Additions and Corrections

Synthesis, Experimental and ab Initio Theoretical Vibrational Circular Dichroism, and Absolute Configurations of Substituted Oxiranes [*J. Am. Chem. Soc.* **1992**, *114*, 6850–6857]. Simeon T. Pickard, Howard E. Smith,* Prasad L. Polavarapu,* Thomas M. Black, Arvi Rauk,* and Danya Yang

Page 6851, Table 1: The heading of column 2 is observed rotation and should read $\alpha^{23-25}_{\mathrm{D}}$, deg (neat, 0.5 dm); footnote *b* also gives an observed rotation and should be α^{25}_{D} –47.02° (neat, 1 dm).

Page 6856, left column, line 25: The rotatory powers for (2*S*,3*S*)-2,3-dimethyloxirane [(2*S*,3*S*)-**5a**] are the observed rotations and should read α^{25}_{D} –19.6° (neat, 0.5 dm) [lit.[22] α^{25}_{D} –47.02° (neat, 1 dm)].

Page 6856, left column, line 31: The rotatory power for (2*S*,3*S*)-2,3-dimethyloxirane-*2,3-d*$_2$ [(2*S*,3*S*)-**5b**] is the observed rotation and should read α^{23}_{D} –19.5° (neat, 0.5 dm).

Page 6856, left column, line 39: The rotatory power for (2*R*,3*R*)-2,3-dimethyloxirane-*2,3-d*$_2$ [(2*R*,3*R*)-**5b**] is the observed rotation and should read α^{25}_{D} +18.1° (neat, 0.5 dm).

Page 6856, left column, line 46: The rotatory power for (2*S*,3*S*)-2,3-dimethyloxirane-*2-d* [(2*S*,3*S*)-**5c**] is the observed rotation and should read α^{25}_{D} –19.2° (neat, 0.5 dm).

Page 6856, left column, line 54: The rotatory power for (2*R*,3*R*)-2,3-dimethyloxirane-*2-d* [(2*R*,3*R*)-**5c**] is the observed rotation and should read α^{25}_{D} +19.0° (neat, 0.5 dm).

A Reaction Kinetic Mechanism for Methane Hydrate Formation in Liquid Water [*J. Am. Chem. Soc.* **1993**, *115*, 8565–8569]. Knut Lekvam* and Peter Ruoff*

Page 8566: The values of rate constants k_2, k_4, and k_5 in Table I were not those used in the simulations. The correct values are the following: $k_2 = 1.05 \times 10^{-13}$ M^{1-f-h} min^{-1}, $k_4 = 1.8 \times 10^{8}$ M^{-1} min^{-1}, and $k_5 = 0.001894$ M^{-f-h} min^{-1}. The errors were due to incorporation of constant water concentrations in the rate constants. The conclusions in the paper were based on the correct values given here, not the incorrect values given in the paper. Reaction M5 should read:

$$f{\cdot}\mathrm{CH_4(aq)} + h{\cdot}\mathrm{H_2O} \underset{k_{-5}}{\overset{k_5[\mathrm{H}]}{\rightleftarrows}} \mathrm{H} \qquad \text{(M5)}$$

Spectroscopic Studies of the Coupled Binuclear Non-Heme Iron Active Site in the Fully Reduced Hydroxylase Component of Methane Monooxygenase: Comparison to Deoxy and Deoxy-Azide Hemerythrin [*J. Am. Chem. Soc.* **1993**, *115*, 12409–12422]. Sabine Pulver, Wayne A. Froland, Brian G. Fox, John D. Lipscomb,* and Edward I. Solomon*

Page 12412, right column, 1st paragraph, end of first sentence: The following reference was inadvertently omitted: McCormick, J. M. Ph.D. Thesis, Stanford University, 1991.

