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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TECHSIGHTING
SOFTWARE

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.

—JOHN A. WASS

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TECHSIGHTING
SOFTWARE

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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