

pH 6.5–7) and heated to 65° to increase the isotope exchange rate. Resonances observed at –72, –400, –772, and –906 ppm are tentatively assigned to the sixfold bridging oxygens (O_A), threefold bridging oxygens (O_B), doubly bridging oxygens (O_C, O_D, O_E), and terminal oxygens (O_F, O_G), respectively, using the labeling scheme shown in Figure 2 and assuming that the more metal atoms an oxo ligand bridges, the further upfield its resonance will lie. Other features in the ¹⁷O spectrum are observed which correspond to degraded species known to coexist with protonated V₁₀O₂₈⁶⁻ species in the pH range 6.5–7.² Future experiments will be carried out to determine the structure(s) of these species.

An important qualitative correlation has been demonstrated between oxygen environment and chemical shift; as further data are gathered more detailed interpretations should be possible.

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ya and F. N. Schoch for obtaining some of the NMR spectra.

References and Notes

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Additions and Corrections

Stereochemistry of Dioxovanadium(V) Complexes. II. The Crystal and Molecular Structures of Ammonium (Dihydrogen ethylenediaminetetraacetato)dioxovanadate(V) Trihydrate [*J. Am. Chem. Soc.*, **93**, 3873 (1971)]. By W. ROBERT SCHEIDT, D. M. COLLINS, and J. L. HOARD,* Department of Chemistry, Cornell University, Ithaca, New York 14850.

Professor E. C. Lingafelter has called our attention to some errors in Table I. The corrected values are given below.

Table I. Atomic Coordinates in Crystalline NH₄[VO₂AH₂]₃·3H₂O

Atom	10 ⁴ x	10 ⁴ y	10 ⁴ z
O ₇	2951 (3)	–267 (2)	344 (1)
O ₉	–4603 (3)	–1591 (2)	1528 (1)
C ₃	4142 (3)	–229 (2)	3120 (2)
C ₄	5169 (3)	–840 (2)	3752 (2)

Molecular Orbital Studies of Hydrogen Bonds. V. Analysis of the Hydrogen-Bond Energy between Lower Excited States of H₂CO and H₂O [*J. Am. Chem. Soc.*, **95**, 7563 (1973)]. By SUEHIRO IWATA and KEIJI MOROKUMA,* Department of Chemistry, University of Rochester, Rochester, New York 14627.

The first term in parentheses of eq 13 should be E₂ⁱ instead of E₁ⁱ. The first term of eq A-3 should have a factor ($\frac{1}{b}$). The denominator of eq A-4 should be (1 ± S_{αμ}²), not (1 + S_{αμ}²)^{1/2}. In the sixth line following eq A-4, √2 should not be there. The numerical factor of the second term of eq A-6 should be 4, not 2√2. All the calculations were done with correct formulas.

Stereochemistry of Low-Spin Cobalt Porphyrins. III. The Crystal Structure and Molecular Stereochemistry of Bis(piperidine)-α,β,γ,δ-tetraphenylporphyrinatocobalt(II) [*J. Am. Chem. Soc.*, **96**, 84 (1974)]. By W. ROBERT SCHEIDT, Department of Chemistry, University of Notre Dame, Notre Dame, Indiana 46556.

The value for the unit cell constant, α, is incorrectly reported in the abstract and the paper. The correct value is α = 104.99 (2)°.

Synthesis and Characterization of a 1,8-Naphthoquinodimethane [*J. Am. Chem. Soc.*, **96**, 2291 (1974)]. By RICHARD M. PAGNI* and CHARLES R. WATSON, JR., Department of Chemistry, University of Tennessee, Knoxville, Tennessee 37916.

In reference 9 of this paper the rate constant at 128.8° is reported as 1.88 × 10^{–5} sec^{–1}. The value should be 1.88 × 10^{–4} sec^{–1}.

A Deuterium Isotope Study of Electrogenative Hydrogenation. Mechanism of Hydrogenation of Ethylene at Positive Potentials [*J. Am. Chem. Soc.*, **93**, 1092 (1971)]. By STANLEY H. LANGER,* IRAJ FEIZ, and COLIN P. QUINN, Department of Chemical Engineering, University of Wisconsin, Madison, Wisconsin 53706.

