

# Additions and Corrections

**The Secondary  $\beta$ -Deuterium Isotope Effect and the Cage Effect in the Thermal Decomposition of Azobis- $\alpha$ -phenylethane** [*J. Am. Chem. Soc.*, **88**, 3775 (1966)]. By STANLEY SELTZER\* and EDWIN J. HAMILTON, JR., Chemistry Department, Brookhaven National Laboratory, Upton, New York 11973.

The abscissa of Figure 2 is incorrect and should read  $2[IV]/[III + IV + V]$ . The caption should read: "A plot of the ratio of rate constants vs. twice the ratio of cross-product to the sum of all products for equal concentrations of starting material."

Line 2, left column of p 3780, should read: " $2[IV]/[III + IV + V] = 0.9967$ ."



Ten lines from the bottom of the right column of p 3779 should read: "The variation of the ratio of cross-product to total product as a function of the ratio of first-order rate constants, in the absence of a cage effect, is shown in Figure 2."

**Mass Spectral Rearrangements of Siliconium Ions. Migration of Electronegative Groups from Carbon to Silicon** [*J. Am. Chem. Soc.*, **91**, 6544 (1969)]. By WILLIAM P. WEBER,\* RAYMOND A. FELIX, and ALVIN K. WILLARD, Department of Chemistry, University of Southern California, Los Angeles, California 90007.

On reexamination of the mass spectra of methyl 3-trimethylsilylpropionate under high resolution conditions, an error in the composition of the  $m/e$  105 ion became apparent. It is not  $C_3H_9SiO_2$  as indicated in eq 3 and Figure 1, but rather  $C_4H_{13}SiO$ . Peak matching high resolution data: calcd for  $C_4H_{13}SiO$ , 105.0732; found, 105.0733. A metastable peak at  $m/e$  68.9 =  $(105)^2/160$  indicates that this ion may be formed directly from the parent ion by loss of  $C_3H_3O$ .

**Stable Carbocations. CXXXVII. Cycloheptenyl, Cyclooctenyl, and Cyclononenyl Cations** [*J. Am. Chem. Soc.*, **94**, 6434 (1972)]. By GEORGE A. OLAH\* and GAO LIANG, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio 44106.

In Table II, cmr shifts for the first and third ions were interchanged and should be:

	$C_1$	$C_3$	$C_2$	$\Delta C_2 - C_1$
	-41.0	-41.0	+48.0	+89.0
	-24.0	-24.0	+57.0	+81.0

**Ambident Behavior of Nitrite Ion. Reactions of 2,4-Dinitrohalobenzenes and 1,2,4-Trinitrobenzene with Sodium Nitrite** [*J. Am. Chem. Soc.*, **95**, 2133 (1973)]. By DAVID H. ROSENBLATT,\* WILLIAM H. DENNIS, JR., and RICHARD D. GOODIN, Physical Research Division, Chemical Laboratory, Edgewood Arsenal, Edgewood Arsenal, Maryland 21010.

An error has been found in the calculation of rate constant  $k_1$  from  $\Delta OD/\Delta t$  for the compounds 2,4-dinitrochlorobenzene (DNCIB) and 2,4-dinitrobromobenzene (DNBrB) for their reactions with nitrite by O-attack. In

Table I the values for  $k_1$  should read, for DNCIB and DNBrB,  $2.5 \times 10^{-5} M^{-1} \text{ min}^{-1}$  and  $2.2 \times 10^{-5} M^{-1} \text{ min}^{-1}$ , respectively. Therefore the N:O ratio of nitrite attack on DNCIB is 70:1 and not 18,000:1, as implied by the previously stated rate constants. This correction has no effect upon the other rate constants nor upon the conclusions stated.

**Structure of the Peptide Antibiotic Amphomycin** [*J. Am. Chem. Soc.*, **95**, 2352 (1973)]. By MIKLOS BODANSZKY,\* GERALD F. SIGLER, and AGNES BODANSZKY, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio 44106.

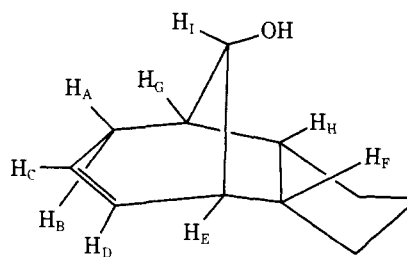
The + sign preceding the name of 3-isododecenoic acid should be deleted.

