

Counteranion Effect on Macrocyclic Complex Materials

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Dinuclear copper (II) macrocyclic complexes derived from the condensation of 4-methyl-2,6-diformylphenol with 1,3-diamine-2-propanol, with different counteranions, $[\text{Cu}_2\text{LCl}_2]\cdot 2\text{H}_2\text{O}$ **1**; $\{[\text{Cu}_2\text{L}(\mu_2\text{-acetate})](\text{acetate})$ **2a** $[\text{Cu}_2\text{L}(\text{acetate})_2(\text{H}_2\text{O})_2]$ **2b** $\}\cdot 6\text{H}_2\text{O}$; $[\text{Cu}_2\text{L}(\text{H}_2\text{O})_2]2(\text{SO}_4\text{H})\cdot 2\text{H}_2\text{O}$ **3**, have been prepared. **1** and **3** crystallize in the triclinic P-1 (#2) space group with $a=7.7223(16)$, $b=9.3901(19)$, $c=10.167(2)$ Å; $\alpha=73.377(3)$, $\beta=85.768(4)$, $\gamma=65.766(3)$ °; $V=643.4(2)$ Å³; $Z=1$ and $a=7.727(5)$, $b=8.663(4)$, $c=11.753(4)$ Å; $\alpha=82.199(6)$, $\beta=85.519(10)$, $\gamma=75.830(11)$ °; $V=754.8(7)$ Å³; $Z=1$ respectively. **2a**, **2b** co-crystallize in the orthorhombic crystal system, Pnma(#62) space group with $a=15.1671(11)$, $b=27.4366(19)$, $c=15.9786(11)$ Å; $V=6649.2(8)$ Å³; $Z=4$. The copper (II) ions present a square base pyramidal geometry in three of the reported complexes, with axially coordinated halogens **1**, a syn-syn acetate ligand **2b** and water molecules **3**. Compound **2a** can be described as having a distorted octahedral environment, with aqua and acetate oxygens in the apices. Compound **2b** which co-crystallized with **2a**, presents a folded structure of the macrocyclic ligand due to the presence of the bridging acetate molecule. Strong antiferromagnetic exchange is observed in all complexes. The correlation between magnetic properties and structure will be discussed.

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