NOTE

Synthesis and Crystal Structure New Zn(II) Coordination Polymer with 4-Connected *sql* Tetragonal Plane Net

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A new coordination polymer $\{[\text{Zn}(\text{5-NO}_2\text{-ip})(\text{bimb})]\cdot\text{H}_2\text{O}\}_n$ (**1**) with 5-nitro-1,3- benzenedicarboxylic acid (5-NO₂-ip) and 1,4-*bis*(1-imidazol-yl)-2,5-dimethyl benzene (bimb) has been prepared by hydrothermal synthesis and characterized by single-crystal X-ray diffraction and EA. Complex, $\{[\text{Zn}(\text{5-NO}_2\text{-ip})(\text{bimb})]\cdot\text{H}_2\text{O}\}_n$ (**1**), is triclinic, space group P-1 with $a = 9.094$ (2) Å, $b = 9.428$ (4) Å, $c = 13.999$ (3) Å, $\alpha = 71.553$ (6)°, $\beta = 87.530$ (6)°, $\gamma = 84.220$ (7)°, $V = 1132.7$ (6) Å³, $Z = 2$, $M_r = 530.79$, $D_c = 1.556$ g/cm³ and $F(000) = 544$. The final refinement gave $R = 0.0416$ and $wR = 0.1102$ for 4125 reflections with $I > 2\sigma(I)$. X-ray diffraction analysis reveals that the complex **1** displays a two-dimensional structure with 4-connected *sql* topology.

Keywords: Zn(II), Coordination polymer, Crystal structure.

The self-assembly of metal-organic frameworks (MOFs) from metal ions and organic moieties is of much current interest in crystal engineering because of their outstanding properties such as gas storage, molecular magnetism and luminescence, which are intimately related to their structures¹⁻⁴. For the construction of MOFs some functional organic ligands, are usually chosen as rigid tectons. It is well-known that carboxylate-metal compounds exhibit various network topologies and remarkable prospect, therefore the construction of novel coordination polymers using metal ions and anionic *O*-donor ligands is a hotspot in the field^{5,6}.

In this paper, we used the 5-nitro-1,3-benzenedicarboxylic acid (5-NO₂-ip) and 1,4-*bis*(1-imidazol-yl)-2,5-dimethyl benzene (bimb) construct a new Zn(II) coordination polymer with a 4-connected *sql* tetragonal plane net.

All reagents and solvents employed were commercially available and used without further purification. Elemental analysis was carried out on a Carlo Erba 1106 full-automatic trace organic elemental analyzer.

Synthesis of $\{[\text{Zn}(\text{5-NO}_2\text{-ip})(\text{bimb})]\cdot\text{H}_2\text{O}\}_n$ (1**):** The mixtures of 5-NO₂-ip (0.5 mmol), Zn(OAc)₂·2H₂O (0.5 mmol), bimb (0.5 mmol), NaOH (1 mmol, 0.04 g) and 12 mL of water were heated to 140 °C for 3 days and then cooled to room-temperature. The colorless crystals were obtained in pure phase, washed with water and ethanol and dried at room

temperature (Yield: 46 % based on Ni). Elemental Anal. Calcd. (%) for C₂₂H₁₉N₅O₇Zn: C, 49.78; H, 3.61; N, 13.19. Found: C, 49.79; H, 3.62; N, 13.17.

X-ray crystallography: Single crystal X-ray diffraction analyses of complex **1** was carried out on a Bruker SMART APEX-II CCD diffractometer equipped with a graphite monochromated MoK α radiation ($\lambda = 0.71073$ Å) by using a ω -scan mode. Empirical absorption correction was applied using the SADABS programs⁷. All the structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 using the program SHELXL 97⁸. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were located by geometrically calculations and their positions and thermal parameters were fixed during the structure refinement.

Crystallographic analysis reveals that the complex $\{[\text{Zn}(\text{5-NO}_2\text{-ip})(\text{bimb})]\cdot\text{H}_2\text{O}\}_n$ crystallizes in the triclinic system P-1 space group. The coordination environment around the Zn(II) center is represented in Fig. 1. It consist of one Zn(II) ion, one 5-NO₂-ip, two halves of bimb ligands and one lattice water molecule. The central Zn(II) exhibits a tetrahedral geometry with N₂O₂ coordination sphere from two 5-NO₂-ip ligands [Zn(1)-O(1) = 1.927 Å and Zn(1)-O(3) = 1.949 Å] and two bimb ligands [Zn(1)-N(1) = 2.017(2) Å and Zn(1)-N(3) = 2.018(2) Å].

Fig. 1. A portion view of complex **1** showing the coordination environment of Zn(II)

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