$$\sum_T \frac{[\chi'_{\mathrm{mol,exp}}(T) - \chi'_{\mathrm{mol,calc}}(T)]^2}{\sigma^2(\chi') + \left(\frac{\partial\chi}{\partial T}\right)^2 \sigma^2(T)}$$

within the framework of regression analysis. The term C/T accounts for the presence of small quantities of (presumably monomeric) paramagnetic impurities, while K accounts for temperature-independent paramagnetism (TIP) and for any minor deviations in the corrections for the diamagnetism of the atoms. The energies E_i of the various components of the ground-state manifold were obtained using the Hamiltonian operator

$$H = -2J(\hat{S}_1 \cdot \hat{S}_2) + g_1\beta\hat{S}_1 \cdot \hat{H} + g_2\beta\hat{S}_2 \cdot \hat{H}$$

where we have assumed that the g values for the two copper atoms are identical; *i.e.*, we have set $g_1 = g_2$. Since we have two $S = {}^1/_2$ centers in the complexes, the Heisenberg term $-2J(\hat{S}_1 \cdot \hat{S}_2)$ in the Hamiltonian gives rise to states with $S = 0$ (singlet) and 1 (triplet) with energies of 0 and $-2J$, respectively. For the hydrogen-bonded complex **1**, the fitting leads to a value of $2J = -4.09$ cm^{-1} with $g = 2.107$, and a value for C equivalent to the presence of 0.8% monomeric Cu(II) impurity. This observed $2J$ value of approximately -4 cm^{-1} for **1** is very much smaller (in magnitude) than those of -56 to -94 cm^{-1} reported for apparently analogous binuclear hydrogen-bonded copper(II) complexes.[13]

As was noted above, the principal difference between the structure of **1** and those of the earlier complexes is the distortion from planarity at the copper centers. Sinn and co-workers[21] have noted that such distortions, defined in the present complex by the dihedral angle τ between the CuO_2 and the CuN_2 planes, can lead to a significant diminution in the magnitude of the value of the triplet energy in copper(II) dimers, and we have rationalized this effect elsewhere.[22] The present result, therefore, demonstrates that these concepts, originally postulated for tightly bound dimeric systems, are equally applicable to the more weakly bound hydrogen-bonded binuclear complexes. If other distorted systems become available, we shall be able to investigate the possible existence of a quantitative correlation between τ and J.

Acknowledgment. This work was supported by the National Science Foundation through Grant No. CHE-9007607 (to D.J.H.) and by the Scientific Affairs Division, North Atlantic Treaty Organization (NATO), through Grant No. CRG 910277 (to D.J.H. and J.G.).

Supplementary Material Available: Hydrogen atom parameters (Table S1), anisotropic thermal parameters (Table S2), and complete bond distances and angles (Tables S3 and S4) (4 pages). Ordering information is given on any current masthead page. Listings of observed and calculated structure amplitudes are available from D.J.H. on request.

---

(17) Countryman, R. M.; Robinson, W. T.; Sinn, E. *Inorg. Chem.* **1974**, *13*, 247.

(18) Hodgson, D. J. *Inorg. Chem.* **1976**, *15*, 3174.

Additions and Corrections

1993, Volume 32

Pierre Braunstein,* Daniele Cauzzi, David Kelly, Maurizio Lanfranchi, and Antonio Tiripicchio: Reactivity of the Cyanometalate $Na[Cp'Mn(CO)_2CN]$ with Titanium, Zirconium, and Hafnium Halides. Crystal and Molecular Structure of the μ-Cyano μ-Oxo Tetranuclear Complex $[Cp_2Zr\{(\mu\text{-}NC)MnCp'(CO)_2\}]_2(\mu\text{-}O)$ ($Cp = \eta\text{-}C_5H_5$; $Cp' = \eta\text{-}MeC_5H_4$).

Page 3375. For $Cp_2Ti[(\mu\text{-}NC)MnCp'(CO)_2]_2$ (**1**), the second ^1H NMR (C_7D_8) assignment should read δ 4.34 (m, 8 H, $2C_5H_4CH_3$). For $Cp_2Hf[(\mu\text{-}NC)MnCp'(CO)_2]_2$ (**3**), the intensities of the IR absorptions should read as follows: IR (C_7H_8) ν(CN) 2020 s, 1995 m cm^{-1}; IR (Nujol) ν(CN) 2037 m, 2019 m, 2008 m, 1991 s cm^{-1}.

Page 3376. For $Cp_2Ti[(\mu\text{-}NC)MnCp'(CO)_2]Cl$ (**8**), the IR (Nujol) values should read as follows: ν(CN) 1995 s cm^{-1}; ν(CO) 1910 m, 1860 s cm^{-1}.