

MS30-P7 The synthesis and crystal structure of Cd(II)-Azoxybenzenetetracarboxylate with 1,4-bis(2-methylimidazol-1yl)butane

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During the last decades, there is a continued interest in the rational design and synthesis of coordination polymers due to not only their application fields such as gas storage/separation, catalysis, luminescence, sensor, but also their fascinating topological structures [1]. Despite the syntheses of a great deal of coordination polymers, it has been still difficult the controllable synthesis of coordination polymers. In the assembly of coordination polymers, several factors, such as, organic ligands, metal ions, pH, solvents, temperature are the key factors [2]. Hence, it is important to choose the organic ligands, metal ions and regulate the reaction conditions for desired structures. In this study, $[\text{Cd}_2(\mu_6\text{-ao}_2\text{btc})(\mu\text{-1,4-bmeib})(\text{H}_2\text{O})_2]_n$ ($\text{H}_4\text{ao}_2\text{btc}$ =3,3',5,5'-azoxybenzenetetracarboxylic acid, 1,4-bmeib: 1,4-bis(2-methylimidazol-1yl)butane) was synthesized and characterized by elemental analysis, IR spectrum, single crystal X-ray diffraction. Complex **1** was prepared by the solvothermal reaction of H_4abtc (0.1 g, 0.279 mmol), $\text{CdCl}_2 \cdot 2.5\text{H}_2\text{O}$ (0.127 g, 0.558 mmol) and 1,4-bmeib ligand (0.061 g, 0.279 mmol) at 100 °C in the mixture of DMF: H_2O (10:2, v:v) in the presence of HNO_3 . The crystal structure of **1** with atom numbering scheme is shown in Fig. 1a. X-ray single-crystal diffraction analysis indicates that complex **1** crystallizes in the triclinic space group *P*. The asymmetric unit of **1** consists of one Cd(II) ion, one half 1,4-bmeib, one half ao_2btc and one aqua ligands. ao_2btc ligand displays new coordination mode in **1** and each ao_2btc ligand acts a decadentate ligand in which 3,3'-carboxyl groups display bidentate chelating mode and 5,5'-carboxyl groups exhibit bidentate chelating and monodentate bridging modes, connecting to six metal centers. Each Cd(II) ions are bridging by 3,3'-and 5,5'-carboxylate oxygen atoms of ao_2btc ligand to form 1D double chains with the 26-membered rings. Adjacent 1D double chains are linked by 5,5'-carboxy groups of ao_2btc with Cd...Cd distance of 3.876 Å to generate 2D planar structures. 2D structures are extended to 3D porous structure by the coordination of 1,4-bmeib ligand (Fig. 1b).

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References

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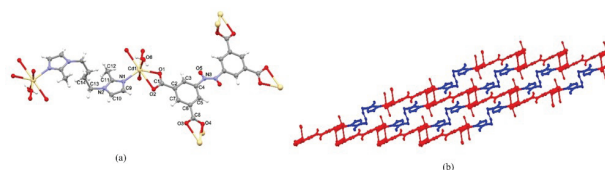


Figure 1. (a) The crystal structure of **1** with the atom labeling and (b) 3D structure of **1**

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