

Template effect of guest cations on topology of copper-cyanide networks

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During the course of our ongoing structural studies on copper cyanide networks, we have determined the structures of twenty to thirty anionic Cu(I)CN networks in which the guest cations are protonated N-substituted diamines or ethanolamines. The various anionic CuCN networks that have been characterized are built up from 2, 3, or 4-coordinated Cu atoms as nodes, either occurring singly or as cuprophilic pairs, and linked by μ_2 or μ_3 CN bridges. We had envisioned that a specific network could accommodate several different cations of similar size, but in fact each cation appears to template its own specific 2D or 3D network. In one or two cases, a given cation can template two different CuCN networks, depending on the reaction conditions. In order to understand the parameters that affect formation of the different networks, we are tabulating formal network topologies, cation guest properties such as volume, shape and electrostatic charge distribution, and hydrogen-bonding between guests and between guests and the CuCN network, looking for correlations that can explain the formation of these diverse structures and enable the deliberate synthesis of new polymers with desired topologies and physical properties.