Trinuclear Copper(II) Complex, Super-Exchange Interactions, Antiferromagnetic Coupling

[Cu_3(L)_3]^3+(LH = 1,3-diaminopropan-2-ol) was synthesized and its crystal structure determined. It crystallizes in the triclinic space group $\overline{P}1$ with $a = 10.504(2)$, $b = 10.856(2)$, $c = 12.519(2)$ Å, $\alpha = 74.41(1)$, $\beta = 70.60(1)$, $\gamma = 63.60(1)^\circ$, $V = 1193.6(3)$ Å³, $Z = 2$. The structure consists of trimeric [Cu_3(L)_3]^3+ units and three perchlorate anions in the asymmetric unit. In the compound three copper(II) ions are linked by 1,3-diamino-2-propanol molecules in such a way that an almost equilateral triangle is formed. The coordination spheres of the three copper(II) ions are slightly different from each other. The coordination geometry of Cu1 is a distorted square pyramid, and that of Cu2 is almost square planar while that of Cu3 is tetrahedrally distorted square planar. The copper(II) centers are separated by average 3.481(2) Å and antiferromagnetically coupled ($-J = 100$ cm$^{-1}$), which follows from temperature-dependent magnetic susceptibility measurements in the temperature range 4.4 to 299 K. The average Cu-O-Cu angle is 128.1(1)$^\circ$ in the super-exchange pathway. As the temperature is increased, the magnetic moment rises from 1.41 $\mu_B$ at 4.4 K to 2.22 $\mu_B$ at 299 K. In the $\chi(T)$ curve no characteristic maximum was observed. The magnetic super-exchange interaction for the title compound is due to the effective overlap of the magnetic orbitals (d$_{x^2-y^2}$) with orbitals of bridging alkoxide oxygen atoms.