TECHSIGHTING
SOFTWARE

Micromanaging References

Modern bibliographic software products facilitate the placement of footnotes and references into scientific manuscripts and allow continuous updating of the citations without requiring the user to reformat the document. Most bibliographic software packages accept references entered manually, copied from CD-ROM databases, or downloaded from standard Web sites such as BIOSIS. Only a few are integrated with Internet browsers that search and download citations from online databases.

Reference Manager 9.5
ISI ResearchSoft
Berkeley, CA
$199.95 (academic); $99.95 (student)
510-559-8592
www.isiresearchsoft.com

One such product is the excellent Reference Manager 9.5, a substantial update of Reference Manager 9 (*1*). The power behind the Reference Manager 9 was its cite-while-you-write capability that enabled users to import references into a document without leaving their word processing program. The software made it very simple to enter new citations in the text by automatically associating the internal citation with the reference listed at the end of the manuscript. Reference Manager 9.5 now adds new features that include "pay-per-view" access to Search ISI, one of the largest and most popular scientific referencing services. Other features of Reference Manager 9.5 include a spell checker with a customizable dictionary.

Reference Manager 9.5 works within word processing programs as an item under the Tools menu. This adds functions to the word processor for importing, searching, and editing citations. Although other bibliographic software packages share these features, Reference Manager 9.5 distinguishes itself by the convenience with which it lets the user search online while simultaneously working on a manuscript, permitting real-time reference entry and updating.

New databases are created in the Database Window, which contains numerous options for managing references. Citations for the database can be retrieved by searching CD-ROM and online bibliographic sources, including Medline and PubMed. Reference Manager 9.5 also provides direct access to ISI databases in two ways. First, the program allows users to directly search the ISI eSource database and download 10 full-record views for $29.95. In addition, current subscribers to the ISI Web of Science database can retrieve information using Reference Manager 9.5 at no additional charge.

The features of Reference Manager 9.5 surpass those of other popular bibliographic software products. Its flexibility in copying reference information between databases and its ability to search 10 databases at one time are noteworthy. The software is simple to use and is an invaluable companion to word processing programs. It is highly recommended for anyone needing a powerful tool for developing local bibliographic databases.

Reference Manager Version 9.5 operates on Windows 95, 98, and NT4 systems with at least 16 MB of RAM and a CD-ROM. The program works with all Windows-compatible word processing software; however, its cite-while-you-write feature was designed for Microsoft Word 95, 97, and 2000 as well as Corel WordPerfect for Windows 7, 8, and 9.

—BRIAN R. SHMAEFSKY

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Reference
1. B. Shmaefsky, *Science* **288**, 1981 (2000).

TECHSIGHTING
SOFTWARE

Plotting the Fit

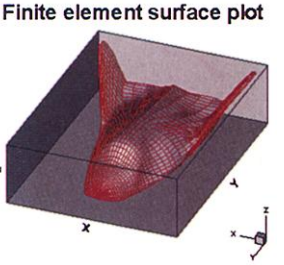
Tecplot 8.0 is a technical graphing software program for creating high-quality, two- and three-dimensional (2D and 3D) graphical representations of complex data. Like many technical programs, Tecplot requires time and effort to master. But the effort is worthwhile because the quality of the graphical output obtained is exceptional. Tecplot is available in a Windows 95, 98, or NT version and a Unix X-Motif version. Instructions and pictures depicting dialog boxes for the Windows and Unix versions are intermixed in the Tecplot manual. This may be somewhat confusing, although the overall formats of the Windows and Motif versions are very similar.

Tecplot 8.0
Amtec Engineering, Inc.
Bellevue, WA
$1295 (Windows)
800-763-7005
www.amtec.com

Tecplot can render 3D surface and volume plots, vector and streamline representations of fluid flow and heat transfer data, mesh plots of linear or curvilinear grid data, finite element representations of real world structures, and contour plots. Tools that allow one to explore the 3D data representations by panning, zooming, and rotating 3D objects are particularly useful for examining complicated graphics. Light source color and shading options can be adjusted to enhance the 3D quality of the graphic. Data can also be examined by slicing along x, y, and z axes or another specified plane.

Tecplot can draw an unlimited number of lines in an x-y plot and has over 100 different symbol types. The program features interactive data adjustment, multiple axes, logarithmic scales, custom labels, and error bars. Line thickness, color and pattern, axis range, and label and tick mark attributes can be easily specified. In scatter plots, the symbol size and color can be a function of a field variable.

Finite element surface plot



Tecplot permits several types of data manipulation, including data smoothing to reduce noise, shifting of cell-centered data, transforming polar coordinates to rectangular, and shifting from 2D to 3D views. There are several interpolation routines available, including kriging, inverse-distance, and linear interpolation. Curve-fitting routines built into Tecplot include polynomial, exponential, power, and spline fits. Variables can easily be weighted before curve fitting. One shortcoming of this program is that user-defined curve fits are not supported.

Macros and plot templates in Tecplot allow for automation of repetitive tasks. Tecplot can be run in batch mode to generate multiple plots.

