Software Comparison Lab

In each of the following experiments, methanol will be constructed, minimized, and various bond lengths and angles measured. Several of the software programs have more than one method that can be used to construct the molecule. The three-dimensional model builder will be the preferred method for these exercises.

1. ACD ChemSketch/3D
(Strictly speaking, this combination is not a molecular modeling program. However, two-dimensional and three-dimensional structures can be drawn, manipulated, minimized using a molecular mechanics based on CHARMM, and molecular properties determined.)

Construct Molecule
Open / ACD / ChemSketch.
Open / ACD / 3D Viewer.
Click on ChemSk at bottom.
Click on C on left tool bar.
Click in workspace. CH_4 appears.
Click on O on left tool bar.
Click on CH_4, drag away, and release. CH_3OH appears.
Click on Clean Structure icon (21^{st} across top).
Click on 3D Optimization icon (23^{rd} across top).
Click on Copy to 3D at bottom.
Rotate by left clicking and dragging. Note that the eclipsed form may be present.

Optimize Molecule
Click 3D Optimization icon (15^{th} across top). Note the staggered form appears.

Measure Properties
Click on Calculate Distance Between 2 Atoms icon (12^{th} across top).
Click on C atom and move cursor to each attached H atom. Record the three C-H bond lengths in the table on the last page of these laboratory directions. Click in the workspace away from the molecule.
Click the O atom and move the cursor to the C and H atoms. Record the C-O and O-H bond lengths. Click in the workspace away from the molecule.
Click on Calculate Angle Between 2 Bonds icon (13^{th} across top).
Click the C, O, and H atoms and record the C-O-H bond angle.
Exit. Do not save.

2. Bio-Rad KnowItAll

(Strictly speaking, this combination is not a molecular modeling program. However, two-dimensional and three-dimensional structures can be drawn, manipulated, minimized using a molecular mechanics based on CHARMM, and molecular properties determined.)

Construct Molecule

Open / KnowItAll.
Click the DrawIt icon (1st down).
Click the Main tool bar.
Click the single bond tool (6th) and click in the workspace.
Click the atom replacement tool (5th) and click on the end of the single bond. Type in OH.

Optimize Molecule

Click Transfer to: 3D ViewIt.
Click OK in the "2D Data Present" warning window.
Click Compute / 3D Structure.

Measure Properties

Click on C atom and move cursor to each attached H atom. Record the three C-H bond lengths in the table.
Click the O atom and move the cursor to the C and H atoms. Record the C-O and O-H bond lengths.
Click the C, O, and H atoms and record the C-O-H bond angle. [Note: This may be incorrect!]
Exit. Do not save.

3. CAChe

Construct Molecule

Open / CAChe / Workspace. (The first time may be a screen listing of installed options.)
Click Drawing Pencil tool (5th down on left). Choose C / sp^3 / blank / single in the drop down windows.
Click in workspace. A black C atom appears.
On drop down menu choose O / sp^3 / blank / single.
Click on C atom and drag away. Release. A red O atom appears bonded to the C atom.
Click Select tool (1st down on left).
Click in workspace. Both atoms appear in full color.
Choose Beautify / Comprehensive. CH_3OH appears.
Click Rotate tool (6th down on left). Left click and drag. The staggered form should be

present.

Optimize Molecule
Choose Experiment / New. Save as ch3oh.csf.
Choose Property of: chemical sample, Property: optimized geometry, Using: PM3.
Click Start. Record the final $\Delta_f H$ value.
Close Experiment Status and Experiment windows.

Measure Properties
Click Select tool. Click on C and shift click on a H atom. Choose Adjust / Atom Distance and record the C-H bond length. Close the window. Repeat for the other two C-H bonds.
Likewise, measure and record the C-O bond length and the O-H bond length.
Click on the C atom and shift click the O and H atoms. Chose Adjust / Bond Angle and record the C-O-H bond angle. Close the window.
Exit. Do not save.

4. Chem3D
(Many chemists use the ChemDraw or the Text tool.)

Construct Molecule
Open / Chem3D.
Click the Single Bond tool (4^{th} down on left).
Click and drag in the workspace. CH_3CH_3 appears.
Click the Text tool (7^{th} down on left).
Click on one of the C atoms and type O in the small window that opens. CH_3OH appears.
Click the Rotate tool (2^{nd} down on left). Left click and drag to rotate. The staggered form should be present.
Click the Select tool (1^{st} down on left) and click in the workspace.

