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Short communication

A mixed valence copper coordination polymer with a new highly self-penetrated topology

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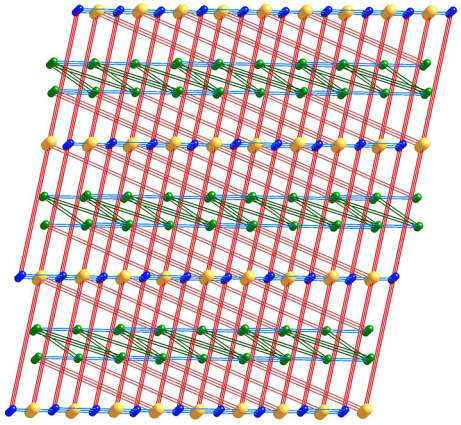
GRAPHICAL ABSTRACT

$\{[Cu_5(oba)_4(bpmp)_3(H_2O)_2]\cdot 10H_2O\}_n$ (pictured, oba = oxybisbenzoate, bpmp = bis(4-pyridylmethyl)piperazine) shows a complicated 3D self-penetrated 3,4,4-connected $(8^3)_2(6.8.10^4)(6^4.8.10)$ topology.



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ABSTRACT

Crystals of $\{[Cu_5(oba)_4(bpmp)_3(H_2O)_2]\cdot 10H_2O\}_n$ (**1**, oba = oxybisbenzoate, bpmp = bis(4-pyridylmethyl)piperazine) were prepared by hydrothermal methods. A single-crystal structure determination showed the presence of $[Cu_5(oba)_4(H_2O)_2]_n$ ribbons with $\{Cu_2(OCO)_4\}$ paddlewheel dimers connected to isolated divalent copper atoms and isolated monovalent copper atoms. These ribbon motifs are pillared into the full complicated 3D coordination polymer net of **1** by long-spanning bpmp tethers. Compound **1** presents the unique example of a self-penetrated 3,4,4-connected $(8^3)_2(6.8.10^4)(6^4.8.10)$ topology. Decameric water molecule clusters entrained within the net play an important stabilization role.

Coordination polymers remain under focused investigation because of their wide potential industrial or environmental applications [1] such as hydrogen storage [2], shape-selective molecular separations [3], detection of toxic contaminants [4], and heterogeneous catalysis for the degradation of organic dyes [5]. A standard approach towards the construction of crystalline coordination polymers is the hydrothermal or solvothermal reaction of a divalent metal salt with an organic dicarboxylic acid and a dipyridyl-type coligand [6]. While the synthetic approach is largely standardized at this juncture, the infinite variety of organic substructures continues to produce molecular structures with a remarkable number of network topologies with rather striking aesthetics [7]. Coordination polymer networks have frequently

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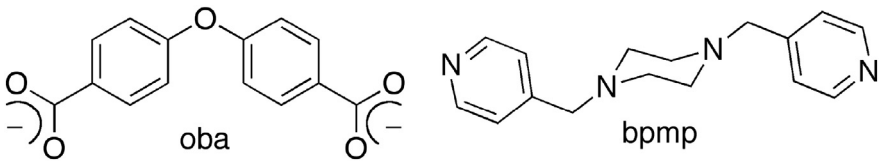

Scheme 1. Ligands used in this study.

