Additions and Corrections

Antibody Catalysis of $B_{Ac}2$ Aryl Carbamate Ester Hydrolysis: A Highly Disfavored Chemical Process. [*J. Am. Chem. Soc.* **1997**, *119*, 2315−2316]. PAUL WENTWORTH, JR., ANITA DATTA, SIMON SMITH, ANN MARSHALL, LYNDA J. PARTRIDGE, AND G. MICHAEL BLACKBURN*

Page 2316: The units in the third and fourth columns of Table 1 should be μM.

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Computer Software Reviews

MacMimic for Macintosh and PowerMac, version 3.0, with MM2(91) and MM3(92). Written by Anders Sundin. Instar Software AB, Ideon Research Park, S-223 70 Lund, Sweden. Phone: +46 46 18 24 70. Fax: +46 46 12 80 22. E-mail: anders.sundlin@orgk2.lth.se. Commercial price $1450 for the package. Academic price $600, and an additional $350 to include MM3.

MacMimic is a molecular display and modeling program for the Macintosh that interfaces with Allinger's molecular mechanics programs MM2 and MM3 and a raytracer (MolRay) for making "photorealistic" displays. MacMimic runs on Macintoshes (and Power Macintoshes) with FPU coprocessing capability with System 7.0 or newer MacOS. MacMimic and files are downloaded with an installer contained on a single 1.4 Mbyte floppy disk, which was not copy protected. MM2(91) and MM3(92) are also each installed from their own disks. After installation the total package occupies 9.8 Mbyte of memory. MacMimic uses 2.8 Mbyte of Ram, and the accompanying MolRay raytracer program 4.1 Mbyte. More memory must be allocated for monitors larger than 14 in. MM2 and MM3 are supplied as parallel modules in Fortran that run in emulation by the Macintosh and take 2 and 7 Mbyte of Ram, respectively. Free updates will be available to licensed users.

A previous review of version 1.0 (see: Porter, N. A.; Scott, D. M. *J. Am. Chem. Soc.* **1991**, *113*, 2801−2802) has a very detailed description of all the features of MacMimic. Version 3.0 is basically the same, but allows all MM calculations to be performed on a FPU-enabled MacIntosh without exporting to a mainframe. The MacMimic software suite package allows the rapid modeling of organic molecules, handled separately or as ensembles. Molecules are built in 3D and color from the fragment files supplied, and user-modified with tools selected and activated from various palettes. There is no capability to generate models from two-dimensional drawings that organic chemists routinely use. However, molecules are smoothly imported and translated from other three-dimensional formats such as pdb files. The molecular models are rotated and manipulated (for example, rotation of a specified dihedral) with mouse-activated buttons on screen palettes and sometimes while a keyboard button is depressed simultaneously. With a group of molecules, single molecules can be selected and manipulated independently. The displays with 256 colors look highly defined and polished on a 14 in. monitor. Motion is very smooth and lucid in real time on a Power Macintosh. To control manipulations, this reviewer personally prefers one-handed controlling with the mouse as the joystick and/or a cluster of buttons on the keyboard, but use of the palette became intuitive rapidly. Molecular surfaces are quickly generated in specified colors from standard van der Waal radii and displayed as dot surfaces, with dot densities as chosen. Once oriented as desired, the model depiction can be printed out in color or black and white, or saved in numerous formats as appropriate—for the accompanying display programs for photorealistic cpk video display (MolRay)—or submitted singly or in batch mode for parallel MM2 or MM3 energy minimization. The MolRay module quickly creates nice half-screen-sized displays of cpk models.

Learning MacMimic was easy from the supplied documentation or with the Help balloons feature of System 7 MacOS. The manual is well-written and split into sections for introduction/installation, tutorials, and later reference. An example tutorial demonstrates the use of the MacMimic interface to perform energy minimization of butane conformers with or without torsion driving in MM2 or MM3. Heats of formation and other calculated physical properties are demonstrated. However, for other routine modeling problems, the need to export from MacMimic into MM2 or MM3 becomes somewhat cumbersome. A few common functional and heterocyclic groups are supplied in sample files, but problems were encountered with others submitted for molecular mechanics calculations. For heterocycles other than those supplied such as furan, pyrrole, and imidazole, messages appear demanding parameters. Practitioners of molecular mechanics are familiar with supplying correct atom-typing, atomic charges, bond lengths, bending constants, etc., but for MacMimic's MM modules, the documentation is not clear about how to create, find, or implement the missing values. Since this software package runs an unadulterated version of the Allinger MM programs, potential users should be ready to supply many parameters, which can be inconvenient, but also crucial to the validity of the model. Although perhaps less scientifically stringent, other available molecular modeling packages supply parameters and accept a wide variety of functional groups in a transparent interface without leaving a program, and some guide the novice user on-the-fly.

Many uses in medicinal chemistry for molecular modeling demand seamless handling of a wide variety of heterocycles and functional groups. Hopefully most practicing medicinal chemists are already aware and familiar with the pitfalls of setting molecular force field parameters. Otherwise the MacMimic package could impart a useful education in the establishment of a personal library of fragments and their parameters for molecular mechanics calculations (which is warranted in many cases anyway). However, such an experience of determining parameters and their validation would probably be most useful to novices such as undergraduates or beginning graduate students. With parameters in hand, the MacMimic package appears useful for calculating physical organic molecular energy parameters, such as heats of formation. MacMimic is very capable of high-quality display, manipulation, and desktop publishing of molecular models. Unfortunately the price of the MacMimic package is comparable to other modeling software for the MacIntosh that are more established, easier to use, and ultimately more versatile because they also serve as transparent interfaces to other modeling applications and/or software suites.