α,3-Dehydrotoluene: Experimental and Theoretical Evidence for a Singlet Ground State [*J. Am. Chem. Soc.* **1993**, *115*, 12611–12612]. Paul G. Wenthold, Scott G. Wierschke, John J. Nash, and Robert R. Squires*

The MCSCF(8,8)/pVDZ energy calculations for the $^1B_1$ state of α,4-dehydrotoluene (compound **4**) and for benzyl radical were inadvertently carried out with a pVDZ basis set incorporating only five d-type polarization functions, instead of the six d-functions used for all other calculations. New calculations using the correct basis set give revised singlet–triplet energy differences ($E_{\mathrm{triplet}} - E_{\mathrm{singlet}}$) and 298 K heats of formation for α,2-, α,3-, and α,4-dehydrotoluene of –7.4, 3.0, and –8.1 kcal/mol and 105.4, 105.2, and 105.6 kcal/mol, respectively. The qualitative conclusions described in this paper are unchanged.

The Cope Rearrangement Revisited Again. Results of ab Initio Calculations beyond the CASSCF Level [*J. Am. Chem. Soc.* **1994**, *116*, 1072–1076]. David A. Hrovat, Keiji Morokuma, and Weston Thatcher Borden*

Page 1075: In footnote 32 the CASSCF energy of the conrotatory transition state for the opening of cyclobutene was incorrectly given as –154.8581 hartrees. The correct number is –154.8872 hartrees, which, at the CASSCF/6-31G* level of theory, puts the transition state 36.6 kcal/mol above cyclobutene and 55.4 kcal/mol above 1,3-butadiene.

Computer Software Reviews *

ChemIntosh. Version 3.3. SoftShell International Ltd.: 715 Horizon Drive, Suite 390, Grand Junction, Colorado 81506 (303-242-7502).List price $599.00; academic discount directly from vendor $399.00; student price $99.00; free demo.

ChemIntosh represents a superb chemical structure drawing program for the Macintosh. This program has undergone a number of upgrades since ChemIntosh II reviewed in 1992 (*J. Am. Chem. Soc.* **1991**, *113*, 2342). The latest revision includes a number of valuable changes and additions, while retaining the "look-and-feel" of previous versions.

The tool pallet is essentially unchanged, with the exception of the inclusion of a separate tool for Kekulé and "circle" forms of benzene (at the sacrifice of the cyclopropane tool, which has been relegated to the built in template collection). (The command key still switches modes of the old tool.) More substantive changes represent significant time saving as well as new features:

Atom labeling is now part of the bond drawing tool. Draw a new bond, hit O and an OH is placed at the end of the bond; N gives an NH_2 group; H a hydrogen; C a CH_3. This feature is "directionally savvy", placing a CH_3 or H_3C at the end of the bond, as appropriate. If a new bond is clicked, it changes into a double bond (click again, into a triple) and the labeling tool understands valence, placing a CH_3, CH_2, or CH group, as appropriate. Further, the atom label tool has a new feature: if the label window is empty (or not displayed), the tool can be used to click on a bond end or intersection of bonds and then to enter atom label text.

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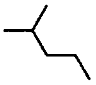
*Unsigned computer software reviews are by the Computer Software Review Editor.

Color is now available. Objects (or pasts thereof) can be selected with the "lasso" tool and then given one of eight standard colors (including white and black). Alternatively, a full color palate is available from a custom color submenue.

The program understands chemical structures (it actually has from the beginning) and can now calculate the molecular formula and weight of a selected structure. It can also check the chemical syntax of structures, reporting on atoms with incorrect valences. Further, structures represented as # # can be easily converted to line drawings, as:

$CH_3CH_2CH_2CH(CH_3)_2 \longrightarrow$ 

A number of different file formats can be opened and saved, including standard chemistry format (.SCF), PICT, Chemdraw 2.x, and Molecular Design MolFiles.

A separate Portfolio utility program is provided that affords a convenient tool for storing both ChemIntosh structures and PICT data. The portfolio is used in a simple and intuitive fashion by copy, paste, and cut operations.