Optimize Molecule
Choose MOPAC / Minimize Energy / Theory / PM3 / Run.
Click the triangle next to the message bar at the bottom. Record the $\Delta_f H$ value.

Measure Properties
Click on the C atom and move the cursor over each C-H bond. Record the C-H bond lengths.
Click on the O atom and move the cursor over the C-O and O-H bonds. Record the C-O bond length and the O-H bond length.
Click on the C atom and shift click on the O and H atoms. Record the C-O-H bond

angle. (Note table of all measurements are available using Analyze / Show Measurements / Show... .)

Exit. Do not save.

5. HyperChem

Construct Molecule

Open / HyperChem.

Double click Draw tool (1st across top). Periodic table appears.

Click C and click in workspace. A blue circle for C appears.

Click O. Click on C atom, drag away, and release. A red-blue line appears.

Close the periodic table.

Double click Select tool (2nd across top). CH_3OH appears.

Click Rotate tool (3rd across top). Left click and drag. The staggered form should be present.

Click Select tool.

Optimize Molecule

Choose Setup / Semi-empirical. Click PM3 and OK.

Choose File / Start Log. Save as ch3ohpm3.log.

Choose Compute / Geometry Optimization. Click OK on any dialog windows.

Choose File / Stop Log. Locate ch3ohpm3.log and open using Notepad or Wordpad. Record the $\Delta_f H$ value. Close the file and delete.

Measure Properties

Click on a C-H bond and record the C-H bond length. Right click in the workspace and repeat for the other two C-H bonds.

Likewise, measure and record the C-O bond length and the O-H bond length.

Click and drag from the C atom and to the H atom on the O. Record the C-O-H bond angle.

Exit. Do not save.

6. PC Model

Construct Molecule

Open / PC Model.

Click Build tool (4th down on left). CH_3CH_3 appears.

Click H/AD tool (6th down on left). H atoms disappear.

Click PT tool (14th down on left). Periodic table appears.

Click O and close the periodic table.

Click the center of one of the C atoms. C changes to red O.

Click H/AD tool. CH_3OH appears.
Rotate by right clicking and dragging. The staggered form should be present.
Choose Edit / Remove LP.

Optimize Molecule
Choose Compute / Minimize(MMX calculation). Record the $\Delta_f H$ value.

Measure Properties
Click Querie tool (13th down on left).
Click the C atom and a H atom and then click in the workspace. Record the C-H bond length. Repeat for the other two C-H bonds, the C-O bond length, and the O-H bond length.
Click the C, O, and H atoms and then click in the workspace. Record the C-O-H bond angle.
Exit. Do not save.

7. Spartan

Construct Molecule
Open / Spartan.
Click the New icon (1st across top). Building tools appear.
Click C atom (1st row, 1st column).
Click in workspace. CH_4 skeleton appears.
Click O atom (2nd row, 3rd column).
Click on one of the yellow ends. CH_3OH appears.
Rotate by left clicking and dragging. The staggered form should be present.

Optimize Molecule
Choose Setup / Calculations. Choose Equilibrium Geometry at Ground State with Semi-Empirical PM3.
Click Submit. Save as ch3oh.spartan.
Click OK to "started" message and OK to "completed" message.
Choose Display / Properties and record the $\Delta_f H$ value. Close.

Measure Properties
Click on the Distance icon (11th across top) and on a C-H bond. Record the C-H bond length. Repeat for the other two C-H bonds.
Click on the C-O bond and record the C-O bond length and click on the O-H bond and record the O-H bond length.
Click on the Angle icon (12th across top) and click on the C, O, and H atoms. Record the C-O-H bond angle.

Exit. Do not save.

Software	$\Delta_f H^o_{298}$ (kcal mol^{-1})	$r_{C\text{-}H}$ Å	$r_{C\text{-}O}$ Å	$r_{O\text{-}H}$ Å	$\angle_{C\text{-}O\text{-}H}$ °
ACD ChemSketch/3D (mm)					
Bio-Rad KnowItAll (mm)					
CAChe					
Chem3D					
HyperChem					
PCModel (MMX)					
Spartan					
Literature	-47.96	1.096±0.01	1.427±0.007	0.956±0.015	108.9±2.0