Asian Journal of Chemistry; Vol. 26, No. 14 (2014), 4531-4532

ASIAN JOURNAL OF CHEMISTRY

http://dx.doi.org/10.14233/ajchem.2014.17454

NOTE

Hydrothermal Synthesis and Crystal Structure of New (4,4)-Connected Ni(II) Coordination Polymer Based on 3,5-di(4'-Carboxylphenyl)benzene and 1,4-*bis*(Imidazol-1-yl)benzene

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Received: 24 February 2014; *Accepted*: 2 May 2014; *Published online*: 5 July 2014; AJC-15517

A new coordination polymers $[Ni_2(L)(HL)_2(bimb)_{2.5}(H_2O)]_n$ (**1**) (H_2L=3,5-di(4'-carboxylphenyl)benzene and bib=1,4-*bis*(imidazol-1-yl)benzene), has been prepared by hydrothermal synthesis. Complex $[Ni_2(L)(HL)_2(bimb)_{2.5}(H_2O)]_n$ (**1**), triclinic, space group P-1 with a = 10.472 (5) Å, b = 13.610 (5) Å, c = 27.738 (5) Å, β = 98.648 (5)° V = 3755 (2) $Å^3$, Z = 2, Mr = 1609.92, D_c = 1.424 g/cm^3, F (000) = 1666 and μ = 0.58 mm^{-1}. The final refinement gave R = 0.0519 and wR = 0.1236 for 5110 reflections with I > 2σ (I). X-ray diffraction analysis reveals that complex **1** shows a three-dimensional structure with a rare (4,4)-connected tcj/hc topological net.

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

The rational design and construction of new coordination polymers based on metal ions and multifunctional bridging ligands is of great research interest not only due to their interesting topologies but also for their potential applications as functional materials in molecular sensing, magnetism, molecular adsorption, nonlinear optics and catalysis[1-6]. The most common strategy used to obtain coordination polymers is employ appropriate bridging ligands capable of binding to several metal centers through direct bond formation. The carboxylate group is one of the most widely used bridging ligands for designing polynuclear complexes with novel structural features and interesting photoluminescent properties. In this paper, we used the 3,5-di(4'-carboxylphenyl)benzene (H_2L) and 1,4-*bis*(imidazol-1-yl)benzene (bib) to construct a new Ni(II) coordination polymer.

All the 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 $[Ni_2(L)(HL)_2(bimb)_{2.5}(H_2O)]_n$ (1): The mixtures of H_2L (0.5 mmol), $Ni(NO_3)_2·6H_2O$ (0.5 mmol,), bib (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 red crystals were obtained in pure phase, washed with water and ethanol and dried at room temperature (Yield: 40 % based on Ni). Elemental Anal. Calcd. (%) for $C_{90}H_{63}N_{10}O_{13}Ni_2$: C, 67.15; H, 3.94; N, 8.70. Found: C, 67.17; H, 3.95; N, 8.69.

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.

The local coordination environments of the Ni(II) metals in complex **1** with atom-numbering schemes are shown in Fig. 1. The two Ni(II) ions are in different coordination environments. Ni1(II) is surrounded by three carboxylate oxygen atoms [Ni1-O, ranging from 2.038 (3) Å to 2.128 (3) Å], two nitrogen atoms [Ni(1)-N(1) = 2.079 (4) Å and Ni(1)-N(9) = 2.107 (4) Å] and one aqueous molecule[Ni(1)-O(15) = 2.063 (3)Å]. Ni2(II) is coordinated by three carboxylate oxygen atoms [Ni2-O, ranging from 2.000 (3) Å to 2.275 (3) Å] and three nitrogen atom [Ni2-N, ranging from 2.051 (3) Å to 2.149 (3) Å].

The H_2L and bib ligands connect the Ni(II) atoms to form a three-dimensional structure. If the Ni(II) atoms and organic ligands can be viewed as nodes and linkers, the 3D structure can be simplified as a (4,4)-connected tcj/hc topological net (Fig. 2).

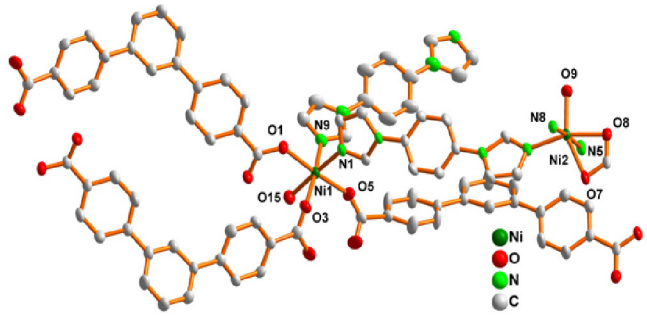

Fig.1. Coordination environment of Ni(II) ions with all hydrogen atoms omitted for clarity

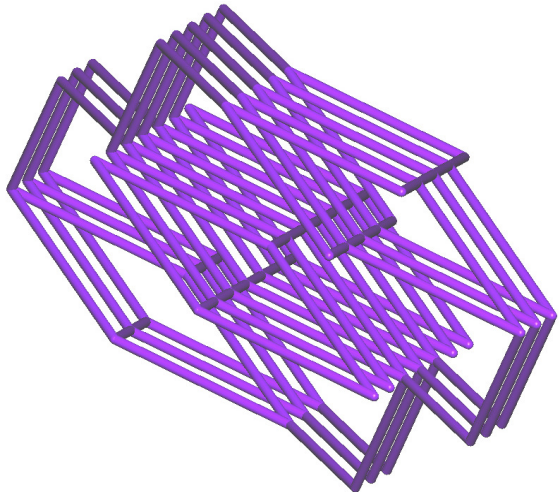

Fig. 2. Topological net for complex **1**

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