**Stereochemistry of  $\alpha$ -Halo Sulfoxides. II. Interdependent Stereochemistry at Sulfur and  $\alpha$ -Carbon in the  $\alpha$ -Halogenation of Sulfoxides** [*J. Am. Chem. Soc.*, **95**, 7431 (1973)]. By PAOLO CALZAVARA, MAURO CINQUINI, STEFANO COLONNA, ROBERTO FORNASIER, and FERNANDO MONTANARI,\* Centro C.N.R. e Istituto di Chimica Industriale dell' Universit , Milan 20133, Italy.

On page 7432, in Scheme I, the notations of absolute configuration (*S*)-(-)-**5b,6b** and (*S*)-(-)-**5a,6a** should be replaced by (*R*)-(-)-**5b,6b** and (*R*)-(-)-**5a,6a**, respectively.

**Photochemical Addition of Benzene to Cyclopentene** [*J. Am. Chem. Soc.*, **95**, 8250 (1973)]. By V. Y. MERRITT, J. CORNELISSE, and R. SRINIVASAN,\* IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598.

The correct structure of VIIIa is



In VIIIc, positions A-E and G are deuterated.

**$^{13}C$  Nuclear Magnetic Resonance Studies of Organometallic Compounds. I. *trans*-Methylplatinum(II) Derivatives** [*J. Am. Chem. Soc.*, **95**, 8574 (1973)]. By M. H. CHISHOLM, H. C. CLARK,\* L. E. MANZER, J. B. STOTHERS, and J. E. H. WARD, Department of Chemistry, The University of Western Ontario, London, Ontario, N6A 3K7, Canada.

Table II, item 14 under other  $^{13}C$  nmr data:  $\delta CH_3$  is 49.0 not 9.2 and  $^2J_{PtCC}$  was not observed and should be denoted  $^2J_{PTCC}^d$ .

Table V, item 8: the left-hand  $|^3J_{PtCNC}|$  value should be  $66(\pm 1)$ , not  $56(\pm 1)$ ; item 15:  $\delta C^1$  should be 52.0, not 41.6, while  $\delta C^2$  should be 41.6, not 52.0.

**Transition Metal Hydroborate Complexes. VI. The Solid-State Structure of  $\mu$ -Bis(cyanotrihydroborato)-tetrakis(tri-**

**phenylphosphine)dicopper(I)** [*J. Am. Chem. Soc.*, **96**, 69 (1974)]. By KENNETH M. MELMED, TING-I LI, JAMES J. MAYERLE, and STEPHEN J. LIPPARD,\* Department of Chemistry, Columbia University, New York, New York 10027.

On page 74, first column, line 39, correct the equation to read  $w = (10.68 - 0.74F + 0.020F^2 - 2.45 \times 10^{-4}F^3 + 1.16 \times 10^{-6}F^4)^{-1}$ .

**Angular Dependence of  $\beta$ -Carbon Atom Hyperfine Coupling Constants** [*J. Am. Chem. Soc.*, **96**, 583 (1974)]. By LEON M. STOCK\* and MICHAEL R. WASIELEWSKI, Department of Chemistry, University of Chicago, Chicago, Illinois 60637.

The value of  $\langle \cos^2 \theta \rangle$  for compound **3** in Figures 1 and 2 is given incorrectly. The correct value is 0.38.

**Synthesis and Luminescence of the Tris(2,2'-bipyridine)iridium(III) Ion** [*J. Am. Chem. Soc.*, **96**, 1959 (1974)]. By C. M. FLYNN, JR., and J. N. DEMAS,\* Department of Chemistry, University of Virginia, Charlottesville, Virginia 22901.

Figure 1: The chemical shift values should read successively  $-89.46$ ,  $-83.77$ ,  $-76.69$ ,  $-63.34$ , and  $-60.04$  ppm.

**A Simple Mechanical Model for Molecular Geometry Based on the Hellmann-Feynman Theorem. I. General Principles and Applications to  $AH_2$ ,  $AH_3$ ,  $AH_4$ ,  $AB_2$ ,  $HAB$ , and  $ABC$  Molecules** [*J. Am. Chem. Soc.*, **96**, 2030 (1974)]. By B. M. DEB, Department of Chemistry, Indian Institute of Technology, Bombay, India.

The summation sign in eq 1 should read

$$\sum_{q \neq p}$$

In Table III the point group of  $SF_4$  was inadvertently shown to be either  $T_d$  or  $D_{2d}$ . The actual symmetry is  $C_{2v}$ , with nonlinear  $SF_2$  fragments. This is also in accord with our predictions based on the transferability of shapes from smaller to higher molecule classes. Similar arguments show that in  $XeO_2F_2$  and  $IO_2F_2^-$  the  $AF_2$  fragment ( $A = Xe, I$ ) would be linear as this is a 22 valence electron  $AB_2$  molecule. The  $AO_2$  fragment, being a 20 valence electron  $AB_2$  molecule, would be bent.

