

# Porous three-dimensional Cd(II) coordination network based on 1,2-bis(4-pyridyl)ethane and formiate ligands

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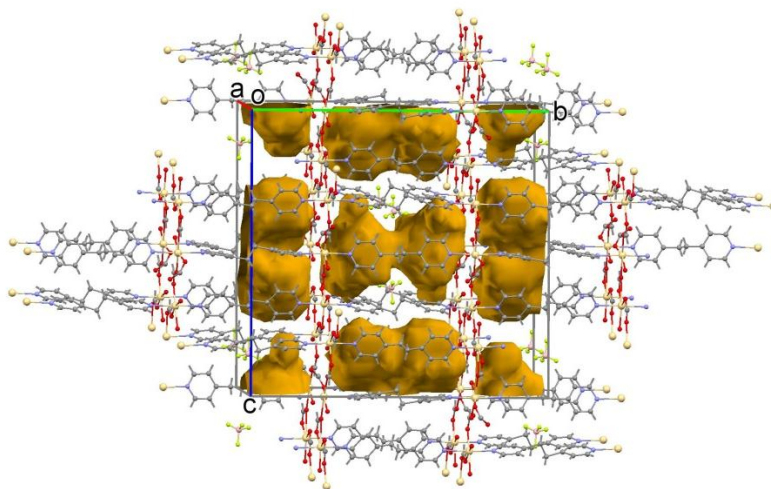
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Metal–organic frameworks (MOFs) represent a new class of porous crystalline materials, which continue to be one of the fastest growing fields in chemistry, with diverse potential applications. MOFs with inherent characteristics such as rigidity, porosity, and overall architecture can be adjusted based upon the choice of the multidentate ligands and the transition metals. The selection of transition metals with versatile coordination geometry as well as multidentate ligands, such as dicarboxylic acids or/and bipyridine-like ligands, with adaptable coordination modes is an efficient way to rationally design MOFs with specific properties and applications.

A new porous Cd(II) coordination polymer  $\{[\text{Cd}_3(\text{HCOO})_5(\text{bpe})_3(\text{H}_2\text{O})_3]\text{BF}_4 \cdot x\text{H}_2\text{O}\}_n$  (**I**) has been prepared by interaction of  $\text{Cd}(\text{BF}_4)_2 \cdot x\text{H}_2\text{O}$  with 1,2-bis(4-pyridyl)ethane (bpe) and glutamic acid in  $\text{CH}_3\text{OH}:\text{dmf}:\text{H}_2\text{O}$  (2:2:1) mixture at 120°C using the hydro/solvothermal condition. Compound has been characterized by IR spectroscopy and single crystal X-ray diffraction method. Crystals of **I** belong to the centrosymmetric monoclinic space group  $P2_1/c$ :  $a=8.5099(3)$ ,  $b=27.8923(8)$ ,  $c=26.5253(7)$  Å,  $\beta = 96.399(3)^\circ$ . The asymmetric part of unit cell contains three cadmium atoms. Two of them Cd1 and Cd2 have similar octahedral  $\text{N}_2\text{O}_4$ -coordination surrounding and coordinate three bridging formate anions and water molecule on the vertexes of square and two nitrogen atoms of bpe ligands in *trans*-positions. The Cd-O and Cd-N distances are in the range 2.256-2.374 Å and 2.300-2.371 Å, respectively. The coordination surrounding of third Cd3 atom may be considered as  $\text{N}_2\text{O}_3$  trigonal-bipyramidal provided by three bridging formate in basal plane and two nitrogen atoms of bpe anions in the vertexes of bipyramid with Cd-O and Cd-N distances in the range 2.284-2.328 and 2.316-2.326 Å, respectively. It should be mentioned that second oxygen atoms of two coordinated formate anions approach to this Cd3 atoms at the distances 2.598 and 2.942 Å and this formate anions may be considered as chelate-bridging and coordination surrounding of Cd 3 and pentagonal-bipyramidal. The  $\text{HCOO}^-$  anion and the bpe ligand have the exo-bidentate-bridging function and unite the cadmium atoms in the 3D network. The crystal structure reveals inclusion of water molecules in the pores of 3D framework. Upon removal of solvent water molecules the total potential solvent accessible voids of 1640 Å<sup>3</sup>, 26.2% of total unit cell volume 6256.9 Å<sup>3</sup>.



**Figure 1.** Fragment of crystal packing with solvent accessible voids shown by yellow

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