d_{z^2} by the low symmetry of the ligand field,[19] so that the 4s participation actually occurs via the d_{z^2} component of the groundstate. The metal hyperfine parameters of the tetragonally compressed CuF_6^{4-} ion are of interest in this context, as here the unpaired electron is located predominantly in d_{z^2}.[20] 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 $K = 0.20$ ($A_z = 85 \times 10^{-4}$, $A_{xy} = 23 \times 10^{-4}$ cm^{-1} via eq 1c,d) corresponding to a fractional unpaired spin density of ~0.032 in the copper 4s orbital. The mixing coefficient of d_{z^2} in the ground state of $(enH_2Cl)_2Zn[Cu]Cl_4$ is $b \approx 0.27$.[6] 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.[21] The value of ~0.011 estimated for the 4s orbital coefficient in the ground state of $(enH_2Cl)_2Zn[Cu]Cl_4$ 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_{x^2} orbital, which is similar to that deduced for the axially symmetric 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.

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

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

(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.[1] 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 $D = 70.6$ 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 $D = 76.8$ cm^{-1}, $E = -0.007$ 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[1] 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 26.7×10^{-4} 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.[2] In this case, $A^e{}_\perp = 2A_\perp$, giving 13.35×10^{-4} cm^{-1} as the correct value for $A_\perp$. This leads to $A_{iso} = 16.13 \times 10^{-4}$ cm^{-1} and $A_{dip} = 2.78 \times 10^{-4}$ cm^{-1}.

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(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. Crecely, 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:

$^1J(^{119}Sn-^{13}C)$, Hz	$^2J(^{119}Sn-C-^1H)$, Hz	ref[a]
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*

[a] First reference for X-ray data, second for NMR values. [b] 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.; Poehler, 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 $Cp_2Ti(Se_2C_2R_2)$ in the preparation of *complexed* (L = Ph_3P, $Ph_2PC{\equiv}CPPh_2$, dppp, CO) metal monodiselenolenes $L_mMSe_2C_2R_2$ and potential preparation of $M(Se_2C_2R_2)_2$.—F. Wudl