**Neglect of Differential Overlap in Calculations of Barriers to Inversion and an Extension of INDO to Calculations Involving Second Row Atoms** [*J. Am. Chem. Soc.*, **96**, 3061 (1974)]. By PHILIP E. STEVENSON\* and DAVID L. BURKEY, Department of Chemistry, Worcester Polytechnic Institute, Worcester, Massachusetts 01609.

There are two computational errors in Table III of our recent publication: The  $F^2$  integral for Si, reported as 0.12046 should be 0.11464; and the  $G^1$  integral for S, reported as 0.27935 should be 0.26044. INDO barriers for  $SiH_3^-$  and  $SH_3^+$  are therefore revised to the values shown below:

	INDO-A		INDO-B	
	$\Delta E$ , kcal/mol	Angle, deg	$\Delta E$ , kcal/mol	Angle, deg
$SiH_3^-$	50.0	96.5	26.0	98.9
$SH_3^+$	25.2	97	6.0	105.6

The preferred geometry of  $N(SiH_3)_3$  is still planar by

both INDO-A and INDO-B. These corrections have no effect on any of the conclusions reported in the paper. Our thanks to Professor M. S. Gordon for drawing our attention to the errors.

**Biosynthesis of Camptothecin. I. Definition of the Overall Pathway Assisted by Carbon-13 Nuclear Magnetic Resonance Analysis.** [*J. Am. Chem. Soc.*, **96**, 5609 (1974)]. By C. R. HUTCHINSON,\* A. H. HECKENDORF, P. E. DADDONA, School of Pharmacy, University of Connecticut, Storrs, Connecticut 06268, E. HAGAMAN, and E. WENKERT, Department of Chemistry, Indiana University, Bloomington, Indiana, 47401.

On page 5611, column 2, lines 16 and 17 should be corrected to read "incorporation of ca. 0.7%, quite in line with the specific incorporation of 0.8–1.8% of radioactively labeled **5a** and 18,19-dihydro-**5a**."

**Calorimetric and Counterion Binding Studies of the Interaction between Micelles and Ions. The Observation of Lyotropic Series.** [*J. Am. Chem. Soc.*, **96**, 5774 (1974)]. By JOHN W. LARSEN\* and LINDA J. MAGID, Department of Chemistry, University of Tennessee, Knoxville, Tennessee 37916.

Column 3 in Table V, headed "Bound  $[OH^-]$ ,  $M$ ," should be deleted.

**A Revised Structure of Vermiculine. A Novel Macrolide Dilactone Antibiotic from *Penicillium vermiculatum*** [*J. Am. Chem. Soc.*, **96**, 5954 (1974)]. By ROBERT K. BOECKMAN, JR.,\* Department of Chemistry, Wayne State University, Detroit, Michigan 48202, JOSÉ FAYOS, and JON CLARDY,\* Ames Laboratory-USAEC and Department of Chemistry, Iowa State University, Ames, Iowa 50010.

The line drawing given for vermiculine (**5**) is incorrect. The bottom atom of the macrocyclic ring is an oxygen, not a carbon as shown. The molecule is a true dimer of the hydroxy acid (**6**) and is correctly depicted in Figure 1.

**A Dynamic Nuclear Magnetic Resonance Study of the Mercury Keto-Enol Tautomerization in Bis(1,1,1,2,2,3,3-heptafluoro-7,7-dimethyl-4,6-octanedion-5-yl)mercury** [*J. Am. Chem. Soc.*, **96**, 6664 (1974)]. By RICHARD H. FISH, Western Regional Research Laboratory, Agricultural Research Service, U.S. Department of Agriculture, Berkeley, California 94710.

Page 6665, first column, line 7 from bottom of page: the sentence should read: "The signal at 5.29 ppm has a  $J_{199Hg-H}$  coupling of 257 Hz at  $-75^\circ$  and can be readily assigned to tautomer **4**, while the signal at 5.54 ppm has a  $J_{199Hg-H}$  of 387 Hz and can be assigned to the methine proton of tautomer **5** (not tautomer **2**). This error also occurs in the next to last sentence of the second column and should read: "Thus the signal at 5.92 ppm was assigned to the enol proton of tautomer **5**" (not tautomer **2**).

Page 6668: structure **10** should be corrected as follows:

