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 $\alpha^{23-25}{}_D$, deg (neat, 0.5 dm); footnote *b* also gives an observed rotation and should be $\alpha^{25}{}_D$ −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 $\alpha^{25}{}_D$ −19.6° (neat, 0.5 dm) [lit.[22] $\alpha^{25}{}_D$ −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 $\alpha^{23}{}_D$ −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 $\alpha^{25}{}_D$ +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 $\alpha^{25}{}_D$ −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 $\alpha^{25}{}_D$ +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:

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

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 ($E_{triplet} - E_{singlet}$) 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.

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