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Book Reviews *

Applications of LC−MS in Environmental Chemistry. Series: Journal of Chromatography Library, Vol. 59. Edited by D. Barceló (CID-CSIC). Elsevier: Amsterdam. 1996. xxii + 543 pp. $281.25. ISBN 0-444-82067-1.

Recent developments in mass spectrometry have afforded new opportunities to devise improved methodologies for characterizing compounds of environmental interest. This volume covers the aspects of using liquid chromatography with mass spectrometry for environmental analysis. The stated goal of this book is to answer a series of questions from the viewpoint of potential users of LC−MS in environmental analysis. These questions include the following: Which interface is the best for a particular problem? What is the sensitivity of a particular LC−MS method? Is there adequate structural information? To answer these questions, 17 authors have contributed to 12 chapters that address many facets of LC−MS in environmental chemistry. The first three chapters cover fundamentals and instrumentation in LC−MS. The next seven chapters describe particular applications of LC−MS in environmental analysis. The final two chapters concentrate on complementary methods for environmental analysis.

The first three chapters of this volume cover adequately the basics of LC−MS. However, the instrument descriptions and jargon make this information more appropriate for users already familiar with mass spectrometry. There is little focus on addressing the concerns of environmental analysis, although extensive references in each of these first three chapters do provide the opportunity for accessing such information. The final two chapters of this volume are good introductions to specific analytical techniques, post column extraction and capillary electrophoresis mass spectrometry, that may find increasing use in the field of environmental analysis. While these two chapters are probably not of general interest to researchers in environmental chemistry, these chapters not only provide excellent descriptions of these specific techniques but also give interested readers an idea of the variety of ways that mass spectrometry can be combined with proven separation methods for environmental problem solving.

The strength of this volume is clearly those chapters describing applications of LC−MS to environmental analysis. The coverage of particular compound classes is broad including such diverse areas as the analysis of dyes (Chapter 4), pesticides (Chapter 5), surfactants (Chapter 6), agrochemicals (Chapter 7), hazardous waste leachates (Chapter 8), organotin compounds (Chapter 9), and seafood toxins (Chapter 10). Each of these chapters is well written with up-to-date references. Numerous figures and tables, which supplement the discussion in the text or provide specific examples of the type of information one may obtain, are included. Each one of these chapters adequately addresses the three goals of this volume, although a few of these chapters are written from the perspective of a particular instrument design which limits their usefulness as a general reference.

As with most edited works, this book permits interested individuals the chance to find information on a particular subject in great detail while learning how such methodologies are applied in other areas of analysis. This work fills a niche in both the environmental chemistry and mass spectrometry literature and provides researchers in this area, for the first time, a useful reference book on the environmental applications of LC−MS. This book is highly recommended for any researchers in the field of environmental analysis, especially those looking to move beyond GC−MS.

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Electrochemical Phase Formation and Growth: An Introduction to the Initial Stages of Metal Deposition. By E. Budevski (Bulgarian Academy of Sciences) and G. Staikov and W. J. Lorenz (University of Karlsruhe). VCH: Weinheim. 1996. xi + 410 pp. DM188.00. ISBN 3-527-29422-8.

This book covers the fundamental aspects of electrochemical growth of crystals and offers rigorous descriptions of the initial steps of electrochemical crystal growth. The first two chapters present the requisite background material. This section is brief but understandable to chemists who are already well versed in electrochemical thermodynamics, Butler−Volmer kinetics, and structural aspects of crystal lattices. Novices may be overwhelmed by the material and thus may require a supplementary text. The authors discuss the thermodynamics and kinetics of 2-dimensional crystal growth by underpotential deposition in Chapter 3, which includes ex situ (ultra-high-vacuum) and in situ (scanning tunneling and atomic force microscopies) characterizations of adsorbed metal species. Chapter 4 delves into overpotential deposition of metals. Chapter 5 concerns the growth of single crystals on electrode surfaces. The formation of polycrystalline structures on surfaces including semiconductor surfaces and their modification by scanning tunneling microscope tips is the subject of Chapter 6.

Overall the book is well referenced and offers a comprehensive review of the literature of electrocrystallization with both classical and recent references (1995). It is a unique monograph since very few others overlap the topics discussed in this book. The strength of this book is the rigor of the treatment of both governing mathematical expressions and the descriptions of electrocrystallization. However, this feature distinguishes it as a monograph focused toward an audience of specialists.

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Kirk-Othmer Encyclopedia of Chemical Technology, Volume 20, Power Generation to Recycling, Glass. Edited by Jacqueline I. Kroschwitz and Mary Howe-Grant. Wiley: New York. 1996. xxviii + 1134 pp. $295.00. ISBN 0-471-52689-4.

This is the 20th volume of a 25-volume encyclopedia set, four volumes being published each year. The Fourth Edition is similar in format to the earlier editions with updates to the entries as necessary and the addition of several new subjects. This volume contains 33 entries ranging from Power Generation to Glass Recycling. This volume does not contain an index; however, paperback indexes are published every four volumes, and the supplement and index volumes are scheduled for publication in 1998.

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*Unsigned book reviews are by the Book Review Editor.