Synthesis, Crystal Structure and Magnetic Properties of a 
(μ-Hydroxo)(μ-Pyrazolato) Dicopper(II) Complex

H. Kara\(^a\), Y. Elerman\(^a\), and K. Prout\(^b\)

\(^a\) Department of Engineering Physics, Faculty of Sciences, University of Ankara,
06100 Besevler-Ankara, Turkey
\(^b\) Chemical Crystallography Laboratory, University of Oxford,
9 Parks Road, OXFORD OX1 3PD, England

Reprint requests to Dr. Y. Elerman E-mail: elerman@science.ankara.edu.tr

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Dinuclear Copper(II) Complex, Super-exchange Interactions, Antiferromagnetic Coupling

Preparation and magnetic properties of a 3,5-dimethylpyrazolate bridged binuclear copper(II) complex \([\text{Cu}_2(L)(3,5-\text{pyz})]\) \((L = 1,3-\text{Bis}(2-\text{Hydroxy-5-Chlorosalicylideneamino})\text{propan-2-ol})\) is reported. The crystal structure determined by X-ray diffraction methods. \((\text{C}_{22}\text{H}_{20}\text{N}_4\text{O}_3\text{Cl}_2\text{Cu}_2)\), triclinic, space group \(\text{P}\bar{1}\), \(a = 9.622(3)\), \(b = 10.921(2)\), \(c = 11.420(3)\) Å, \(\alpha = 100.73(2)\), \(\beta = 94.04(2)\), \(\gamma = 108.08(2)\) \(^\circ\), \(V = 1110.2(5)\) Å\(^3\), \(Z = 2\). Two copper(II) ions in a square-planar coordination are bridged via alkoxide oxygen and 3,5-dimethyl pyrazolate nitrogen atoms to form a dinuclear unit. The metal coordination sphere is four-coordinate, planar with an \(\text{N}_2\text{O}_2\) donor set. The dihedral angle between the two coordination planes is 166.83\(^\circ\).

There are significant intermolecular interactions between neighbouring binuclear entities. The shortest intermolecular \(\text{Cu}(1)\cdot\cdot\cdot\text{Cu}(1)\) distance is 3.383(1) Å and the \(\text{Cu}(1) - \text{O}(1)\) distance is 2.666(3) Å \((i = 1 - x, -y, 1 - z)\). The variable-temperature magnetic susceptibility measurement for a powdered sample of the complex was carried out in the temperature range 5 - 350 K and analysed to obtain values of the parameter \(J\) in the exchange Hamiltonian \(\hat{\mathcal{H}} = -2J\mathbf{S}_\text{Cu} \cdot \mathbf{S}_\text{Cu}\); \(2J = -164\) cm\(^{-1}\). The magnetic moment at 300 K is about 2.42 \(\mu_B\), and 0.22 \(\mu_B\) at 5 K. The weak antiferromagnetism of the present complex is reasonably explained in terms of the orbital countercomplementary effect based on Hoffmann’s theory for super-exchange interaction.