Additions and Corrections

A Stable Crystalline Carbene [*J. Am. Chem. Soc.* **1991**, *113*, 361–363]. ANTHONY J. ARDUENGO, III,* RICHARD L. HARLOW, and MICHAEL KLINE

Two reports[1] describing the isolation of a compound which possesses a very interesting duality between λ^3-phosphinocarbene and λ^5-phosphaacetylene structures have come to our attention. These two references should be included in our ref 7. We are grateful to Prof. G. Bertrand for bringing this work to our attention.

(1) (a) Igau, A.; Grutzmacher, H.; Baceiredo, A.; Bertrand, G. *J. Am. Chem. Soc.* **1988**, *110*, 6463. (b) Igau, A.; Baceiredo, A.; Trinquier, G.; Bertrand, G. *Angew. Chem., Int. Ed. Engl.* **1989**, *28*, 621.

The Complementary Redox Properties of Viologens and Pyromellitimides: A New Class of Organic Conductors [*J. Am. Chem. Soc.* **1991**, *113*, 376–377]. STEPHEN L. BUCHWALTER,* REVATHI IYENGAR, ALFRED VIEHBECK, and TERRENCE R. O'TOOLE

Page 377: Equation 1 of this communication should read as follows:

$$1^0 + 2 \rightleftharpoons 1^{\bullet+} + 2^{\bullet-} \qquad (1)$$

Computer Software Reviews

ChemWords. Version 1.1 (for Microsoft Word 4.0). Scientific Software: 17 Country Squire Ct., St. Louis, MO 63146. List price $50.00; no academic discount.

ChemWords 1.1 is a supplemental dictionary for use with the spelling checker of Microsoft Word 4.0 running on Macintosh systems. It includes approximately 32 000 words that cover a wide range of fields, for example chemistry, biochemistry, pharmacology, and toxicology. Proper names of many famous chemists, a range of chemical structural names, and a diverse selection of functional groups are included. It was not possible to check the accuracy of spellings within the dictionary other than to perform a relatively limited scan (of ca. 500 words) from which no errors were uncovered.

The dictionary is trivial to install and once Word 4.0 is informed of its location, it is automatically loaded along with the regular Word and user dictionaries. Because of its low price, it should serve as a cost-effective tool for most chemists. ChemWords 1.0 is also available from ACS Scientific Software.

James K. Whitesell, *University of Texas*

MacMimic. Version 1.1. InStar Software: IDEON Research Park, S-223 70 Lund, Sweden. List price $1500.00; academic discounted price $1000.00.

MacMimic is a computer application for building, displaying, and comparing molecular structures on the Macintosh II computer. The program also comes with a Macintosh version of MM2(87) and the structure building program (MacMimic) can be used to format structures for MM2 input. This interface makes the use of the MM2 program extremely convenient and this is probably the most powerful feature of the application. MacMimic can be used to import structures from Chem 3D and the Brookhaven Protein or Cambridge Crystallographic Database files and to export structures on an MM2/format file or to Chem 3D.

MacMimic provides the following features.

A 256-color monitor is required and MacMimic has a suggested memory size of 1.5 M as does the MM2(87) application. A hard disk is essential for easy use of the applications.

The MacMimic application does allow for easy construction of complex organic molecules. A thorough reading of the manual and working through the tutorial is recommended for the user to become reasonably proficient with the structure building commands. Some users may find the icon–palette interface somewhat non-intuitive compared to programs such as Chem 3D which offer access to most features through the common Macintosh pull-down menus. With practice, however, structures can be built very rapidly.

The structure building and display routines incorporate some particularly useful features. Default geometric parameters generally create reasonable conformations, and geometries are appropriately changed simply by modifying atom type and hybridization. A structure can be easily converted to its enantiomer and the configuration of individual atoms can also be quickly changed. Complex ring systems can be constructed by fusing separate structures, and the program allows the user to undo the last performed structure modification, even after graphical manipulation of the structure.

Structures can be displayed in ball and stick or stick models and atoms and groups can be easily identified by color. Graphical output to other applications or to color or black and white printers is straightforward, and black and white laser-printer output can differentiate atomic types by gray-scale with 6.0 or later versions of Laser Writer and Laser Prep. Color is used to indicate atom type, but individual atoms or whole structures can be painted in other colors. Optional depth cueing is useful when viewing large molecules, especially proteins.

The application allows for easy and continuous sizing and reorientation of structures along x, y, and z axes, in contrast to Chem 3D. Several structures can be manipulated in the same window or in separate windows and there is a very useful "compare" feature that allows for assessment of structural similarities. Pseudoatoms can be placed in the center of a number of atoms and up to eight models can be RMS fitted simultaneously. Bond lengths, bond angles, and torsion angles can be easily set and can be continuously, interactively changed.

The MM2(87) interface is extremely powerful. MacMimic structures or converted Chem 3D structures can be output as MM2 atom type files which are read by the MM2 program. The MacMimic implementation of MM2(87) is of the authentic program developed by Allinger and co-workers. No changes have been made to the computational part of the program nor to the force-field or force-field parameters.

Computational options such as dihedral drivers, restricted motion, electrostatics, heats of formation, etc. of MM2(87) are fully implemented. The interface allows selection of minimization options, including addition of new or changed force constants, for either direct or batch

minimization or for the creation of a standard format MM2(87) card input file. Once converted to a VAX text file, these input files could be submitted to VAX MM2(87) without editing. Identical calculations performed on a VAX 8350 were completed in one-third to one-fifth the time required by a first-generation Macintosh II with a MC68020 processor. The full output of the Macintosh MM2 calculation is written to a text file that reports the resulting steric energy, the number of atoms and bonds in the molecule, the optimized coordinates with MM1 atom type numbers, and a list of bonds. This file can be used as input to the structure program (MacMimic) which displays the minimized structure. Another text file contains standard MM2(87) output which can be read by any text editor. Input to MM2(87) is thus very easy to achieve and data output and display of the minimized structure is also very convenient.

The MacMimic user's guide and the MM2(87) user's manual are very helpful, and appendices that include MM2 potential functions, atom types, and standard input files will be useful for those users that do not have extensive experience with this method. A modest library of MM2 structures comes with the program, and it is easy to add to this library and to use filed structures as starting points for building new compounds.

MacMimic and MM2(87) for the Macintosh make implementation of the Allinger force-field on the Macintosh a simple and effective process. With fast Macintosh II computers now available, chemists interested in the structure of organic molecules will find MacMimic to be a powerful, although expensive, alternative to some existing VAX and Macintosh programs. The MacMimic structure drawing application is reasonably easy to use and has several features not found elsewhere while other competing programs have more sophisticated displays and output to printers or word processors.

Ned A. Porter and Daniel M. Scott, *Duke University*

*Book Reviews**

Advanced Practical Organic Chemistry. By M. Casey, J. Leonard, B. Lygo, and G. Procter (University of Salford). Routledge, Chapman & Hall: New York. 1990. xii + 264 pp. $37.95. ISBN 0-412-02461-6.

This book is intended to be a guide covering the most up-to-date techniques commonly used in organic synthesis and it performs this task admirably. In general, the book brings together in one convenient volume many of the techniques and "tricks of the trade" necessary to be a practicing organic chemist. The beauty of this book is the simple straightforward presentation of these techniques. A chemist when confronted with a new technique or reaction type could consult this work and at the very least know how to get started carrying out or analyzing the reaction.

Specifically, the chapters of this book address the following: keeping a notebook, general laboratory equipment, purification of solvents and reagents, handling of compressed gases, typical setupts for carrying out reactions and monitoring them, typical workup and characterization procedures, an introduction to the chemical literature, and an introduction to "special" procedures such as catalytic reduction, photolysis, and ozonolysis. In addition, several appendices are included describing properties of common solvents and gases, pK_a's of common acids and bases, properties of common Lewis acids, and reactivity tables for common oxidizing and reducing reagents.

As can be seen from the above listing, this book covers many areas of direct interest to the practicing organic chemist. Therefore, it is strongly recommended as a laboratory reference guide for all academic and industrial chemists involved in the laboratory practice of organic chemistry.

James G. Davidson III, *Parke-Davis*

Dictionary of Drugs. Chemical Data, Structures and Bibliographies. Edited by J. Elks and C. R. Ganellin. Chapman and Hall: London, New York, Tokyo, Melbourne, and Madras. 1990. Two-volume set. Volume I: xiii + 1303 pp. Volume II (Indexes): vii + 755 pp. $1099.00 ISBN 0-412-27300-4.

The main purpose of this two-volume reference work as stated by the editors is to provide the definitive source of concise, easily accessed factual data on all of the most significant drugs currently in use or late development worldwide. The Dictionary is primarily intended for use by the medicinal and pharmaceutical chemist as an aid to research.

Volume I is the Drug Dictionary which contains over 6000 alphabetical entries which are also numbered to assist ready location. Entries include all drugs for which generic names have been assigned, pharmacologic agents in advanced stages of clinical trials, and substances which have been used in traditional folk remedies. The individual substance monographs are consistent with the *Dictionary of Organic Compounds*, Fifth Edition, and provide structure diagrams showing stereochemistry where applicable and selected references to synthesis, analysis, pharmacologic studies, and general review articles. The primary literature citations have been reviewed through July 1989. Additional components of each monograph include a listing of trade names and synonyms and the therapeutic uses of the substance.

Volume II contains five carefully constructed and extremely useful indexes. The Name Index lists every name used in the Dictionary including the primary entries, isomers, and derivatives. The Molecular Formula Index lists all molecular formulae in Hill convention order. The CAS Registry Number Index lists all Chemical Abstracts Service registry numbers used in the Dictionary. The Type of Compound Index classifies all drugs listed in the Dictionary under one or more of approximately 200 headings related primarily to pharmacologic activity. The Structure Index provides reduced size structural formulae of all compounds in entry number order to allow rapid identification of structurally similar compounds.

The *Dictionary of Drugs* is a comprehensive and extremely useful reference which fully meets the goals set forth by the editors. The multiple indexes make the information in the Dictionary readily accessible. Since the continued usefulness of the Dictionary or any reference covering the rapidly changing area of drug development depends on the availability of current information and updated listings of new drugs, the publication of supplements and/or new editions will be essential. The frequency and method by which this information will be made available has yet to be determined; however, the cost of these updates must also be considered in the decision to acquire this reference work.

Cary E. Johnson, *The University of Michigan College of Pharmacy*

Atoms and Quanta. By Daphne F. Jackson (University of Surrey, United Kingdom). Surrey University Press: London. 1989. x + 215 pp. $29.95. ISBN 0-12-379075-1.

This is a textbook aimed at first-year physics undergraduates; it is also suitable for chemistry undergraduates with a strong background in elementary physics, perhaps as a supplementary source for physical chemistry. Students should be familiar with elementary classical mechanics and electricity and magnetism. The book has chapters on the structure of atoms, photons and their interactions, elementary quantum theory and the experiments related to its development, the nucleus, and instrumentation related to nuclear structure. Roughly one-eighth of the book addresses experimental considerations. Historical theories and ideas involved in the evolution of quantum theory are presented: Bohr model, planetary models, Rutherford's model of the atom. Each chapter has problems, though not extensive (usually about ten or fewer); solutions are provided for some exercises. Nearly all problems are numerical in nature and often require more insight and thought than the accompanying material. The text includes many figures of experimental data and illustrations of concepts described in the text.

The book has a strong physics orientation in its discussion. Extensive discussion of the photon and its characterization, the Compton effect, and electron and ion motion especially with fields are included. In the elementary discussion of the Schrödinger equation, the time-independent derivation is motivated from a classical wave equation and a number of simple one-dimensional examples are provided: electrons in a beam, electrons in a box, free electrons in a metal, electrons in a periodic potential, and one-electron atoms. Chemical bonds are only briefly discussed. Nuclear processes are discussed with some detail for α and β decay (with neutrinos included). Several nuclear models are discussed. The text does not include any of the more recent nuclear physics ideas, for example those involving quarks.

While the text is not as explanatory as I would prefer for course adoption, the book is an excellent source book for supplementary text. It takes many ideas and, if not fully explained quantitatively, does include qualitative descriptions. *Atoms and Quanta* can provide additional ma-

*Unsigned book reviews are by the Book Review Editor.