Relation between Magnetic, Spectroscopic and Structural Properties of Binuclear Copper(II) Complexes of Pentadentate Schiff-base Ligand, Semi-empirical and ab-initio Calculations

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The synthesis and characterization of $[Cu_2(L^1)(3,5\ prz)]$ (L^1=1,3-Bis(2-hydroxy-3,5-chlorosalicylideneamino)propan-2-ol) **1** and of $[Cu_2(L^2)(3,5\ prz)]$ (L^2=1,3-Bis(2-hydroxy-bromosalicylideneamino)propan-2-ol) **2** are reported. The compounds were studied by elemental analysis, infrared and electronic spectra. The structure of the $Cu_2(L^1)(3,5\ prz)]$ complex was determined by x-ray diffraction. The magnetochemical characteristics of these compounds were determined by temperature-dependent magnetic susceptibility measurements, revealing their antiferromagnetic coupling. The superexchange coupling constants are 210 cm^{-1} for **1** and 440 cm^{-1} for **2**. The difference in the magnitude of the coupling constants was explained by the metal-ligand orbital overlaps and confirmed by ab-initio restricted Hartree-Fock (RHF) calculations. In order to determine the nature of the frontier orbitals, Extended Hückel Molecular Orbital (EHMO) calculations are also reported.

Key words: Dinuclear Copper(II) Complex; Antiferromagnetic Coupling; Overlap Interaction; Countercomplementary Effect; ab-initio Restricted Hartree-Fock Molecular Orbital Calculation.