

## Properties of Molecules

In this exercise we will study some of the features of two freeware programs: ACD ChemSketch/3D Viewer (<http://www.freechemsketch.com/>) and BioRad KnowItAll (<http://www.knowitall.com/academic/>). We will study some of the properties that can be calculated for formaldehyde, a simple molecule.



Literature values for the molecular parameters from the JANAF tables are  $r(\text{C-H}) = 1.12 \pm 0.01 \text{ \AA}$ ,  $r(\text{C=O}) = 1.21 \pm 0.01 \text{ \AA}$ ,  $\angle(\text{H-C-H}) = 118 \pm 2^\circ$ . The point group of formaldehyde is  $\text{C}_{2v}$ .

### 1. ACD ChemSketch/3D Viewer



Open ACD/ChemSketch

open the 3D Viewer by clicking on ACD/Labs and 3D Viewer  
click on ChemSketch at bottom


Construct formaldehyde

click the Draw Normal icon  and the C icon (atoms column at left)  
click in the workspace to produce  $\text{CH}_4$

*You may wish to save the methane molecule that appears for use in another presentation. To do this, click File / Save As, choose the folder or USB drive destination, name the file as methane, choose MDL[V2000] mol as the type, and click Save.*

click the O icon (atoms column at left)  
click on the  $\text{CH}_4$  and drag to produce  $\text{H}_3\text{C-OH}$   
click and drag a second time to produce  $\text{H}_2\text{C=O}$   
click on the Clean Structure icon  or choose Tools / Clean Structure  
click on the 3D Optimization icon 


Generate the name of the compound

click on the Generate Name for Structure icon 


Optimize using molecular mechanics

click Copy to 3D at the bottom  
click the 3D Optimization icon

Measure and Record Bond Lengths

click on the Bond Length icon   
click on the C atom and a H atom  
record the bond length that appears in the Internuclear Distance window  
close the Internuclear Distance window  
repeat for the other C-H bond  
compare to the JANAF values

Measure and Record Bond Angles

click on the Angle icon   
click on a H atom, the C atom, and the other H atom  
record the bond angle that appears in the Bond Angle window  
compare to the JANAF values

Predict various Molecular Properties

click on ChemSketch at the bottom

click Tools / Calculate / All Properties

Try a couple of simple compounds of your choice.

Close

## 2. BioRad KnowItAll

Open BioRad KnowItAll

Construct formaldehyde

click the DrawIt icon in the left column



click the single bond tool  in the Main menu

click once in the workspace to produce a single bond

click a second time on the bond to form a double bond

click the label tool  and click on one end of the double bond

type O

Optimize using molecular mechanics

click Transfer to: 3DViewIt

click OK in the warning message window

click Compute / 3D Structure


Measure and Record Molecular Symmetry, Bond Lengths, and Bond Angles

using the top menu, click Transfer to: SymApps

record the atom coordinates, bond lengths, bond angles, etc. are available in tabular form by expanding the “trees”

Study the symmetry of the molecule

click the entry for the point group in the table

click the Orbit XY icon 

rotate the molecule and symmetry elements by holding the left mouse button down and using the mouse

observe the character table for the molecule by either clicking Compute / Character Table or clicking the Compute Character Table icon

Determine the IUPAC Name

return to Chemistry / DrawIt

click Transfer to: IUPAC NameIt

click ok in the warning message window

Try a couple of simple compounds of your choice.

Close