One of the most attractive features of Tecplot is the publication-quality graphics it produces. The sidebar tools make it very easy to add, delete, move, or resize text and geometries. Properties of the graphics such as data representations, axes, and legends can be altered quickly from multitabbed dialog boxes. Complex layouts can display multiple graphs either side-by-side or laid over each other. Axis and plot features can be linked so that when a parameter, such as scaling, is

Tech.Sight is published in the third issue of each month. Contributing editor: Kevin Ahern, Department of Biochemistry and Biophysics, Oregon State University. Send your comments by e-mail to techsight@aaas.org

changed in one graph, it is changed simultaneously in all corresponding ones. A feature that allows data to be animated by time or other plot parameters makes for powerful data presentation. Tecplot also includes a built-in Web publishing feature, and the Tecplot Web site has a gallery of plot graphics generated by Tecplot users from a variety of disciplines.

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Modeling Molecules

Gaussian 98W is a software product for Windows, Unix, and VMS systems that models molecular systems using atomic properties, molecular coordinates and the basic laws of quantum mechanics. The program calculates physical chemical indices, such as potential energy surfaces, excitation energies, and substituent effects. Computations may be made for systems in the gas phase or in solution, in the ground or excited states. Other molecular properties calculated by the program include molecular energies and structures, bond and reaction energies, transition states, molecular orbitals, multipole moments, atomic charge and electrostatic potentials, vibrational frequencies, and thermochemical properties. Gaussian 98W can also diagram reaction pathways. The software is a powerful tool for teaching physical chemistry or thermochemistry at undergraduate and graduate levels.

Gaussian 98W and GaussViewW
Gaussian, Inc.
Carnegie, PA
$600/$1500 and $500/$1000 (academic/commercial)
412-279-6700
www.gaussian.com

GaussViewW (the "W" in each program name stands for the Windows version) is a graphical user interface for Gaussian 98W, which will appeal primarily to novices, for building molecules and controlling the program. Experienced users may also appreciate having the original option of keyboard control of the program. The Save Image option in GaussViewW can be used to quickly create chemical structures and surfaces in a form suitable for publication. The program allows one to view Gaussian 98W calculation results, such as optimized molecular structures, molecular orbitals, atomic charges, electron density surfaces, electrostatic potential surfaces, as well as animations of normal modes corresponding to vibrational frequencies. Users can also set up and run Gaussian calculations from this interface, which can be a huge help for the novice because instead of having to write many lines of code, one can simply build a molecule in GaussViewW. From this, Gaussian 98W derives and uses the resulting bond lengths, bond angles, and dihedral angles for calculations.

Building a molecule is simple—one clicks on the fragment box to select structures and then clicks in the view box to add the selected fragment. Aliphatic and ring structures are available, and a Bio option allows addition of amino acids or nucleosides. By selecting the Element button, a user can choose any atom from the periodic table. The Inquire button allows one to find bond length and interatomic angles for any portion of a molecule.

Gaussian 98W is more than a simple program that draws molecular structures and performs calculations. Users should be knowledgeable in physical chemistry and have some understanding of the application of quantum mechanical calculations for electronic structure studies to derive maximum benefit from the package. The quality of results produced by the program depends on how problems are defined. Similarly, the accuracy of analyses depends greatly on the investigator's knowledge of the system, as well as the accuracy of any guesses or compromises made in specifying the problem.

Gaussian 98W comes with a Reference guide, a User's Reference, and *Exploring Chemistry with Electronic Structure Methods*, a wonderful book that introduces the workings of the program and the theory behind the calculation methods.

The available technical support is excellent. The Gaussian Web site provides news about the program and its features. Online help is particularly useful for experienced users.

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TECHSIGHTING
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Electronic Teacher

Bonding II provides electronic instruction on the basics of chemistry. Packaged on a Macintosh/Windows hybrid CD-ROM, the tutorial contains a narrated set of modules covering fundamental concepts for a freshman-level chemistry class.

Bonding II
CyberEd, Inc.
Paradise, CA
$129.95
www.cybered.net/index.html

The CD-ROM is organized into three domains: Presentation, Testing, and Interaction. The Presentation module takes the form of narration, broken into 54 segments, and the entire module can be viewed in about an hour. Users can view these sequentially or navigate with the Jump Presentation option. Concepts covered in this section include atomic orbitals, valence shells, covalent bonds, Lewis structures, multiple bonds, valence share electron pair repulsion (VSEPR), molecular shapes, bond angles, polarity, orbital hybridization, σ and π bonds, and intermolecular forces. As a whole, the narrations are quite clear and integrated well with illustrative graphics. The voice of the narrator is pleasant, but it is overused in places (for example, in some places it reads print that appears on the screen). The sound recordings have considerable background hiss.

A particular strength of the Presentation module is its coverage of VSEPR theory and molecular shapes. Here, users can clearly view orbital shapes and understand molecular structures arising from them.

In addition to the Presentation module, the disk also has a Testing mode, which largely consists of multiple choice questions. The selection of questions is fairly extensive and covers the material well. Both "pre-tests" and "post-tests" are available to assess a student's change in learning. There is also a so-called Interactive mode, which consists primarily of testing as well. It is designed to provide a more visual environment for learning, but the user-controlled actions are simplistic (e.g., dragging answers to a desired spot) and unintuitive in places.

Shortcomings of the disk include a lack of coverage of all molecular orbitals (only *s* and *p* are discussed) and the absence of stoichiometry from the lessons. One error, which could be very confusing to students, was noticed in the testing section for the Lewis diagrams. The program incorrectly tells students that their answer is wrong unless they orient electrons in one particular configuration.

Despite these weaknesses, Bonding II provides a clear explanation of many of the basic principles of chemistry for beginning students, and it can serve as a useful learning tool that can easily be integrated into an instructional program.

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