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.

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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-

*Unsigned book reviews are by the Book Review Editor.

sions is given a careful treatment in Chapter 6. The authors derive the Landau–Zener–Stueckelberg formula by means of a novel perturbative calculation in the adiabatic representation; while this is more complicated than Zener's derivation, it has the advantage of giving the Stueckelberg phase. Classical-path methods such as the Tully–Preston surface hopping algorithm are described in some detail. Finally, Chapter 7 gives a short survey of surface scattering.

The range of topics discussed in a book of this size keeps the authors from exploring any of them in detail; instead, they direct the reader to the many excellent review articles. In some places, unfortunately, the discussion is brief to the point of obscurity. I was not happy with the discussion of action-angle variables in sections 3.3 and 3.6—it places too much emphasis upon the harmonic oscillator and could be misleading. I doubt that a student who has no background in formal classical mechanics will be able to get much out of the discussion of canonical generating functions on p 57. I would also have preferred a more leisurely discussion of the rotational sudden approximations. The IOS gets a good treatment but the physical significance of the CS approximation, that it neglects coriolis coupling arising from rotation of the collision plane, is not brought out.

These are minor complaints about what is overall an excellent introduction to the subject. I highly recommend the book for a course in second-semester quantum mechanics, or as a supplement to a book such as Levine and Bernstein for a course in chemical kinetics and dynamics.

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Quadrupole Storage Mass Spectrometry. Chemical Analysis. Volume 102. By Raymond E. March and Richard J. Hughes (Trent University). John Wiley & Sons: New York. 1989. xx + 471 pp. $69.95. ISBN 0-471-85794-7.

This book appeared with coincidentally appropriate timing close to the Nobel Prize Award to Paul and Dehmelt for quadrupole ion trap work. However, its focus is very definitely on the operation and application of quadrupole traps as mass spectrometers and chemical reactors, without detailed attention to the quadrupole-trap activities of the physics community. The emergence of the quadrupole ion storage trap (QUISTOR) as a mass spectrometric device with mass resolution, mass range, versatility, and sensitivity sufficient to interest the chemical, analytical, and mass spectrometric communities has been an unexpected, striking development of recent years.

The authors are able to do a successful job of combining an instructional primer, a detailed exposition of the theory and operation of the device, a historical survey, and a comprehensive, up-to-date review of the literature of the technique and its applications. Reasonable success in all of these aims should earn the book praise from a wide audience.

An opening chapter by J. F. J. Todd offers a well-conceived introduction to the history, principles, and applications of the device at a low level of detail, interesting to the casual as well as the serious reader. The second chapter describes principles and theory in considerable detail, progressing from an elementary level. The extensive third chapter on the physics of the ion trap extends this exposition to the design and operation of practical devices. These nearly 200 pages on theory, design and operation reach a substantial level of mathematical sophistication, but the exposition is carried through with enough blow-by-blow detail to be accessible to most chemists with even modest mathematical tools. Many illustrations, diagrams, actual numerical data, and sample calculations (but not a number of careless and typographical errors) are welcome aids to learning. Substantial parts would be usable in an undergraduate analytical instrumentation course. The choice, organization, and presentation of this instructional portion of the book are excellent. The authors are not gifted in presenting complex material clearly, however, and more effort than should be necessary is often needed to follow the sequence of argument.

The remaining four chapters explore a wide range of topics in applying various QUISTOR techniques to problems in ion chemistry and chemical analysis. The last two chapters concentrate on the commercial instruments developed and sold by Finnigan MAT that have played a central role in disseminating this new technology into the chemical community, overcoming a perception of extreme difficulty and expense of the technique in the bands of physicists. The briefer, useful exposition in the theory and operation of the QUISTOR mass spectrometer which begins Chapter 6 might well be read before Chapter 2.

As is natural for a new technique, the chemical studies described in these chapters display some elements of reinventing the wheel, as for instance in the area of ion photochemistry familiar to this reviewer, whose study by other techniques is still at a higher level of development and sophistication. The versatility and potential for important contributions of the quadrupole-trapping mass spectrometer are nevertheless displayed very clearly.

The book is attractively produced, with good indexing, an interesting table of patents, a bibliography, a thesis list, and 451 references up to 1988. Coming at a time when the initial evolution of this new mass spectrometric approach seems fairly mature and when extensive application is underway, this is a timely and largely successful book that should be widely interesting to physical and analytical chemists.

