

Super-Exchange Interaction in a *Chair*-Piperazine Bridged Dicopper(II/II) Complex: Synthesis, Crystal Structure, Magnetic Properties and Molecular Orbital Calculations

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Reaction of the μ -bis(tridentate) ligand H_3L' ($L' = 1,3$ -bis[N-(5-chloro-2-hydroxybenzylidene)-2-aminoethylene]-2-(5-chloro-2-hydroxyphenyl)imidazolidine) with copper(II) chloride dihydrate gives the *chair*-piperazine bridged complex $[Cu_2(\mu-L)Cl_2]$. The halves of the binuclear complex are related by crystallographic inversion symmetry. The intramolecular Cu...Cu separation is 6.954(3) Å. Temperature-dependent magnetic susceptibility measurements of the complex show a weak intramolecular antiferromagnetic coupling. The super-exchange coupling constant (J) is -10.5 cm^{-1} . Semi-empirical 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, Super-Exchange Interactions, Antiferromagnetic Coupling, Schiff Base, Imidazolidine