Computer Software Reviews

ChemWindow. Reviewed Version 1.0. Current Version 1.3. SoftShell International Ltd.: 2754 Compass Drive, Suite 375, Grand Junction, CO 81506. Phone: 303-242-7502. FAX: 303-242-6469. Compatible with Windows 3.0 or 2.X. List Price $295.00; academic discounted (20%) price $236.00; student discounted (80%) price $59.00. The ChemWindow demo and molecular mass calculator are free.

ChemWindow is a molecular drawing program derived from SoftShell's ChemIntosh desk accessory for the Macintosh; files can be exchanged between ChemWindow and ChemIntosh. The features are similar to previously reviewed packages [Molecular Presentation Graphics (PC). *J. Am. Chem. Soc.* **1987**, *109*, 3177; ChemIntosh and ChemPanion (Mac). *J. Am. Chem. Soc.* **1987**, *109*, 6905–6906; ChemText (PC). *J. Am. Chem. Soc.* **1987**, *109*, 7240–7241; WIMP (PC). *J. Am. Chem. Soc.* **1988**, *110*, 4099; ChemDraw (Mac). *J. Am. Chem. Soc.* **1988**, *110*, 7260–7261; ChemConnection Desk Accessory (Mac). *J. Am. Chem. Soc.* **1989**, *111*, 8327]. The program is a Microsoft Windows application; if you do not have Windows, a run-time version is included with the package. The system requirements are the same as for Microsoft Windows. In general, the software will run on any IBM or 100% compatible computer and is available on 1.2 Mb or 720 Kb diskettes. In order to take advantage of this product and the Windows environment you will need a mouse, graphics adapter, hard disk drive, and a Windows supported printer or plotter.

Drawing structures with ChemWindow is quick and easy since the mouse provides complete control over the structural lines being drawn and text placement. There are ten bond types available: forward wedge, backward (or hashed) wedge, hashed, dashed, wavy (or squiggle), bold, dot, and normal (single, double, or triple). Several types of arrows are available: reaction, equilibrium, resonance, retrosynthetic, and solid or dotted curved. Four fonts are available for plotter text: Modern, Roman, Sans Serif, and Script. Proportional spacing is optional for the Roman and Sans Serif typefaces. If a printer is installed and selected, the fonts native to that device are available.

The manual is thorough, but it is somewhat difficult to read due to variable line spacing in places where small graphics are included. On-line help is available from the Options menu; once selected, the mouse is used to click on an item to access the pertinent help information. In conjunction with the manual, the help facility provides all the information necessary to perform an operation.

The menu arrangement is straightforward and provides complete control of all the available tools such as the length and thickness of bonds as well as the size of a ring to be drawn. Selection of the Fonts menu option not only allows one to change the font style but also allows the choice of bold, italic, superscript, and subscript types. A series of palette tools located just below the pull-down menus allow rapid access to the many types of drawing functions (bonds, rings, text, etc.).

While using this program only a few disadvantages were discovered. A significant inconvenience is the manner in which files are saved in different formats; ChemWindow (CW), encapsulated postscript (EPS), and WordPerfect Graphics (WPG) formats are supported. This function allows saving a file in only one of these formats at a time; only files saved in the ChemWindow format can be retrieved and edited. If you want to save a file in two formats (i.e., .CW so the file can be edited, and .WPG for importing the drawing into Word Perfect), you must execute the file save twice. Unfortunately, there is no macro facility that would allow this procedure to be automated. The vendor indicates that version 1.3 corrects this problem. ChemWindow also lacks an enlarged view, which makes drawing (editing) complicated structures more difficult.

A very useful feature is the ability to position structures based on rulers, which can be turned on and off, positioned at the top and left of the drawing area. Structures can also be selected and aligned horizontally (vertically) in a drawing relative to the left (top), center, or right (bottom) of each graphic by selecting the Arrange option on the menu.

The choice of rings available on the menu includes 3–8-membered carbocycles. The six-membered ring also has options for chair and boat forms as well as a benzene form. Fused-ring systems can easily be created by clicking on the point of initial attachment and rotating the resulting ring for the fusion to occur.

Since ChemWindow is a Windows application, drawings can be exported to the Clipboard and transferred to another program. Drawings in other documents originally created by ChemWindow may be edited by importing them via the Clipboard.

As an added bonus SoftShell includes another Windows program called MMCalc, which calculates molecular weights, exact masses (for high-resolution MS), or percent composition (for elemental analyses) from an entered molecular formula. Formulas are entered in a free format fashion without spaces, parentheses are allowed, and isotopes are indicated with the "^" character (i.e., ^{13}C would be entered as "^13C").

In conclusion, ChemWindow is an excellent program for creating and editing publication quality chemical drawings and would be a good addition to any chemists' software portfolio. If you are shopping for a drawing program, ChemWindow should be on your list.

George R. Newkome, Gregory R. Baker, and Charles N. Moorefield,
University of South Florida

Book Reviews*

Introduction to the Theory of Atomic and Molecular Collisions. By J. N. Murrell and S. D. Bosanac (The University of Sussex). John Wiley & Sons: New York. 1989. viii + 199 pp. $69.95. ISBN 0-471-92365-6.

Although molecular collisions are the primary events in chemical reaction dynamics, the quantum-mechanical education of physical chemists has traditionally emphasized bound-state problems. Now that theory is able to make quantitative predictions of cross sections and rate constants, and even to challenge experimental results on simple systems, the time has come to redress this situation. There are several good textbooks on scattering theory written by physicists, which are directed toward nuclear, atomic, or high-energy applications. The serious students must eventually master the formalism developed in these texts, but they first ought to acquire an elementary overview of the characteristic problems posed by molecular collisions. The excellent monographs by Child (1974) and Levine (1969) are out of date in many respects, and in any case they are probably too difficult for a first introduction. There is a real need for an *elementary* introduction to collision theory, suitable for advanced undergraduates or beginning graduate chemistry students who have had a semester of basic quantum mechanics.

The authors of the book under review have succeeded remarkably well in presenting the basic classical and quantum theory of elastic, inelastic, and reactive collisions using only elementary methods. Having taught some of this material at the first-year chemistry graduate level, I appreciate the authors' achievement; this book will be extremely useful to instructors as well as students. Chapters 1 and 2 set the tone: quantum scattering theory is introduced from the elementary time-independent point of view, based upon stationary solutions of the Schrödinger equation satisfying (intuitively motivated) asymptotic boundary conditions, and applied to the central force problem. Of course, this is followed by the Ford-Wheeler analysis of the semiclassical limit via the WKB phase shift and a study of classical-quantum correspondence in rainbow and glory scattering. The insights developed here are drawn upon in later chapters, in discussing rotational rainbows and interference effects in vibrational excitation. Chapters 3 and 4 develop the classical, semiclassical, and quantum-mechanical treatments of inelastic collisions. The S-matrix and its cousins are introduced here, again from the strictly time-independent perspective (via the Jost matrices), as are the close-coupling equations and the distorted-wave and sudden approximations. Classical S-matrix theory also makes a brief appearance. Chapter 5 deals with reactive scattering. Naturally, the classical theory dominates here, but there is some qualitative discussion of quantum procedures, in particular of the hyperspherical coordinate method that is probably the easiest to explain at this level. The difficult problem of electronically nonadiabatic colli-

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