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Volumes of Proceedings

Comparative Biochemistry of Parasitic Helminths. Edited by Eva-Maria Bennet, Carolyn Behm, and Christopher Bryant (Australian National University). Chapman and Hall: London and New York. 1989. 180 pp. $65.00. ISBN 0-412-32730-9.

This little volume is far pleasanter to read than one would expect on being confronted by the cover, which features a horrifying close-up view of the business end of a Great Worm, Scourge of the Cosmos, seemingly straight out of a pseudoscience movie. Inside, however, there are no more pictures of creepy creatures, but only graphs, reaction pathways, etc. These are parts of the 13 papers from the Sixth International Congress of Parasitology, held in Australia at an undisclosed date (which appears to have been in 1987). The papers treat metabolism in helminths, schistosomes, nematodes, and other nasties and tell something about antiparasitic drugs. Most books have a subject index, some also have author indexes, but this one has a Helminth index.

Photosensitizing Compounds: Their Chemistry, Biology and Clinical Use. CIBA Foundation Symposium 146. Edited by Gregory Bock and Sara Harnett. John Wiley & Sons: New York and Chichester. 1989. viii + 241 pp. $57.95. ISBN 0-471-92308-7.

The CIBA Foundation sponsors symposia on biological, medical, and chemical research, generally multidisciplinary. One of them, held in London in March 1989, included the 15 papers in this volume, which also contains an introduction and a summing up by the Chairman, T. J. Dougherty, and transcripts of the discussions following each paper. The papers range from those that are essentially chemical to those that are clinical. Chemotherapy of cancer is a prominent theme. The subject index is thorough.

Dynamic Properties of Biomolecular Assemblies. Edited by S. E. Harding (University of Nottingham) and A. J. Rowe (University of Leicester). Royal Society of Chemistry: Cambridge. 1989. viii + 373 pp. $86.00. ISBN 0-85186-896-7.

This typescript volume contains the texts of 20 papers from a symposium held in Nottingham in 1988. The symposium aimed "to bring together scientists from both the 'colloid' and 'biophysical chemistry' traditions". Eight of the papers are devoted to techniques; five to dynamics of protein, nucleic acid, and protein–nucleic acid assemblies; and seven to dynamics of glycoconjugates and membranes. A substantial subject index is included.

Catalysis in Petroleum Refining 1989. Studies in Surface Science and Catalysis 53. Edited by D. L. Trimm (University of New South Wales), S. Akashah (Kuwait Institute for Scientific Research), M. Absi-Halabi (Kuwait Institute for Scientific Research), and A. Bishara (Kuwait Institute for Scientific Research). Elsevier: Amsterdam and New York. 1990. xii + 603 pp. $197.50. ISBN 0-0444-88211-1.

At a 1989 conference held in Kuwait there were five plenary lectures, 28 papers, and two panel discussions. All are reproduced from typescript in this volume. The emphasis is, of course, on industrial application. A list of participants occupies the inordinately large space of 15 pages, with more than 50% unused white space, whereas a subject index, which would have made the book more useful, is not present in any form.

Mycotoxins and Phycotoxins '88. Edited by S. Natori, K. Hashimoto, and Y. Ueno. Elsevier: Amsterdam and New York. 1989. ix + 484 pp. $168.50. ISBN 0-444-88028-3.

This is a collection of papers from the 7th International Symposium on the title subject, held in Tokyo in 1988. The subject includes fungal toxins, especially those produced by molds (e.g., aflatoxin) and toxins produced in algae. The papers deal with the hazards, pathology, detection, decontamination, etc., as well as the more chemical aspects, such as isolation, structure determination, and biochemistry. The papers are reproduced in typescript; there is no index.

Chemistry and Significance of Condensed Tannins. Edited by Richard W. Hemingway (U.S. Department of Agriculture) and Joseph J. Karchesy (Oregon State University). Plenum: New York and London. 1989. xi + 553 pp. $110.00. ISBN 0-306-43326-5.

The first North American Tannin Conference was held in Port Angeles, WA, in 1988. The attendance of 69 was only a little larger than the number of authors contributing papers. The papers are a mixture of review articles and reports of new research and are arranged under

eight headings: Introduction, Biogenesis, Structure, Analytical Methods, Reactions, Complexation, Biological Significance, and Specialty Chemicals. The papers are set in type and the Editors express their hope that the book will serve as a monograph on tannins. However, the presence of abstracts of each paper and the presentation of much experimental research of the authors leaves an obvious impression of a volume of proceedings. Nevertheless, the papers are well endowed with tables of data, historical reviews, and references. A substantial index enhances the reference value of the work. A noteworthy feature of the reference citations is the inclusion of the full titles of the cited works.

