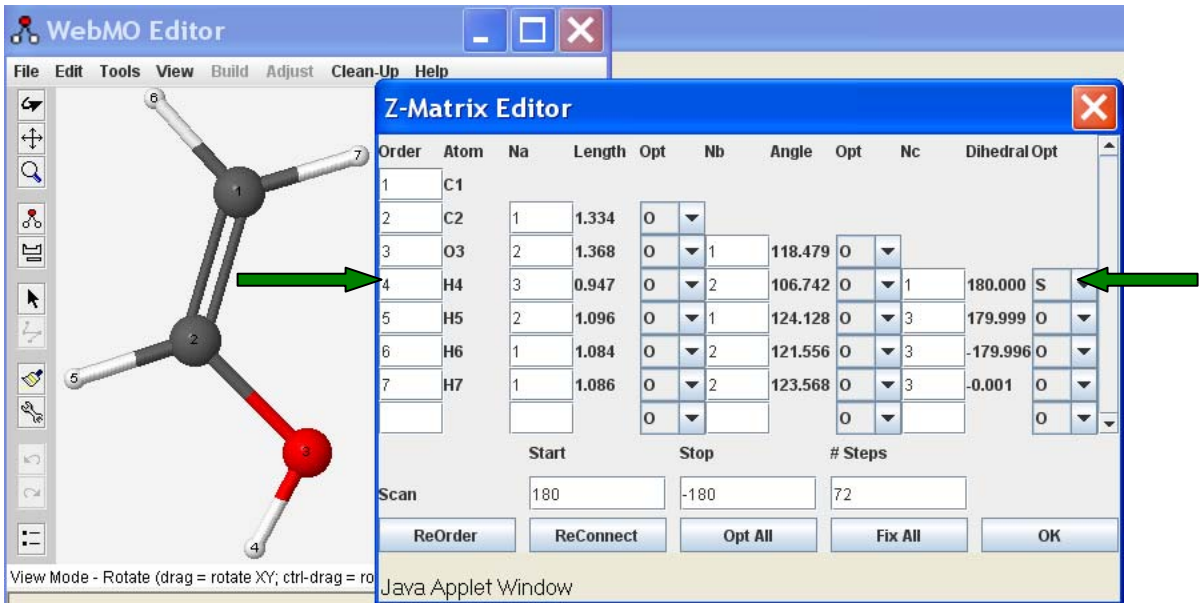
Exercise 3 – Determining the Optimum Structure for Ethenol (Vinyl alcohol)

Build a model of ethanol by drawing the C=C-O backbone, followed by Clean-Up > Comprehensive-Mechanics. The model builder will generate one of the two Structures shown.



Click the Adjust tool (Arrow, 6th down). Define a dihedral angle by clicking on the hydroxyl H atom, hold the Shift key, then click in turn on the O-C=C atoms.

Choose Tools > Z-matrix. In the pull down menu next to the dihedral angle, chose "S", and type in the Start, Stop, and # Steps as shown below. (Hint: Be sure to use the atom numbers to help find the dihedral angle of interest).



Click OK in the Z-matrix Editor, then click Close Editor. Click the blue continue arrow.

Choose Gaussian or Mopac as the engine.

Choose/Type in the following:

Job Name: C2H4OScan
Calculation: Coordinate Scan
Theory: PM3
Basis Set: 3-21G (or default)
Charge: 0
Multiplicity: Singlet

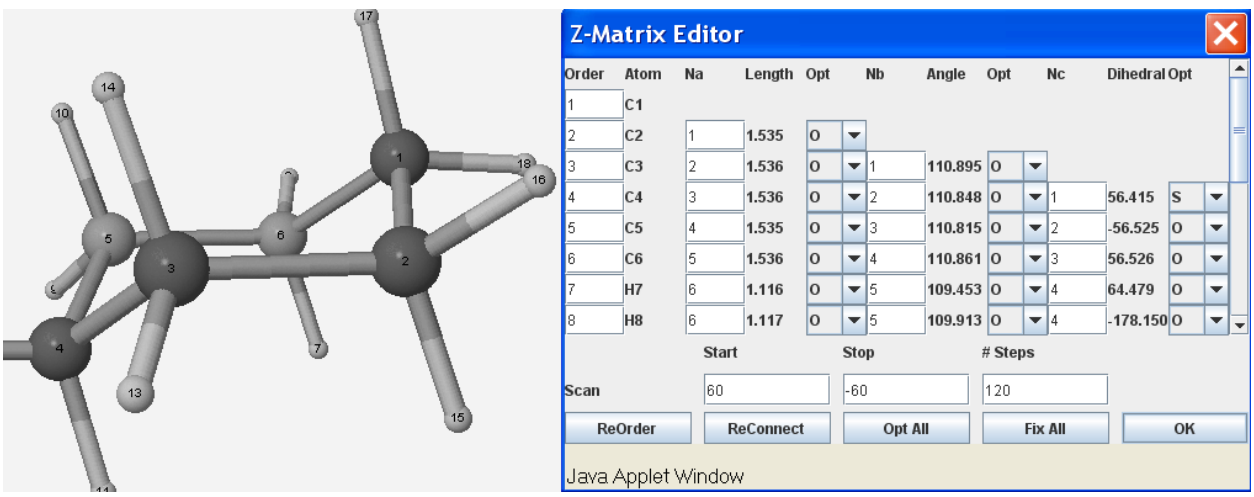
Click the blue continue arrow. When the job is complete, open the file and scroll down to the Coordinate Scan data. Click on the magnifying glass in the title bar.

On the graph that appears, use your mouse to record the energies of conformer **I** _____kcal mol^{-1}; conformer **II** _____ kcal mol^{-1}, and the barrier _____kcal mol^{-1}. Which conformer is more stable? _____

Exercise 4 – Determining the Energy Map for Cyclohexane

Build a molecule of cyclohexane. (Note: Try to place the atoms at the corners of a regular hexagon for best results).

Choose Tools > Z-matrix. As in Exercise 3, identify a dihedral angle consisting of the "head", two "seat", and the "foot" C atoms. Use the Adjust Tool and click the "head" and the other three atoms in order around the ring. (Note: Refer to the atom numbers to help). In the Z-matrix Editor window, enter the Start, Stop, and # Steps as shown. Click OK, followed by Close Editor.



Click the blue continue arrow, choose Gaussian or Mopac as the engine, then Choose/Type in the following:

Job Name: C6H12Scan
Calculation: Coordinate Scan
Theory: PM3
Basis Set: 3-21G (or default)
Charge: 0
Multiplicity: Singlet

Click the blue continue arrow. When the job is complete, open the file and scroll down to the Coordinate Scan data. Click on the magnifying glass in the title bar. On the graph, use the mouse to position the cursor to collect the data below.

Record the energy values of the chair conformer (global minimum) _____ kcal mol^{-1}, the half-chair conformer (global maximum) _____ kcal mol^{-1}, the

twist-boat conformer (local minimum) _____ kcal mol^{-1}, and the boat conformer (local maximum) _____ kcal mol^{-1}.

Which conformer is the most stable? _____ What is the energy difference between the two stable conformers? _____ kcal mol^{-1} (literature 4.0 – 5.5 kcal mol^{-1})

What is the potential energy barrier between the two stable conformers? _____ kcal mol^{-1} (literature 10.0 – 11.0 kcal mol^{-1})

What is the potential barrier between the twist-boat and boat conformers? _____ kcal mol^{-1} (literature 1.4 – 1.6 kcal mol^{-1})