

$d_{z^2}$  by the low symmetry of the ligand field,<sup>19</sup> so that the 4s participation actually occurs via the  $d_{z^2}$  component of the groundstate. The metal hyperfine parameters of the tetragonally compressed  $\text{CuF}_6^{4-}$  ion are of interest in this context, as here the unpaired electron is located predominantly in  $d_{z^2}$ .<sup>20</sup> In this case the hyperfine parameters calculated by using eq 1c,d and the conventional  $g$  shift expressions (4c,d) are very similar, as is expected for a complex of a ligand of this kind, but both are in poor agreement with experiment (Table I). Satisfactory agreement may be obtained by using a value of  $K = 0.20$  ( $A_z = 85 \times 10^{-4}$ ,  $A_{xy} = 23 \times 10^{-4} \text{ cm}^{-1}$  via eq 1c,d) corresponding to a fractional unpaired spin density of  $\sim 0.032$  in the copper 4s orbital. The

(19) Smith, D. W. *Inorg. Chim. Acta* **1977**, *22*, 107.

(20) Hitchman, M. A.; McDonald, R. D.; Reinen, D. *Inorg. Chem.*, in press.

mixing coefficient of  $d_{z^2}$  in the ground state of  $(\text{enH}_2\text{Cl})_2\text{Zn}[\text{Cu}]\text{Cl}_4$  is  $b \approx 0.27$ .<sup>6</sup> However, it should be noted that a coefficient of  $b = 0.5$  corresponds to an orbital of the form  $d_{2x^2-z^2-y^2}$ , which is equivalent to  $d_{z^2}$ , with  $x$  defined as the symmetry axis.<sup>21</sup> The value of  $\sim 0.011$  estimated for the 4s orbital coefficient in the ground state of  $(\text{enH}_2\text{Cl})_2\text{Zn}[\text{Cu}]\text{Cl}_4$  thus implies a value of  $\sim (0.5^2/0.27^2) \times 0.014 = \sim 0.038$  for the mixing coefficient in the above unconventional  $d_{z^2}$  orbital, which is similar to that deduced for the axially symmetric  $\text{CuF}_6^{4-}$  complex.

**Acknowledgment.** The receipt of a Humboldt Research Fellowship and the help and hospitality of Professor D. Reinen, Fachbereich Chemie, University of Marburg, are gratefully acknowledged.

(21) Hitchman, M. A. *J. Chem. Soc. A* **1979**, 4.

## Additions and Corrections

1984, Volume 23

**E. I. Onstott,\* Laura B. Brown, and E. J. Peterson\*:** Desolvation Method for Assessment of Crystallization Energies and Ion Crowding in Rare-Earth Perchlorates, Chlorides and Nitrates.

Page 2432. In Table I the second entry in the last column should read -1391. In Table III the saturated molality datum for dysprosium nitrate is in error; it should read 4.738 in column 2, according to a recent correction in the literature. (Spedding, F. H.; Derer, J. L.; Mohs, M. A.; Rard, J. A. *J. Chem. Eng. Data* **1985**, *30*, 242). We have recalculated data for dysprosium nitrate that should read as follows: column 3, 11.715; column 5, 0.5235; column 6, 0.175; column 7, 383; column 8, 2189. The last datum reveals that the work of crystallization in the nitrate series is a maximum for gadolinium nitrate rather than for dysprosium nitrate.—E. I. Onstott

**Joshua Telser and Russell S. Drago\*:** Reinvestigation of the Electronic and Magnetic Properties of Ruthenium Butyrate Chloride.

Page 3115. An error was discovered in the equation for the exponential form of the zero-field susceptibility for an  $O_h$ ,  $S = 3/2$  complex with axial zero-field splitting.<sup>1</sup> The correct equation for  $\chi_{\perp}$  ( $\chi_{\parallel}$  is correct as written) is as follows:

$$\chi_{\perp} = \frac{Ng_{\perp}^2\beta^2}{kT} \frac{4 + (3kT/D)(1 - \exp(-2D/kT))}{4(1 + \exp(-2D/kT))}$$

The magnetic susceptibility data were fitted by using this correct equation. This gave values of  $D = 70.6 \text{ cm}^{-1}$ ,  $g = 2.09$ , and  $g_{\perp} = 2.11$ . These are in much better agreement with values obtained previously by using the full spin Hamiltonian for an  $O_h$ ,  $S = 3/2$  system with axial zero-field splitting. In addition, the susceptibility data were fitted here by using the spin Hamiltonian, but allowing rhombic distortion. This gave  $D = 76.8 \text{ cm}^{-1}$ ,  $E = -0.007 \text{ cm}^{-1}$ ,  $g_z = 2.022$ ,  $g_x = 2.134$ , and  $g_y = 2.137$ . Within experimental error, these values are identical with those obtained with only axial distortion. A true axial system is also suggested by the crystallographic and EPR data.

