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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 $\{[Zn(5\text{-}NO_2\text{-}ip)(bimb)]\cdot H_2O\}_n$ (**1**) with 5-nitro-1,3- benzenedicarboxylic acid (5-NO_2-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, $\{[Zn(5\text{-}NO_2\text{-}ip)(bimb)]\cdot H_2O\}_n$ (**1**), is triclinic, space group P-1 with a = 9.094 (2) , b = 9.428 (4), c = 13.999 (3) Å, α = 71.553 (6) °, β = 87.530 (6)°, γ = 84.220 (7) °, V = 1132.7 (6) $Å^3$, Z = 2, M_r = 530.79, D_c = 1.556 g/cm^3 and F(000) = 544. The final refinement gave R = 0.0416 and wR = 0.1102 for 4125 reflections with I > 2σ (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 structures[1-4]. 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-NO_2-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 $\{[Zn(5\text{-}NO_2\text{-}ip)(bimb)]\cdot H_2O\}_n$ (1): The mixtures of 5-NO_2-ip (0.5 mmol), $Zn(OAc)_2\cdot 2H_2O$ (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 $C_{22}H_{19}N_5O_7Zn$: 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 (λ = 0.71073 Å) by using a ω-scan mode. Empirical absorption correction was applied using the SADABS programs[7]. All the structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 using the program SHEXL 97[8]. 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 $\{[Zn(5\text{-}NO_2\text{-}ip)(bimb)]\cdot H_2O\}_n$ 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-NO_2-ip, two halves of bimb ligands and one lattice water molecule. The central Zn(II) exhibits a tetrahedral geometry with N_2O_2 coordination sphere from two 5-NO_2-ip ligands [Zn(1)-O(1) = 1.927Å and Zn(1)-O(3) = 1.949Å] and two bimb ligands[Zn(1)-N(1) = 2.017(2) Å and Zn(1)-N(3) = 2.018(2) Å].

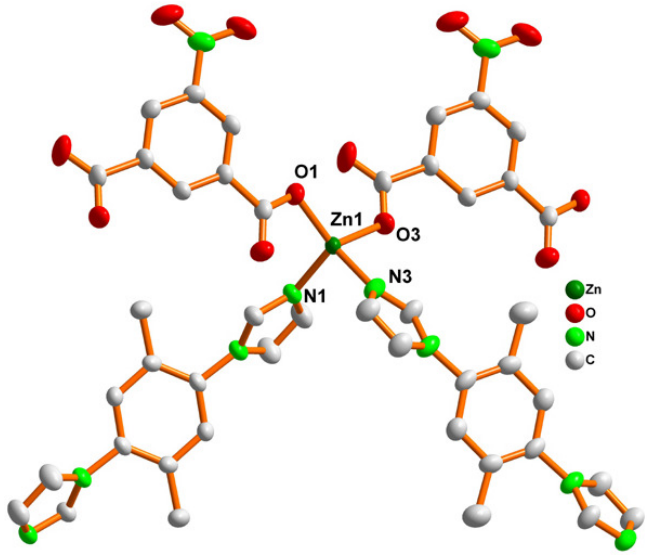

Fig. 1. A portion view of complex **1** showing the coordination environment of Zn(II)

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