Recently, it was brought to our attention that computational errors led to the reporting of incorrect predicted mass spectra of deuterated ethanes in this paper. Corrected spectra calculated on the basis of assumptions given in this report are now presented in Table I. Use of these spectra resulted in corrected labeled ethane distributions which are

Table I. Predicted Spectra of Deuterated Ethanes, Based on Ethane- d_0 ^a

<i>m/e</i>	<i>d</i> ₀	<i>d</i> ₁	<i>d</i> ₂	<i>d</i> ₃	<i>d</i> ₄	<i>d</i> ₅	<i>d</i> ₆
28	187.30	53.07	9.02	0	0	0	0
29	12.67	126.66	84.90	27.06	0	0	0
30	100	10.56	78.51	95.52	54.13	0	0
31	0	100	8.44	42.84	84.85	90.20	0
32	0	0	100	6.33	19.66	53.06	135.32
33	0	0	0	100	4.22	8.97	0
34	0	0	0	0	100	2.11	10.77
35	0	0	0	0	0	100	0
36	0	0	0	0	0	0	100

^a Ionization potential, 12 eV; gain, 10; pressure, 47 μ ; current, 35 μ A.

Table II. Corrected Ethane Product Distribution. Electrogenative Hydrogenation of Ethylene with Deuterium^a

Sample	0.514	A	B	C	D	E	F
<i>E</i> _{obsd} , V	Open	0.219	0.143	0.100	0.070	0.044	0.031
<i>I</i> , mA	circuit	5.3	46	118	180	265	330
% conversion	0	1.04	9.17	23.8	34.3	49.4	54.9
Ethanes							
<i>d</i> ₀	0	14.2	10.1	13.6	17.9	20.3	18.0
<i>d</i> ₁	0	18.9	30.9	29.3	29.4	30.1	30.4
<i>d</i> ₂	0	23.0	27.1	23.5	21.8	21.4	22.5
<i>d</i> ₃	0	17.2	9.4	11.8	11.5	12.5	12.4
<i>d</i> ₄	0	12.5	9.7	11.4	10.5	9.6	10.0
<i>d</i> ₅	0	9.4	9.6	7.9	6.9	4.9	5.2
<i>d</i> ₆	0	4.7	3.3	2.5	2.2	1.3	1.5

^a Run D54, temp 24°, pressure 746 mm, *R*_{int} = 0.25 ohm, gas flow = 4.5 ml/min.

Table IV. Comparison of Observed and Calculated Distribution of Deuterated Products from Ethylene and Deuterium in Electrogenative Reaction with D₂O–2*N* Perchloric Acid-*d*₁ Electrolyte Recalculated

	A		B		C		D		E		F	
	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd
Ethylenes												
<i>d</i> ₁	33.5	34.4	21.4	21.2	12.8	12.4	10.5	9.1	8.2	6.6	4.5	2.6
<i>d</i> ₂	19.1	11.8	12.4	8.5	8.5	5.3	6.5	3.8	4.9	3.0	2.8	1.5
<i>d</i> ₃	8.1	8.7	5.2	5.4	3.9	3.3	2.5	2.2	1.8	1.6	1.7	0.9
<i>d</i> ₄	1.9	6.0	1.2	3.4	0.8	1.7	0.4	1.1	0.3	0.6	0.2	0.4
Ethanes												
<i>d</i> ₀	2.1	5.6	5.9	6.2	9.2	10.5	13.3	15.0	15.9	17.9	15.4	17.1
<i>d</i> ₁	10.0	7.4	20.2	19.0	23.9	22.6	26.9	24.6	29.2	26.5	30.8	28.7
<i>d</i> ₂	12.5	9.0	17.5	16.6	20.6	18.2	21.9	18.3	22.8	18.8	25.0	21.3
<i>d</i> ₃	7.6	6.8	10.2	5.8	13.0	9.1	12.4	9.6	12.1	11.0	14.1	11.8
<i>d</i> ₄	3.7	4.9	4.6	6.0	5.8	8.8	4.6	8.8	4.0	8.4	5.1	9.5
<i>d</i> ₅	1.3	3.7	1.3	5.9	1.5	6.1	0.9	5.8	0.7	4.3	1.0	4.9
<i>d</i> ₆	0.2	1.8	0.2	2.0	0.13	2.0	0.06	1.8	0.04	1.1	0.06	1.4

given in Table II. With the new ethane distributions, we have recalculated statistical parameters for the addition of hydrogen or deuterium to ethylene as shown in Table III. Because of the qualitative nature of our earlier discussion, the new statistical parameters are consistent with the argument there. The only significant change is in the value of *q* which is indicative of a high probability of addition of deuterium from the electrolyte in the initiating step of hydrogenation (see eq 12).

