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Dinuclear Copper(II) Complex, Antiferromagnetic Coupling, Overlap Interaction

\([\text{Cu}_2(\text{L})(\text{O}_2\text{CMe})]\cdot\frac{1}{2}\text{H}_2\text{O} \quad \text{(L = 1,3-bis (2-hydroxy-5-chlorosalicylideneamino)propan-2-ol)}\)

was synthesized and its crystal structure determined. \((\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_5\text{Cl}_2\text{Cu}_2)\cdot\frac{1}{2}\text{H}_2\text{O}, \text{monoclinic, space group } P 2_1/c, a = 20.660(10), b = 9.618(2), c = 21.810(10) \text{Å}, \beta = 109.3(8)^\circ, V = 4090(2) \text{Å}^3, Z = 8.\) The crystal contains two independent dicopper(II) complexes and an uncoordinated molecule of water in the asymmetric unit. In both molecules of the asymmetric unit, the two copper(II) ions are bridged by the alkoxo group of the ligand and by an acetato group. Magnetic susceptibilities of the complex in the solid state were measured over the temperature range 4.6 - 308 K. The title compound shows weak antiferromagnetic coupling with a best fit \(J\) value of \(-89.6 \text{ cm}^{-1}\), which is interpreted in terms of a compensation effects of the different bridging ligands which participate in the super-exchange interactions. \textit{Ab initio} restricted Hartree-Fock calculations have shown that the acetato bridge and the alkoxide bridge contribute to the magnetic interaction countercomplementarily to reduce antiferromagnetic interaction.