

Additions and Corrections

Longithorone A: Unprecedented Dimeric Prenylated Quinone from the Tunicate *Aplidium longithorax* [*J. Am. Chem. Soc.* **1994**, *11*, 12125–12126]. XIONG FU, M. BILAYET HOSSAIN, DICK VAN DER HELM,* AND FRANCIS J. SCHMITZ*

The spelling of the genus name in the title and text should be *Aplidium*, not *Aplyidium*.

JA9550236

Energy Transfer in Rigidly-Linked Heterodinuclear Ru(II)/Fe(II) Polypyridyl Complexes: Distance and Linkage Dependence [*J. Am. Chem. Soc.* **1995**, *117*, 5881–5882]. S. L. LARSON, S. M. HENDRICKSON, S. FERRERE, D. L. DERR, AND C. MICHAEL ELLIOTT*

Page 5881, the first sentence of the third paragraph should read as follows: Molecular mechanics calculations were conducted employing Biograf³ software on all of the dinuclear Fe–Fe and Ru–Fe complexes.

Page 5881, footnote 3 should read as follows: The Dreiding force field was employed (Mayo, S. L.; Olafson, B. D.; Goddard, W. A. *J. Phys. Chem.* **1990**, *94*, 8897). Partial charges were obtained using QEq (Rappé, A. K.; Goddard, W. A. *J. Phys. Chem.* **1991**, *95*, 3358). Annealed dynamics was used as the conformational searching procedure (Castonguay, L. A.; Rappé, A. K. *J. Am. Chem. Soc.* **1992**, *114*, 5832).

JA955024Y

Analysis of the Jahn–Teller Effect in Matrix Isolated Cyclooctatetraene Mononegative Ion Using Magnetic Circular Dichroism Spectroscopy [*J. Am. Chem. Soc.* **1994**, *116*, 11109–11119]. CINDY SAMET,* JANNA L. ROSE, SUSAN B. PIEPHO,* JOSEPH LAURITO, LESTER ANDREWS, AND PAUL N. SCHATZ*

Professor David F. Bocian has pointed out to us that the spin–orbit coupling constant we used ($\zeta_{2p_C} = 32 \text{ cm}^{-1}$) is inappropriate for a planar π -electron system because, as first shown by

McClure,¹ both one- and two-center spin–orbit terms are zero in that case. Thus a much smaller value of ζ_{2p_C} is appropriate. We have therefore refit our moment data allowing ζ_{2p_C} to vary. Approximately equally good best fits were obtained for a ζ_{2p_C} value anywhere in the range 0–0.2 cm^{-1} . The fit for $\zeta_{2p_C} = 0.1 \text{ cm}^{-1}$ is shown by the solid line in our new Figure 5. This fit is seen to be distinctly better than our previous fit using $\zeta_{2p_C} = 32 \text{ cm}^{-1}$ (dashed line). The resulting changes in ground state parameters are as follows: $\lambda_{JT}(\text{new}) = 1.30$ vs $\lambda_{JT}(\text{old}) = 1.59$; $\Delta(\text{new}) = 4.4 \text{ cm}^{-1}$ vs $\Delta(\text{old}) = 13.5 \text{ cm}^{-1}$; $E_{JT}(\text{new}) = 964 \text{ cm}^{-1}$ vs $E_{JT}(\text{old}) = 1442 \text{ cm}^{-1}$. Thus the crystal field splitting (Δ) is significantly smaller and the Jahn–Teller splitting is about 1.7 rather than 2.5 times the zero-point energy so that each COT^- is less strongly trapped in one of the two Kekule-like structures than previously calculated. These changes have no effect on our calculation of excited state properties.

We thank Professor Bocian for pointing out this error and acknowledge helpful correspondence with Professor D. S. McClure.

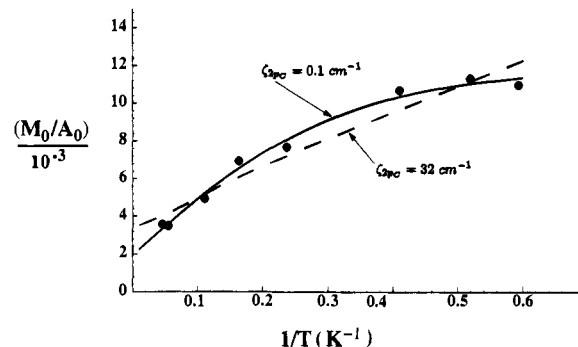


Figure 5. Ratio of zeroth MCD and absorption moments vs $1/T$. The filled circles are the experimental points, and the solid and dashed curves are respective best fits using $\zeta_{2p_C} = 0.1$ and 32 cm^{-1} , respectively.

(1) McClure, D. S. *J. Chem. Phys.* **1952**, *20*, 682–686.

JA955022D

Book Reviews *

Taxane Anticancer Agents: Basic Science and Current Status. Edited by Gunda I. Georg (University of Kansas), Thomas T. Chen (University of Tennessee), Iwao Ojima (State University of New York at Stony Brook), and Dolatra M. Vyas (Bristol-Myers Squibb PRI). American Chemical Society: Washington, DC, 1994. xiii + 353 pp. \$99.95. ISBN 0-8412-3073-0.

ACS Symposium Series No. 583. Developed from a symposium sponsored by the Division of Chemical Health and Safety, Medicinal Chemistry, and Organic Chemistry at the 207th National Meeting of the American Chemical Society, San Diego, CA, March 13–17, 1994.

JA955276Z

Allelopathy: Organisms, Processes, and Applications. Edited by Inderjit (University of Delhi), K. M. M. Dakshini (University of Delhi), and Frank A. Einhellig (Southwest Missouri State University). American Chemical Society: Washington, DC, 1994. x + 381 pp. \$99.95. ISBN 0-8412-3061-7.

ACS Symposium Series No. 582. Developed from a symposium sponsored by the Botanical Society of America Section of the American Institute of Biological Sciences, Ames, IA, August 1–5, 1993.

JA955270+

*Unsigned book reviews are by the Book Review Editor.

Modeling the Hydrogen Bond. Edited by Douglas A. Smith (University of Toledo). American Chemical Society: Washington, DC, 1994. x + 300 pp. \$74.95. ISBN 0-8412-2961-3.

ACS Symposium Series No. 569. Developed from a symposium sponsored by the Division of Computers in Chemistry at the 206th National Meeting of the American Chemical Society, Chicago, IL, August 22–27, 1993.

JA955279B

Structure and Reactivity in Aqueous Solution: Characterization of Chemical and Biological Systems. Edited by Christopher J. Cramer and Donald G. Truhlar (University of Minnesota). American Chemical Society: Washington, DC, 1994. ix + 438 pp. \$99.95. ISBN 0-8412-2980-5.

ACS Symposium Series No. 568. Developed from a symposium sponsored by the Division of Physical Chemistry at the 207th National Meeting of the American Chemical Society, San Diego, CA, March 13–18, 1994.

JA955272U