

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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References and Notes

- (1) H. T. Evans, Jr., *Perspect. Struct. Chem.*, **4**, 1–59 (1971).
- (2) D. L. Kepert, "Comprehensive Inorganic Chemistry", Vol. 4, J. C. Bailar, H. J. Emeléus, R. Nyholm, and A. F. Trotman-Dickinson, Ed., Pergamon Press, Oxford, 1973, pp 607–672.
- (3) (a) J. A. Jackson and H. Taube, *J. Phys. Chem.*, **69**, 1844 (1965); (b) B. N. Figgis, R. G. Kidd, and R. S. Nyholm, *Can. J. Chem.*, **43**, 145 (1965); (c) R. G. Kidd, *Can. J. Chem.*, **45**, 605 (1967).
- (4) G. A. Tsigdinos and C. J. Hallada, *Inorg. Chem.*, **9**, 2488 (1970).

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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