

Open and closed forms of the interpenetrated [Cu-2(Tae)(Bpa)(2)](NO3)(2) center dot nH(2)O: magnetic properties and high pressure CO2/CH4 gas sorption

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Resumen

Two closed and one open structural forms of the interpenetrated [Cu-2(Tae)(Bpa)(2)](NO3)(2) center dot nH(2)O (H(2)Tae = 1,1,2,2-tetraacetylene, Bpa = 1,2-bis(4-pyridyl) ethane) cationic coordination polymer have been synthesized. Three crystallographically related interpenetrated "ths" cationic nets encapsulate water molecules and nitrate anions giving rise to the closed structural forms of [Cu-2(Tae)(Bpa)(2)](NO3)(2) center dot nH(2)O. Depending on the location of water molecules and nitrate groups, two different closed forms with 5.5 and 3.6 crystallization water molecules have been obtained. The thermal activation of the closed structures gives rise to a 29% expansion of the unit cell. This closed to open transformation is reversible, and is triggered by the loss or uptake of solvent. The high pressure gas adsorption experiments show similar selectivity values towards CO2 for CO2/CH4 mixtures to that showed by some metal organic frameworks without unsaturated metal sites, and isosteric heats for CO2 adsorption similar to that for the HKUST-1 compound.

Palabras clave

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