Food Colloids. Edited by R. D. Bee (Unilever Corporation), P. Richmond (AFRC), and J. Mingins (AFRC). Royal Society of Chemistry: London. 1989. x + 406 pp. $111.00. ISBN 0-85186-826-6.

This is a collection of 26 papers and 11 poster presentations from a 1988 symposium held in England. There are papers on beer foams, solid foams, froths, and Edible Food Foams and Sponges, as well as more limited subjects, such as Continuous Sausage Processing (is the sausage or the process continuous?), and surfactants in cream liqueurs. There seems to be something for all tastes.

Structure and Function of Biofilms. Life Sciences Research Report 46. Edited by W. G. Characklis (Montana State University) and P. A. Wilderer (Technische Universität Hamburg). John Wiley & Sons: New York and Chichester. 1989. xiii + 387 pp. $103.00. ISBN 0-471-92480-6.

This book is a "report" of a Dahlem Workshop held in Berlin in 1988. There are 17 individual papers, an introduction, four "group reports", and one "minority opinion", beside a glossary, a list of participants, and contributor and subject indexes. The Dahlem Konferenzen has a most unusual format, involving a selection of Group Agenda, followed by Group Discussions, then Reports, and finally a second meeting of the Groups to revise their reports. The interesting procedure is described in the forepages.

Modelling of Molecular Structures and Properties. Studies in Physical and Theoretical Chemistry 71. Edited by J.-L. Rivail (University of Nancy). Elsevier: Amsterdam and New York. 1990. xxiv + 788 pp. $269.25. ISBN 0-444-88714-8.

An international meeting held in Nancy in 1989 was the occasion for the many papers reproduced from typescript in this volume. They are grouped under five headings: Theoretical Advances and Basic Methodology, Molecular Modelling in Chemistry, Molecular Modelling in Biophysics, Modelling–NMR Joint Study of Biomolecules, and Computational Science. A list of the participants, including their affiliations with full addresses, is included. There is no index, but a terminating discussion of five pages appears in abbreviated form.

Acid–Base Catalysis. Edited by K. Tanabe, H. Hattori, T. Yamaguchi, and T. Tanaka (Hokkaido University). VCH: New York and Weinheim. 1990. xvix + 532 pp. $140.00 ISBN 0-89573-891-0.

The 48 papers in this volume are reproduced from typescripts and are grouped under four heading: Organic Synthesis, Characterization, Design and Preparation of Catalyst, and Catalytic Features. The emphasis of the program is on surface catalysis, and the treatment ranges from the theoretical to the practical. The symposium at which they were presented was held in Sapporo in 1988. A 4-page subject index is included.

Surfactants in Solution. Volume 7. Edited by K. L. Mittal (IBM Corporation). Plenum: New York and London. 1989. xvx + 510 pp. $115.00. ISBN 0-306-4332-X.

This is one of four volumes that constitute the proceedings of the Sixth International Symposium on the title subject, held in New Delhi in 1986. The subtitle is Aggregation of Surfactants, and Structure, Dynamics and Characterization of Micelles. It is a collection of reviews and (mostly) reports of original research, reproduced from typescript. A list of contributors, with a biographical paragraph about each, and a 4-page index complete the volume.

Biosynthesis of Branched Chain Amino Acids. Edited by Z. Barak (Ben-Gurion University of the Negev), D. M. Chapman (Ben-Gurion University of the Negev), and J. V. Schloss (E. I. Dupont de Nemours and Company). VCH: New York and Weinheim. 1990. ix + 530 pp. $120.00. ISBN 0-89573-961-5.

A "workshop" on the title subject was held in Beersheba in 1988 and gave rise to the 25 papers in uniform type that make up this volume. Some of the papers are concerned with inhibition of synthesis. The majority of papers are about microorganisms, but there is also a little about higher plants. An extensive subject index and a list of contributors complete the volume.

Insect Neurochemistry and Neurophysiology 1989. Edited by A. B. Bořkovec and Edward P. Masler (United States Department of Agriculture). Humana: Clifton. 1990. xii + 480 pp. $79.50. ISBN 0-89603-168-3.

The Third International Conference on the title subject, held at the University of Maryland in 1989, was the source of this book of proceedings. It begins with six reviews of roughly 30 pages each. These are followed by reports of original research, arranged in three groups: neurochemistry; neurophysiology, and neuroanatomy. A list of participants (with addresses), an index of contributors, and a 14-page subject index complete the work.