A corrected comparison of observed and calculated values of labeled ethylenes and ethanes is given in Table IV. Agreement between observed and calculated values is improved.

Ground States of Molecules. XXV. MINDO/3. An Improved Version of the MINDO Semiempirical SCF-MO Method [*J. Am. Chem. Soc.*, **97**, 1285 (1975)]. By RICHARD C. BINGHAM, MICHAEL J. S. DEWAR,* and DONALD H. LO, Department of Chemistry, The University of Texas at Austin, Austin, Texas 78812.

Table III. Recalculated Statistical Parameters

Current output (mA)	<i>p</i>	<i>q</i>	<i>r</i>	<i>s</i>
5.3	3.8	3.15	10.4	0.90
46	6.2	2.48	6.40	0.28
118	14.5	1.63	7.16	0.16
180	22.8	1.05	8.21	0.12
265	31.9	0.90	8.40	0.10
330	51.8	1.04	6.89	0.11

The first summation in eq 2 should be:

$$\sum_{k \neq i}^{(m)} q_k (g_{ik} - 0.5h_{ik})$$

Equation 3 should be:

$$F_{ik}(mm) = 0.5p_{ik}(3h_{ik} - g_{ik})$$

These errors were due to an uncorrected page from an earlier draft being accidentally included in the final manuscript. The correct version was given in the original MINDO paper (N. C. Baird and M. J. S. Dewar, *J. Chem. Phys.*, **50**, 1262 (1969)) and has been used in all our calculations.

Radical Production from the Interaction of Closed Shell Molecules. II. The Reaction of Organic Sulfides with *tert*-Butyl Peroxybenzoates [*J. Am. Chem. Soc.*, **97**, 1580 (1975)]. By WILLIAM A. PRYOR* and WILLIAM H.

HENDRICKSON, JR., Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana 70803.

In line 2 on page 1581 the words "Equation 2a" should have been followed by a colon, *not* placed in parentheses. The same is true of "Equation 2b" which occurs five lines below eq 3 and "Equation 3" which occurs two lines below that. The point is that the sentences following these words discuss each of the equations referred to, not the sentences which precede them.

Additions to Bicyclic Olefins. VIII. Electrophilic Addition of Trifluoroacetic Acid and Deuteriotrifluoroacetic Acid to Norbornene and Related Bicyclic Olefins. Evidence for the Capture of the Unsymmetrical (Classical) 2-Norbornyl Cation [*J. Am. Chem. Soc.*, **97**, 2469 (1975)]. By HERBERT C. BROWN* and KWANG-TING LIU, Richard B. Wetherill Laboratory, Purdue University, West Lafayette, Indiana 47907

On page 2474, first column, 14 lines down, the sentence, "The 2-norbornyl cation has not been captured in unsymmetrical form in some 11 different reactions," should read: "The 2-norbornyl cation has now been captured in unsymmetrical form in some 11 different reactions."

Study of Olefin Proportions from E2 Reactions of Secondary Alkyl Bromides. Mechanistic Implications [*J. Am. Chem. Soc.*, **97**, 2477 (1975)]. By IRVING N. FEIT,* ILENE KAIN BREGER, ANTONIA M. CAPOBIANCO, THOMAS W. COOKE, and LARRY F. GITLIN, Department of Chemistry, C. W. Post College of Long Island University, Greenvale, New York 11548.

On page 2479, one sentence is repeated and another left out. Lines 14-11 from the bottom of the right-hand column should read:

"... weak base. Ring strain is advanced as the explanation for the unexpectedly slow reactions of the alicyclic tosylates. Rather than invoke . . ."

A Fluxional, Catalytically Active Metal Cluster, Ni₄[CNC(CH₃)₃]₇ [*J. Am. Chem. Soc.*, **97**, 2571 (1975)].

By V. W. DAY* and R. O. DAY, Department of Chemistry, University of Nebraska, Lincoln, Nebraska 68508, and J. S. KRISTOFF, F. J. HIRSEKORN, and E. L. MUETTERTIES,* Cornell Material Science Center and Spencer T. Olin Chemistry Laboratories, Cornell University, Ithaca, New York 14853.

Line 14, left column of page 2572 should read, "... and shorter than the 2.508 Å value . . ."

The Structure of Heptakis(*tert*-butyl isocyanide)molybdenum(II) Hexafluorophosphate, a Seven-Coordinate Complex with C_{2v} Monocapped Trigonal Prismatic Geometry [*J. Am. Chem. Soc.*, **97**, 2697 (1975)]. By DAVID L. LEWIS and STEPHEN J. LIPPARD,* Department of Chemistry, Columbia University, New York, New York 10027.

In the Abstract, change $Z = 4$ to $Z = 8$.

On page 2698, left column, line 27 should read: (00 $\bar{1}$), (110), ($\bar{1}\bar{1}0$), ($\bar{1}10$), and (1 $\bar{1}0$); etc.

Carboxyl-Assisted Hydrolyses. Synthesis and Hydrolysis of Diphenyl *cis*-2-(3-Carboxy)norbornyl Phosphates [*J. Am. Chem. Soc.*, **96**, 6492 (1974)]. By S. STONEY SIMONS, JR.,* James Bryant Conant Laboratories, Harvard University, Cambridge, Massachusetts 02138.

A hydroxyl, not a carbamyl, group was found to induce a lithium aluminum hydride reduction from the more hindered side of a molecule.²⁰ This correction can only strengthen the structural assignment of **10**, though since now no example is known of an amide group altering the predicted stereochemistry of a metal hydride reduction.

Direct Synthesis of Fluorocarbon Peroxides. III. The Addition of Chloroperoxytrifluoromethane to Olefins [*J. Am. Chem. Soc.*, **97**, 13 (1975)]. By NYAL WALKER and DARRYL D. DESMARTEAU,* Department of Chemistry, Kansas State University, Manhattan, Kansas 66506.

On page 15, first column, under *erythro*-CF₃OOCFHCFHCl, $J_{BD} = 13.3$, $J_{BE} = 3.9$, and $J_{CD} = 4.1$ Hz.

Book Reviews

MTP International Review of Science. Series One on Physical Chemistry. Volumes 1-4, 6, 7, 10-13. Consultant Editor: A. D. BUCKINGHAM (University of Cambridge). Butterworth and Co., London, and University Park Press, Baltimore, Md. 1972. 3357 pp. \$24.50 per volume.

The publisher of this encyclopedic compendium of reviews has set out to provide regular, authoritative appraisals of the recent advances achieved in entire fields of physical chemistry. This first 13-volume series deals principally with the period 1967-1971, and further series are scheduled to be issued every two years. Three of the volumes (5, 8, and 9) have been reviewed elsewhere in this Journal.

The authorship is international and distinguished. The discipline of physical chemistry has been carefully subdivided by consultant editor A. D. Buckingham into structural units. Separate volumes, in the charge of subeditors, have been devoted to each unit. Each subeditor has in turn organized a group of some six to ten authors who have contributed reviews.

From a purely organizational point of view the coordination of this large group of authors and editors has been accomplished successfully. In the series as a whole, there is an appropriate choice of material, authorship, and balance between the description of technical details and theory. This balance is satisfactory both for the general professional reader and the expert. Thus the publishers' stated formal aims seem to this reviewer to have been successfully carried out.

However, one might have hoped for more than an array of independent reviews. After all, the publisher has created something of a new medium for the presentation of modern scientific ideas, by commissioning reviews of such wide coverage at one time. It seems a pity therefore that no noticeable effort was made to exploit the potentially unique possibilities of the medium. The work fails to provide the reader with an overview of physical chemistry as a whole today. There is almost no general, historical, or philosophical perspective to the work. Physical chemistry is presented as an array of separate areas rather than as an integrated, living branch