

Additions and Corrections

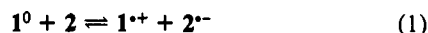
A Stable Crystalline Carbene [*J. Am. Chem. Soc.* 1991, 113, 361–363]. ANTHONY J. ARDUENGO, III,* RICHARD L. HARLOW, and MICHAEL KLINE

Two reports¹ 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.; Baccaredo, A.; Bertrand, G. *J. Am. Chem. Soc.* 1988, 110, 6463. (b) Igau, A.; Baccaredo, 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:



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