The following review is the second in a series of articles surveying free online resources of potential interest to chemists. The first article appeared in the July-Aug 2006 CI*, p. 26.*

Free Information Resources for Chemists, Part 2

by Leslie Glasser

Chemical Informatics

Structure representation is an important support to chemical understanding. A long history and wide applicability make RasMol and the related MDL Chime plugin two of the most important chemical display programs available (RasMol is now known as "Protein Explorer" <www.umass.edu/microbio/rasmol>, although it can be used for much more than protein structures; MDL Chime can be downloaded at <www.mdli.com> or <www.umass.edu/microbio/chime>, where further information on molecular visualization is provided). In addition, the World Index of Molecular Visualisation Resources <molvis.sdsc.edu/visres> provides a comprehensive listing of programs, tutorials, and examples for molecular visualizations.

Structure drawing, naming, and query programs are also available for free downloading for noncommercial uses. KnowItAll ChemWindow Edition <www.knowitall.com/academic/welcome.html> from Bio-Rad provides access to spectroscopic information, Elsevier offers a number of free-to-academics programs <www.mdli.com/solutions/solutions_for/academics>, including its MDL ISIS/Draw program, and ACD/Labs offers ChemSketch <www.acdlabs.com/download/#free>. ChemAxon provides a wide range of Java-based chemical toolkits that can be accessed through at <www.chemaxon.com/forum/ftopic193.html> based on its Marvin program for viewing chemical reactions and queries. The toolkits available provide facilities for the prediction of structure-based properties; structure and reaction searching and database handling; structure canonization, transformations, and library enumerations; pharmacophore and structure-based screening, clustering, and diversity analysis; and (promised for the near future) drug design.

The important ORTEP program, used for crystal-structure drawing (and adaptable to single molecules), can be found in version ORTEP-III at <www.ornl.gov/sci/ortep/ortep.html>.

INFOTHERM <www.infotherm.de> is a database of thermophysical properties maintained by Berlin's FIZ-Chemie, where search on the Internet is available free of charge for pure substances and by subscription for mixtures. INFOTHERM is updated monthly.

Mathematical Applications

Having access to data fitting and symbolic mathematics is important. An enormous range of mathematical software, much of which is free, is available through the Department of Mathematics at the University of Haifa <http://math.haifa.ac.il/msoftware.html>. Drawing simple graphs can generally be accomplished by using the facilities available in the spreadsheet program; however, for greater versatility, the free GNU Project graph-drawing program Gnuplot (version 4.0 at <www.gnuplot.info>) is enormously powerful and will perform most tasks rapidly and more than satisfactorily. New users will face an initial steep learning curve, but once it is overcome, the effort expended will generally be found to have been well worthwhile.

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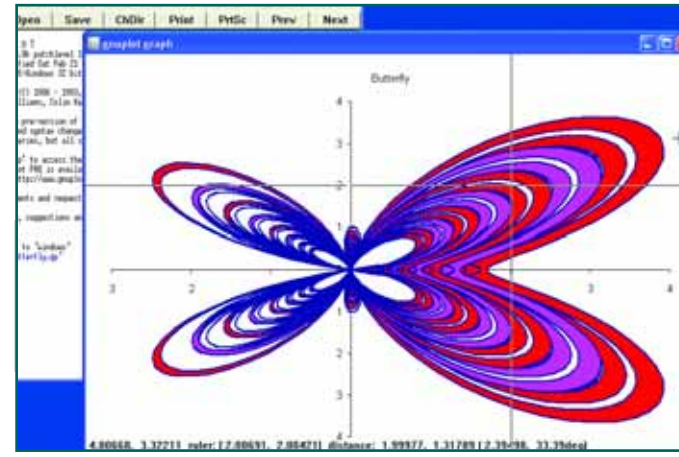

Sample output from Gnuplot, copied from <www.gnuplot.info>.