

Crystal Structure and Magnetic Exchange Interaction in a Binuclear Copper(II) Schiff Base Complex with a Bridging *m*-Phenylenediamine Ligand

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Condensation of 2-hydroxy-3-methoxybenzaldehyde with *m*-phenylenediamine (1,3-diaminobenzene) (*m*-pda) gives the ligand [*N,N'*-bis(2-hydroxy-3-methoxybenzylidene)-1,3-diaminobenzene] which reacts with cupric acetate to give the complex [Cu₂(L-*m*-pda)₂]·2H₂O, [L = 2-hydroxy-3-methoxybenzaldehyde]. The molecular structure of the complex [Cu₂(L-*m*-pda)₂]·2H₂O has been determined by single-crystal X-ray analysis. (C₄₄H₄₀Cu₂N₄O₈)·2H₂O, triclinic, space group *P* $\bar{1}$. Two [Cu(L-*m*-pda)] fragments, related by an inversion center, are connected by *m*-phenylene groups to form a binuclear unit. The coordination geometry around each copper(II) can be described as a distorted tetrahedron formed by the N₂O₂ donor set of the Schiff base ligands. The intramolecular Cu...Cu separation is 7.401(6) Å. The magnetic susceptibility of the complex in the 5–301 K temperature range can be rationalized by the parameters $J = -0.4 \text{ cm}^{-1}$ and $g = 2.17$. This indicates a weak intramolecular antiferromagnetic interaction. Extended Hückel molecular orbital (EHMO) calculations have been performed in order to gain insight into the molecular orbitals that participate in the super-exchange pathway.

Key words: Dinuclear Copper(II) Complex, Antiferromagnetic Interactions, Super-Exchange Interactions, Schiff Base, Molecular Orbital Calculation