

## EDU 104 lab Molecular Visualization Links



**Chime (CHemical mIME):** A Browser plug-in that has been around for a long time. Many sites still exist, while others are converting to Jmol. To download the plug-in requires registration:

<http://www.mdli.com/downloads/downloadable/index.jsp>

Examples:

- 1) <http://molvis.sdsc.edu/atlas/morphs/water10/water10r.htm>
- 2) <http://www.umass.edu/microbio/chime/ir-spect/index.htm>
- 3) <http://faculty.otterbein.edu/DJohnston/symmetry/chime/index.html>
- 4) [http://www.umass.edu/microbio/chime/index.html#martz\\_tutorials\\_chime](http://www.umass.edu/microbio/chime/index.html#martz_tutorials_chime)
- 5) <http://www.wellesley.edu/Chemistry/Flick/molecules/newlist.html>

**Jmol:** There are several options, an *applet* that can be integrated into web pages, an *application* that runs on the desktop, or the *viewer* that can be integrated into other java applications. For more information on the capabilities, go to: <http://jmol.sourceforge.net/>

Examples:

- 1) <http://virtual-museum.soils.wisc.edu/displays.html>
- 2) <http://jmol.sourceforge.net/demo/>
- 3) <http://www.dcu.ie/~pratta/jmgallery/JGALLERY.HTM>
- 4) <http://undergrad-ed.chemistry.ohio-state.edu/>
- 5) <http://www.jce.divched.org/JCEWWW/Features/MonthlyMolecules/index.html>

**Cortona VRML Client:** A browser plug-in that has different some different capabilities. The plug-in must be downloaded from: <http://www.parallelgraphics.com/products/cortona/>

Examples:

- 1) <http://www.chm.davidson.edu/ChemistryApplets/AtomicOrbitals/AtomicOrbitals.html>
- 2) <http://bohr.winthrop.edu/vrml/vrml.html>


**Protein Data Bank:** The Protein Data Bank currently has nearly 53,000 proteins, nucleic acids, protein/nucleic acid complexes, and other biomolecules for which the structures have been determined via X-ray diffraction and other techniques. These structures can be viewed in a variety of formats, including Chime, VRML, and Protein Explorer. See: <http://www.rcsb.org/pdb/>





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**Formaldehyde Studies:** In this exercise we will study some of the features of two freeware programs: **ACDChemSketch/3D Viewer** and **BioRad KnowItAll**. 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  $r(\text{C-H}) = 1.12 \pm 0.01 \text{ \AA}$ ,  $r(\text{C=O}) = 1.21 \pm 0.01 \text{ \AA}$ , H-C-H bond angle =  $118 \pm 2^\circ$ . The point group of formaldehyde is  $\text{C}_{2v}$ .

**ACD ChemSketch/3D Viewer:** Available for download at: <http://www.freechemsketch.com/>

- 1) Open ACD/ChemSketch  
open the 3D Viewer by clicking on ACD/Labs and 3D Viewer  
click on ChemSketch at bottom left
- 2) Construct formaldehyde  
click the Draw Normal icon () and the C icon (on the left)

- click in the workspace to produce CH<sub>4</sub>
- click the O icon (on the left)
- click on the CH<sub>4</sub> and drag to produce H<sub>3</sub>C-OH
- click and drag a second time to produce H<sub>2</sub>C=O
- from the top menu, choose Tools > Clean Structure
- click on the 3D Optimization icon ()
- click Copy to 3D at the bottom
- 3) Optimize using molecular mechanics
  - click the 3D Optimization icon again ()
  - from the top menu, choose View > and experiment with the first six options listed
- 4) Measure and Record Bond Lengths
  - click on the Bond Length icon ()
  - click on the C atom and the O atom
  - record the bond length that appears in the Internuclear Distance window
  - close the Internuclear Distance window
  - measure the C-H bond distance in the same way
  - compare to the JANAF values
- 5) 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
- 6) Predict various Molecular Properties
  - click on ChemSketch at the bottom
  - click Tools > Calculate > All Properties
- 7) Try a couple of simple compounds of your choice.
- 8) Close

**BioRad KnowItAll:** Available for download at: <http://www.knowitall.com/academic/>

- 1) Open BioRad KnowItAll
- 2) Construct formaldehyde
  - click the DrawIt icon
  - click the single bond tool () in the Main menu
  - click once in the workspace to produce a single bond
  - click a second time to form a double bond
  - click the label tool () and click on one end of the double bond
  - type O
- 3) Optimize using molecular mechanics
  - using the top menu, click Transfer to: 3DViewIt
  - click OK in the warning message window
  - click Compute / 3D Structure
- 4) Measure and Record Molecular Symmetry, Bond Lengths, and Bond Angles
  - using the top menu, click Transfer to: SymApps
  - The atom coordinates, bond lengths, bond angles, etc. are available in tabular form by expanding the “trees”
- 5) Determine the IUPAC Name

return to Chemistry / DrawIt  
click Transfer to: IUPAC NameIt  
click ok in the warning message window

- 6) Try a couple of simple compounds of your choice.
- 7) Close

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**Molecular Workbench:** Available for download at: <http://mw.concord.org/modeler/>

The *Molecular Workbench* (MW) software is a free, open-source modeling program specifically designed for use in science education. Powered by a set of real-time molecular simulation engines that compute and visualize the motion of particles interacting through force fields, in both 2D and 3D, it provides a simulation platform for teaching and learning science through atomic-scale reasoning. Many important concepts in physics, chemistry, and biology that are otherwise too abstract to understand can be visualized with dynamical and interactive simulations.

Start Molecular Workbench

Choose either the Library of Models or the Activities Center and investigate

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**NetLogo:** Available for download at: <http://ccl.northwestern.edu/netlogo/download.shtml>

NetLogo is a programmable modeling environment particularly well suited for modeling complex systems developing over time. Modelers can give instructions to hundreds or thousands of independent "agents" all operating concurrently. This makes it possible to explore the connection between the micro-level behavior of individuals and the macro-level patterns that emerge from the interaction of many individuals. The program allows students to open simulations and "play" with them, exploring their behavior under various conditions. It is also an authoring environment which enables students, teachers and curriculum developers to create their own models. It is simple enough that students and teachers can easily run simulations or build their own. It is also advanced enough to serve as a powerful tool for researchers in many fields.

The program has extensive documentation and tutorials. It also comes with a Models Library, which is a large collection of pre-written simulations that can be used and modified. These simulations address many content areas in the natural and social sciences, including biology and medicine, physics and chemistry, mathematics and computer science, and economics and social psychology. Several model-based inquiry curricula using NetLogo are currently under development.

Open Netlogo

Choose Files > Models Library and expand the Chemistry and Physics folder  
Click on "Polymer Dynamics" and choose Open at the bottom of the new window  
All Netlogo models run as described below

In the Polymer Dynamics window, click Setup followed by Go

Click Go a second time to stop the model

Click Setup to return to the starting configuration

Repeat the above steps to investigate other Models and find something you can use in your classroom