

SC07 Chemistry Session Links

Chime (CHEMical mIME): A Browser plug-in that is no longer supported. Many sites still exist, while others are converting to Jmol. To download the plug-in requires registration at: <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
- 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.ill.fr/dif/3D-crystals/vrml/buckeyb.wrl>
 - 2) <http://www.chm.davidson.edu/ChemistryApplets/AtomicOrbitals/AtomicOrbitals.html>
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Project Interactivate: A set of interactive Java-based activities for exploration in science and mathematics, available at: <http://www.shodor.org/interactivate/>

Examples:

- 1) Search for *function*, click on *Function Flyer*, and type $1*\sin(1*x+0)+0$ in the box
- 2) Search for *data*, click on *Data Flyer*, type in some data that approximates a function
- 3) Search for *stopwatch* and click on the link

The Computational Science Education Reference Desk (CSERD): A collection of useful applets that can be used as educational tools. Go to: <http://www.shodor.org/refdesk/> and type in the search term *chemistry*. ~230 chemistry-related links appear.

Examples:

- 1) Search for *ideal gas* and click on *Molecular Model for an Ideal Gas*
 - 2) Search for *structure* and click on *Reciprocal Net*
 - 3) Search *kinetics* and click on *Michaelis-Menten Kinetics*
 - 4) Search for a chemistry term you are interested in and see what you find
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Odyssey: A teaching program for introductory and general chemistry classes that utilizes molecular simulations to provide an interactive environment for learning and exploration. For more information, visit: <http://www.wavefun.com/products/odyssey/odyssey.html> A demo version is available at: http://www.wavefun.com/products/demo_odyssey_univ.html

WebMO: A free Web-based interface to computational chemistry packages. Information can be found at: <http://www.webmo.net/> A demo server is available to try out small jobs (up to one minute of CPU time) at: <http://buchner.chem.hope.edu/~webmodemo/cgi-bin/webmo/login.cgi>

A number of free computational engines are available, including GAMESS, MOPAC, and Tinker

We will be using **WebMO Pro**, which is NOT free, and includes graphics capabilities. We will also use the Gaussian computational engine for some exercises, which is not free.

WebMO Pro access via the BobSCEd Cluster at Earlham College:

<http://bobsced.cluster.earlham.edu/cgi-bin/login.cgi>

You will be provided with a login and password for use at SC07.

If you would like to receive permanent login credentials, contact Shawn at: ssendlin@ncu.edu

Further computational chemistry resources are here: <http://www.computationalscience.org/ccce/>

VenSim PLE (VenSim Personal Learning Edition): This is a free systems dynamics software package that allows modeling of time-dependent phenomena such as chemical kinetics. A free version of the program is available for download at: <http://www.vensim.com/freedownload.html>

If you have questions, please contact:

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