Computer-Enhanced Analytical Spectroscopy. Volume 2. Edited by Henk L. C. Meuzelaar (University of Utah). Plenum: New York and London. 1990. xvii + 318 pp. $65.00. ISBN 0-306-43276-5.

This volume contains papers from the Second Hidden Peak Symposium on the title subject, held in 1988. They are reproduced in uniform typeface and arranged in chapters, in two groups: Unsupervised Methods (Spectral, Deconvolution, and Data Reduction) and Supervised Methods (Expert Systems, Modeling, and Quantitation). A 6-page subject index is included.

Antioxidant Nutrients and Immune Functions. Advances in Experimental Medicine and Biology. Volume 262. Edited by Adrianne Bendich (Hoffman LaRoche, Inc.), Marshall Phillips (United States Department of Agriculture), and Robert P. Tengardy (Colorado State University). Plenum: New York and London. 1990. xi + 171 pp. $59.50. ISBN 0-306-43396-6.

Twelve typescript papers, an epilogue, a list of participants, and a short subject index make up this volume, which is derived from a symposium organized by the Agriculture and Food Chemistry Division of the American Chemical Society in 1988.

Phase Transitions in Soft Condensed Matter. NATO ASI Series B: Physics. Volume 211. Edited by Tormod Riste (Institute for Energy Technology) and David Sherrington (Imperial College of Science, Technology, and Medicine). Plenum: New York and London. 1989. ix + 391 pp. $89.50. ISBN 0-306-43394-X.

The NATO Advanced Study Institute held in Norway in April 1989 produced the many typescript reports of original research in this volume, which has an index of $2^1/_2$ pages and an 8-page list of participants.

Man and His Ecosystem. Volumes 1–5. Edited by L. J. Brasser and W. C. Mulder. Elsevier: Amsterdam and New York. 1989. lxxx + 2246 pp. $683.00. ISBN 0-444-87467-4.

An important five-day congress sponsored by The International Union of Air Pollution Prevention Associations was held in the Hague in 1989. Its proceedings consists of 369 papers in five volumes, reproduced from typescript. The five volumes represent five themes: Man (Human Health and Dose-Response Relationships); Indoor Air; Animals and Plants, Materials; The System (monitoring air pollution); and The Man-Made System (emissions, control, economic aspects, etc.). Indexes of contributors and of keywords are included in Volume 5.

New Developments in Selective Oxidation. Studies in Surface Science and Catalysis 55. Edited by G. Centi and F. Trifiro (Universita degli Studi di Bologna). Elsevier: Amsterdam and New York. 1990. xii + 892 pp. $197.50. ISBN 0-444-88694-X.

This volume of typescript papers resulted from an international symposium held in Rimini in 1989. The emphasis of the papers was on industrial chemistry and catalysis, but fundamental aspects were not neglected. A large section is devoted to oxidation by hydrogen peroxide and oxygen. Transformations of alkanes to functionalized derivatives make up another large section. Electro- and photooxidation is a small section. The final section is on surface catalysis. An index of contributors and a short subject index complete the volume.

Polymers in Information Storage Technology. Edited by K. L. Mittal (IBM Corporation). Plenum: New York and London. 1989. ix + 457 pp. $95.00. ISBN 0-306-43390-7.

A symposium on the title subject was held at the ACS National Meeting in Los Angeles in 1988. The typescript papers in this volume arose from it. They are collected under five rubrics: Photochemical Aspects of Optical Recording, Physicochemical Considerations in Optical Recording, Polymer Physics: Relevance to Optical Recording, Bulk/Surface Chemical Considerations in Magnetic Recording, and Physicochemical Aspects of Magnetic Recording. An appendix gives biographical information about the contributors, and there is a good index.

Large Lakes. Ecological Structure and Function. Edited by Max M. Tilzer (University of Constance) and Colette Serruya (Isreali Oceanographic Institute). Springer-Verlag: New York and Berlin. 1990. xviii + 691 pp. $150.00. ISBN 0-387-52103-8.

The 36 papers in this typescript volume are the result of a symposium held in Konstanz in 1987. They are collected in six parts, one of which, Particle Transport and Chemical Fluxes, has a significant amount of chemistry in it. A particularly timely paper has the title Biological Transfer and Sedimentation of Chernobyl Radionuclides in Lake Constance. The other parts are primarily biological or hydrological. The index is very thorough.