

tion.²⁰ Taken together, these spectroscopic data verify that the structure of [Cu(II)-PMB]⁺, as shown in Figure 1, remains intact in solution.

The X-band EPR spectrum of **4** has been run in glycerol/water glass (3:7)¹⁹ at 100 K. The spectrum, shown in Figure 2, is distinctly different from that of Cu(II)-BLM. Noteworthy are the feature around the $g = 2$ region and the A value (190 G vs 183 G for Cu(II)-BLM²). It is clear from Figure 2 that the coordination structure of copper in Cu(II)-BLM is better represented by [Cu(II)-PMA]⁺ (square-pyramidal N₅ chromophore), and this in turn indicates that the amide function of the β -aminoalaninamide moiety of BLM is not bonded to copper through the oxygen atom in Cu(II)-BLM. Since coordination of the deprotonated primary amido nitrogen of β -aminoalaninamide to copper(II) is only reported at pH 9 or above,^{14,21-23} the present

work suggests that the amide group of the β -aminoalaninamide moiety of BLM does not at all participate in coordination to copper in Cu(II)-BLM at physiological pH.

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Supplementary Material Available: Tables of selected bond distances and bond angles, anisotropic displacement coefficients, and H atom coordinates for **4** (2 pages); a table of observed and calculated structure factors (16 pages). Ordering information is given on any current masthead page.

(20) Belford, R. L.; Calvin, M.; Belford, G. *J. Chem. Phys.* **1957**, *26*, 1165.

(21) (a) Sigel, H.; Prijs, B.; Martin, R. B. *Inorg. Chim. Acta* **1981**, *56*, 45.

(b) Kroneck, P. M. H.; Vortisch, V.; Hemmerich, P. *Eur. J. Biochem.* **1980**, *109*, 603.

(22) Spectral parameters of **4** in aqueous phosphate buffer do not change in the pH range 7-9.

(23) One of the reviewers has suggested a reason for deprotonation of only one amide group of PMBH. The deprotonation is driven by the increase in CFSE that occurs when the Cu atom is coordinated by N instead of O in the basal (xy) plane. Since the CFSE effect of the more distant donor in the axial z direction is much smaller, the N-H bond presumably remains intact.

Additions and Corrections

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Linqing Ma, Scott R. Wilson, and John R. Shapley*: Synthesis and Characterization of Heptarhenium Carbido Clusters with (η^2 -Olefin)iridium Capping Moieties.

Page 5134. In Table I, the chemical formula is missing Ir. Also in Table I, footnote *a*, the expression for w contains an R instead of an F . In the first paragraph following the heading Crystallographic Study, the end of the 10th line should read as follows: ...were collected by scanning $\pm h, \pm k, +l...$. In footnote 13, the asterisks should be deleted from the cell parameters, since they are expressed in real space.

Pages 5135-5136. In the section following the heading Solid-State Structure of [PPN]₂[Re₇C(CO)₂₁Ir(C₂H₄)(CO)], replace sentences 3 and 4 with the following sentences: Since the 1,4-bicapped octahedral anion (vide infra) is not centrosymmetric, an inversion disorder problem was encountered in the structural determination, which caused the apparent superposition of the Re(CO)₃ and Ir(C₂H₄)(CO) capping moieties. The positions of rhenium and iridium capping moieties were successfully separated and refined; however, only three octahedron skeletal rhenium atom positions were resolved, since positions of their center of symmetry disordered counterparts (Re2', Re3', Re4') were crystallographically indistinguishable.

This revision removes the previous use of the term "2-fold" disorder and replaces it with the more accurate term "inversion" disorder. We thank Professor Richard E. Marsh for discussions that indicated the need for clarifying this point.—Scott R. Wilson and John R. Shapley