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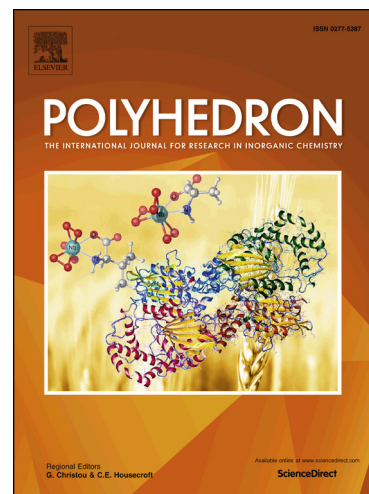
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Structure and characterization of physicochemical and magnetic properties of new complex containing monobridged oxygen copper(II) dinuclear cation

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Abstract

The crystal and molecular structure of the new copper(II) complex with nitrilotriacetate (nta) and 1,10-phenanthroline (phen) ligands of the $[\text{Cu}(\text{phen})_2\text{Cu}(\text{nta})(\text{phen})]_2[\text{Cu}(\text{Hnta})_2] \cdot 20\text{H}_2\text{O}$ molecular formula has been determined. The compound comprises the dianionic mononuclear entity, $[\text{Cu}(\text{Hnta})_2]^{2-}$, and two monocationic dinuclear units, $[\text{Cu}(\text{phen})_2\text{Cu}(\text{nta})(\text{phen})]^+$, in which the Cu(II) ions are bridged by one oxygen atom of the nta ligand in the rarely found $\mu_{1,1}\text{-O}$ bridging mode. The complex was characterized by spectroscopic (IR, FIR and EPR) methods and magnetic measurements as well as thermogravimetry (TG). The magnetic measurements revealed an antiferromagnetic coupling between the Cu(II) ions in the dinuclear unit. Based on the experimental data supported by density functional theory (DFT) calculations the correlation between the coordination mode of the Cu(II) ions and magnetic properties of the compound studied has been discussed.

Keywords: Copper, Nitrilotriacetate, Structure elucidation, Magnetic measurements, Density functional calculations

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