A "magnifier" tool is included that can increase size to 800% and reduce to 12%. The window of the magnifier can be adjusted to encompass only a small portion of the screen or enlarged to cover the entire work area.

Overall, this version of ChemIntosh represents a significant improvement over previous releases and is highly recommended.

SciWords. Pool, Heller, and Milne, Inc.: 9520 Linden Avenue, Bethesda, Maryland 20814 (301-493-6595). $50.00 per copy; $45.00 Government/Academic (Windows Word 6.0 $70.00).

SciWords is a scientific dictionary for use on both Macintosh and IBM compatible systems with a number of word processing programs including WordPerfect and Word. It contains a large number of scientific terms as well as a standard collection of English words.

Installation on a Macintosh for Word (Version 5) is simple, as the file contains both standard as well as scientific words and replaces the dictionary supplied with Word. The file is copied to a directory (it need not be that containing Word) and then selected as the main dictionary using Tools→Preferences→Spelling→Main Dictionary.

The format of this dictionary is such that its contents cannot be viewed directly. As a result, evaluations of its accuracy and breadth could only be made indirectly. In terms of breadth, the dictionary contains a large number of chemical terms not present in Word's dictionary such as abiotic, acetal, alcoholysis, and maxima (the vendor states that the dictionary contains 75 000 sientific words from chemistry, physics, and biology). This comparison was made by spell checking an index for a sophomore organic textbook with the two dictionaries separately. Accuracy is more difficult to evaluate, as a presumption of misspelling in the dictionary is required. One quirk of the dictionary is that it does not always recognize accented letters, and "Kekulé" and "Schrödinger" are indicated as misspelled with "Kekule" and "Schrodinger" the suggested replacements. (Microsoft Word's dictionary recognizes neither.) There are also two separate dictionaries available which focus on agricultural and environmental terms.

Book Reviews

Advances in Enzymology and Related Areas of Molecular Biology. Volume 65. Edited by Alton Meister (Cornell University Medical College). John Wiley & Sons: New York. 1992. viii + 436 pp. $84.95. ISBN 0-471-527602.

There are few series that have been as influential or have maintained such high standards of excellence and timeliness as *Advances in Enzymology*. Volume 65 is no exception. Chapters in this volume are Traffic ATPases: A Superfamily of Transport Proteins Operating from *Escherichia coli* to Humans; The Respiratory Burst Oxidase; Pro- and Antioxidant Functions of Quinones and Quinone Reductase in Mammalian Cells; The Redox Centers of Ribonucleotide Reductase of *Escherichia coli*; Long Range Intramolecular Linked Functions in the Calcium Transport ATPase; Hydrogen-Bonding in Carbohydrates and Hydrate Inclusion Compounds; Methylation of mRNA; and Mammalian Nitric Oxide Synthase.

Collectively these chapters contains much of interest to diverse groups of chemists. Two chapters focus on ATPase transport proteins, covering both structural and mechanistic aspects of transport linked to ATP hydrolysis. Four chapters (those on the respiratory burst oxidase, quinones, ribonucleotide reductase, and nitric oxide synthase) cover various aspects of the roles of radicals and radical reactions in biology. Investigators in bioorganic and bioinorganic chemistry, in particular, may find these chapters interesting and informative. The chapter on hydrogen bonding emphasizes cooperativity in hydrogen bonding, as evident in the structures and energetics of hydrogen-bonding networks in the crystal structures of carbohydrates and hydrate inclusion compounds. The chapter on mRNA methylation concentrates on the detection and possible biological significance of internal methylation of adenosine residues. The level of the chapters is such that the discussions are accessible to investigators who are new to a particular area and to graduate students. At the same time the coverage is generally up-to-date; literature citations appear to extend through 1991, with some 1992 (in press) citations. All the articles are well-referenced, and the titles of references are included. Another feature of this series, which greatly increases its utility as an entry into the literature, is the author index that lists each author whose work is referenced. Overall this volume is an excellent addition to a distinguished series.

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