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3D Interpenetrated Network Based on 1,3-Benzenedicarboxylate and 1,2-Bis(4-Pyridyl) Ethane

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Abstract : Solid coordination networks (SCNs) are materials consisting of metal ions or clusters that are linked by polyfunctional organic ligands and can be designed to form tridimensional frameworks. Their structural features, as for example high surface areas, thermal stability, and in other cases large cavities, have opened a wide range of applications in fields like drug delivery, host-guest chemistry, biomedical imaging, chemical sensing, heterogeneous catalysis and others referred to greenhouse gases storage or even separation. In this sense, the use of polycarboxylate anions and dipyridyl ligands is an effective strategy to produce extended structures with the needed characteristics for these applications. In this context, a novel compound, [Cu4(m-BDC)4(bpa)2DMF]•DMF has been obtained by microwave synthesis, where m-BDC is 1,3-benzenedicarboxylate and bpa 1,2-bis(4-pyridyl)ethane. The crystal structure can be described as a three dimensional framework formed by two equal, interpenetrated networks. Each network consists of two different CuII dimers. Dimer 1 have two coppers with a square pyramidal coordination, and dimer 2 have one with a square pyramidal coordination and other with octahedral one, the last dimer is unique in literature. Therefore, the combination of both type of dimers is unprecedented. Thus, benzenedicarboxylate ligands form sinusoidal chains between the same type of dimers, and also connect both chains forming these layers in the (100) plane. These layers are connected along the [100] direction through the bpa ligand, giving rise to a 3D network with 10 Å2 voids in average. However, the fact that there are two interpenetrated networks results in a significant reduction of the available volume. Structural analysis was carried out by means of single crystal X-ray diffraction and IR spectroscopy. Thermal and magnetic properties have been measured by means of thermogravimetry (TG), X-ray thermodiffractometry (TDX), and electron paramagnetic resonance (EPR). Additionally, CO2 and CH4 high pressure adsorption measurements have been carried out for this compound.

Keywords : gas adsorption, interpenetrated networks, magnetic measurements, solid coordination network (SCN), thermal stability
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