Additional errors in the literature<sup>1</sup> equations for susceptibilities were discovered and the correct versions are given below:

for  $S = 1$

$$\chi_{\perp} = (Ng_{\perp}^2\beta^2/kT)\{(2kT/D) \times (1 - \exp(-kT/D))/[1 + 2 \exp(-kT/D)]\}$$

for  $S = 5/2$

$$\chi_{\perp} = (Ng_{\perp}^2\beta^2/kT)\{[9 + (4kT/D) \times (1 - \exp(-2D/kT)) + (9kT/2D)(\exp(-2kT/D) - \exp(-6kT/D))]/4(1 + \exp(-2kT/D) + \exp(-6kT/D))\}$$

Page 3118. By use of an EPR simulation program for  $S = 1/2$  systems, a value for  $A_{\perp}$  of  $26.7 \times 10^{-4} \text{ cm}^{-1}$  was obtained. However, this

is an effective  $A$  value,  $A^e$ , and must be converted to  $A_{\perp}$  for an  $S = 3/2$  system.<sup>2</sup> In this case,  $A^e_{\perp} = 2A_{\perp}$ , giving  $13.35 \times 10^{-4} \text{ cm}^{-1}$  as the correct value for  $A_{\perp}$ . This leads to  $A_{\text{iso}} = 16.13 \times 10^{-4} \text{ cm}^{-1}$  and  $A_{\text{dip}} = 2.78 \times 10^{-4} \text{ cm}^{-1}$ .

(1) O'Connor, C. J. *Prog. Inorg. Chem.* **1982**, *29*, 203.

(2) Kasai, P. H. *J. Chem. Phys.* **1968**, *49*, 4979.

—Joshua Telser, Vincent M. Miskowski, Russell S. Drago, and Ngai M. Wong

1985, Volume 24

**Leigh C. Porter and Robert J. Doedens\*:** Preparation and Crystal Structure of a Diamagnetic Copper(II) Trichloroacetate Complex Containing a Nitroxyl Radical Ligand.

Pages 1006, 1008. The nitroxyl ligand was named incorrectly. The correct name is 2,2,5,5-tetramethylpyrrolinyl-1-oxy.—Robert J. Doedens

**Wilmont F. Howard, Jr., Roger W. Crecey, and Wilfred H. Nelson\*:** Octahedral Dialkyltin Complexes: A Multinuclear NMR Spectral Solution Structural Study.

Page 2206. In Table IV, the last three columns were incorrectly printed because of a computer system error that occurred after the author had returned galley proof. The correct version of columns 4–6 is as follows:

<sup>1</sup> J( <sup>119</sup> Sn- <sup>13</sup> C), Hz	<sup>2</sup> J( <sup>119</sup> Sn-C- <sup>1</sup> H), Hz	ref <sup>a</sup>
977	99.3	10, 2
630	68.7	42, b
664	84.0	42, 23
664	84.0	43, 23
	81.6	28, 28
	81.5	29, 29
880	98.1	32, b

<sup>a</sup> First reference for X-ray data, second for NMR values. <sup>b</sup> This work.

—Wilmont F. Howard, Jr.

**F. Wudl,\* E. T. Zellers, and S. D. Cox:** Simplified Procedure for the Preparation of Metal Diselenolenes.

Page 2865: Reference 4 should read: Wudl, F.; Nalewajek, D. J. *Chem. Soc., Chem. Commun.* **1980**, 866 and references therein. Chiang, L.; Pochler, T. O.; Bloch, A. N.; Cowan, D. O. *Ibid.* **1980**, 866. Bolinger, C. M.; Rauchfuss, T. B. *Inorg. Chem.* **1982**, *21*, 3947. The latter describes the use of  $\text{Cp}_2\text{Ti}(\text{Se}_2\text{C}_2\text{R}_2)$  in the preparation of complexed ( $\text{L} = \text{Ph}_3\text{P}$ ,  $\text{Ph}_2\text{PC}\equiv\text{CPPH}_2$ ,  $\text{dppp}$ ,  $\text{CO}$ ) metal monodiselenolenes  $\text{L}_m\text{MSe}_2\text{C}_2\text{R}_2$  and potential preparation of  $\text{M}(\text{Se}_2\text{C}_2\text{R}_2)_2$ .—F. Wudl