

MS36-P9 Controlled Stepwise Synthesis of a Cu MOF: From Magnesium Precursor to Mesoporous Material

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A three-dimensional copper metal-organic framework (MOF) has been synthesized from a magnesium precursor and copper sulfate crystallized in space group $I2_13$. The effective free volume calculated by PLATON analysis after removing the entire guest molecules amount approximately 54.8 percent of the crystal volume (8773 Å³ of 16007 Å³ unit cell volume). Topological analysis was carried out by *GTECS3D* to obtain an insight in to the structure [*Z. Kristallogr. Suppl.*, **2012**, 32, 117.]. The structure can be viewed as a 4-connected topology with a Vertex symbol 3.3.10₂,10₂,10₂,10₂, which corresponds to a *1cv* net. The 3D⁺ intersecting channel system has a cross section of approximately 9 Å. In addition, the oxygen atoms of sulfate ions and methyl groups from the ligand are exposed toward the channel, which facilitate the trapping of polar guests.

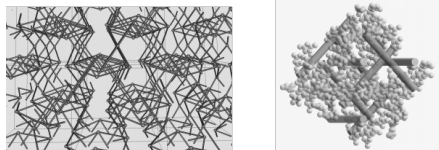


Figure 1. 1cv network structure of the Cu MOF (left); 3D channel net running along the *a*, *b* and *c* axes (right).

Keywords: Metal Organic Framework, Copper, Mesoporous Material, Polar Guests

MS37 Molecular compounds and MOFs at ambient conditions and under high pressure

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MS37-P1 Metal-Hydride Organic Frameworks (HOF)-new solids for gas adsorption and separation

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Due to daily increase in energy demand it is a great task to explore and use a sustainable and carbon-free energy systems. Hydrogen, as clean and easily productive (from water and renewable energy) is possible future energy carrier. Problem of its safe and efficient storage can be solved by solid state storage-through chemical bonding in crystalline compounds or by physical adsorption in porous materials[1].

Metal-hydride organic frameworks (HOF) are a novel hybrid materials designed by combining molecular building blocks of light-weight complex hydrides with organic linkers developed for coordination frameworks. They will be based on crystal engineering principles of coordination frameworks and have new properties (guest-host interactions, dehydrogenation properties) defined by the nature of the unique complex-hydride ligands. HOFs present new type of frameworks due to flexibility of the BH₄⁻ which allows other cation coordination than usually available in coordination frameworks. Also, directional anionic ligands other than hydrides can be used. We used imidazoles or its derivatives because the metal-imidazolate-metal angle of 145° is very similar to metal-borohydride-metal angle observed in Mg(BH₄)₂[2].

We will present first results on mono- and bi-metallic mixed anion (borohydride and imidazolate) frameworks based on Zn²⁺ node and light alkali metal cations (Li⁺, Na⁺). For synthesis we used ball-milling procedure under inert atmosphere, solvent free and liquid-assisted grinding with different solvents (DMF, DMSO, THF, acetonitrile). Starting reactants were NaBH₄, NaIm, Him, 2-MeIm,