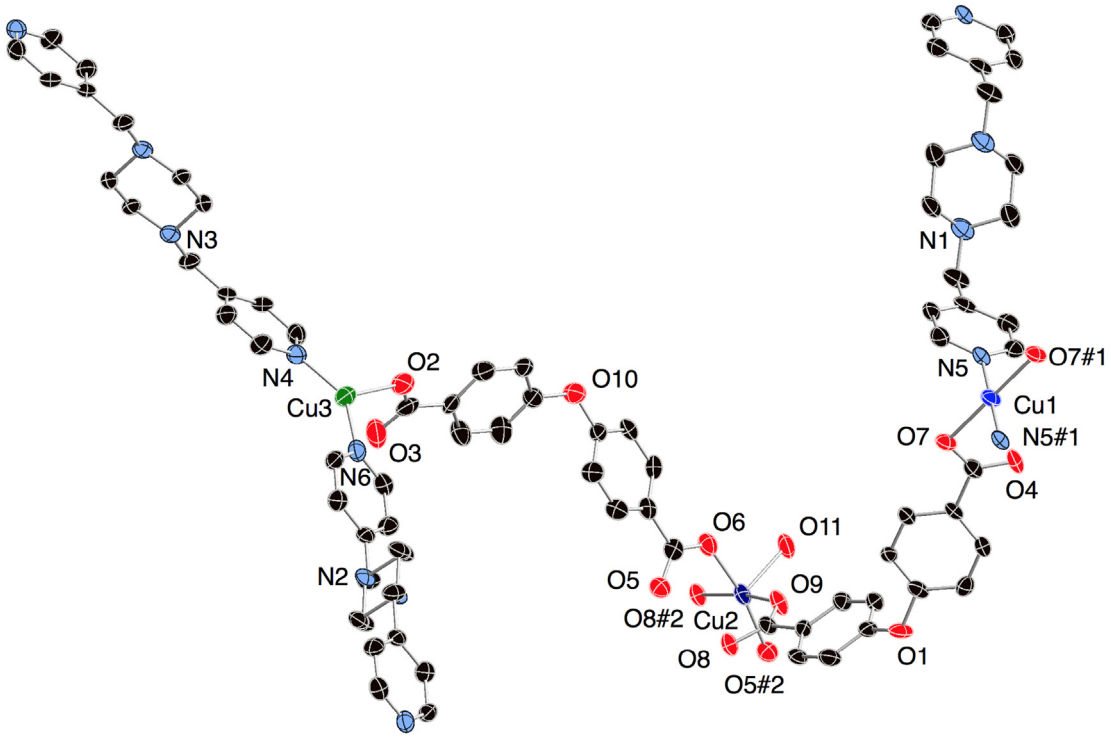

Fig. 1. Coordination environments in **1**. Thermal ellipsoids are drawn at 50% probability. Symmetry transformations: #1 $-x, -y, -z+1$; #2 $-x-1, -y+2, -z+1$.

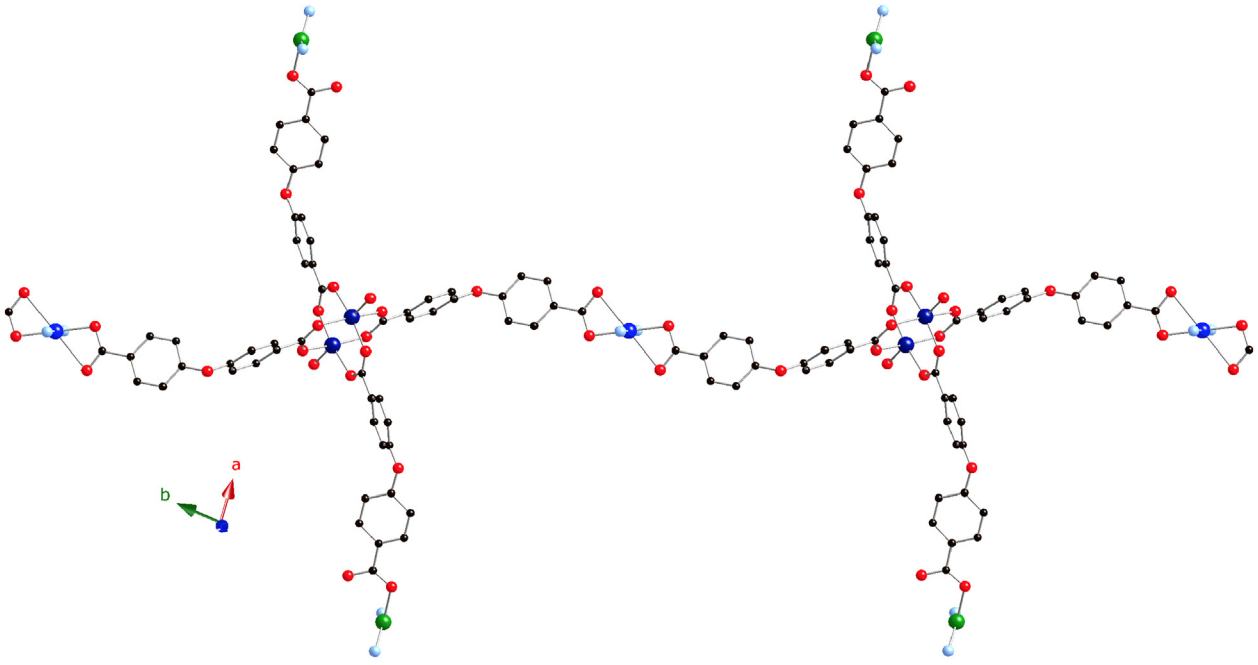

Fig. 2. $[Cu_5(oba)_4(H_2O)_2]_n$ neutral ribbon motif in **1**, showing Cu2-based $\{Cu_2(OCO)_4(H_2O)_2\}$ paddlewheel dimeric units and isolated Cu1 and Cu3 atoms.