

METAL-ORGANIC FRAMEWORK:
STRUCTURE AND MAGNETIC PROPERTIES
OF $[\text{Cu}_3(\text{BTC})_2(\text{L})_x(\text{CuO})_y]_n$ ($\text{L} = \text{H}_2\text{O}, \text{DMF}$)

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ABSTRACT:

The compounds $[\text{Cu}_3(\text{BTC})_2(\text{L})_x(\text{CuO})_y]$, with BTC (benzene 1,3,5-tricarboxylate) and L (H_2O or DMF) were prepared using electrochemical synthesis. Structural and morphologic characterizations were performed by X-ray diffraction and scanning electronic microscopy. The $[\text{Cu}_3(\text{BTC})_2(\text{L})_x(\text{CuO})_y]$ contain dimeric $[\text{Cu}_2(\text{O}_2\text{CR})]_4$ units with three possible spin configurations arising from Cu(II) $3d^9$ states and Cu–Cu δ bond. We observed an unusual very strong antiferromagnetic coupling in temperatures ranging from 100K to 350K for $[\text{Cu}_3(\text{BTC})_2(\text{H}_2\text{O})_3(\text{CuO})_y]_n$. The inverse susceptibility versus temperature shows a linearity from 20K up to 65K fitting the Curie–Weiss law, for $\text{L} = \text{DMF}$. The CW X-band electron paramagnetic resonance spectroscopy (EPR) was important to explore the coordination state for DMF in the network. It was observed that DMF is located in an equatorial geometry of the coordination network experimenting interactions from the nitrogen and copper ions.

Graphical Abstract

The compounds $[\text{Cu}_3(\text{BTC})_2(\text{L})_x(\text{CuO})_y]$, with BTC (benzene 1,3,5-tricarboxylate) and L (H_2O or DMF) were prepared using electrochemical synthesis. Structural and morphologic characterizations were performed by X-ray diffraction and scanning electronic microscopy. Experimental X-ray diffraction patterns showing the isostructural relationship among the $[\text{Cu}_3(\text{BTC})_2]$ -MOF series: (a) HKUST-1, CIF theoretically calculated, (b) $[\text{Cu}_3(\text{BTC})_2(\text{H}_2\text{O})_3]$, blue, synthesized at 25°C , octahedral crystal format (c) $[\text{Cu}_3(\text{BTC})_2(\text{DMF})_x(\text{CuO})_y]$, green, synthesized at 50°C , hexagonal crystal format, and. XRD pattern of the CuO nanoparticles showing a single-phase and monoclinic structure. Lattice parameters are $a = 4.84 \text{ \AA}$, $b = 3.47 \text{ \AA}$, $c = 5.33 \text{ \AA}$. The intensities and peaks positions are in agreement with the reported values (JCPDS- cards file No. 05-661).

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