Asian Journal of Chemistry; Vol. 26, No. 20 (2014), 7073-7074

ASIAN JOURNAL OF CHEMISTRY

http://dx.doi.org/10.14233/ajchem.2014.17401

NOTE

Cobalt(II) Coordination Polymer Based on Dicarboxylate and Nitrogen-Containing Ligands

YUJING WANG

Yucheng People's Hospital, Yucheng 251200, Shandong Province, P.R. China

Corresponding author: E-mail:whyull@yeah.net

Received: 15 February 2014; *Accepted*: 9 June 2014; *Published online*: 25 September 2014; AJC-16071

A new coordination polymers [Co(5-NO_2-ip)(bimb)]$_n$ (**1**) [5-NO_2-ip = 5-nitro isophthalic acid, bimb = 1,4-*bis*(1-imidazol-yl)-2,5-dimethyl benzene], has been prepared by hydrothermal synthesis. Complex [Co(5-NO_2-ip)(bimb)]$_n$ (**1**), is monoclinic, space group $P2_1/c$ with a = 10.228 (5) Å, b = 16.804 (5) Å, c = 12.488 (5) Å, β = 91.771 (5)° V = 2145.3 (15) Å^3, Z = 4, M_r = 506.34, D_c = 1.568 g/cm^3, F (000) = 1036 and μ = 0.85 mm^{-1}. The final refinement gave R = 0.0321and wR = 0.0809 for 4072 reflections with I > 2σ(I). X-ray diffraction analysis reveals that complex **1** shows a two-dimensional (2D) layer structure and features a three-dimensional supramolecular structure.

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

In recent years, the design and construction of inorganic-organic hybrid materials with tunable physical properties have attracted extensive interest in the field of chemistry[1]. The research in this field has provided numerous examples of rationally designed sundry coordination polymers possessing interesting structural motifs and significant properties in catalysis, gas adsorption, magnetism, DNA recognition and so on[2-6]. But research remains a distant prospect since we can hardly control the extended structures or local coordination modes of individual components, even the chemical composition of the final products. Therefore, the design and construction of coordination polymers on the basis of the different metal ions and ligands is still a great challenge for chemists[7,8].

In this paper, we used the 5-nitroisophthalic acid and 1,4-*bis*(1-imidazol-yl)-2,5-dimethyl benzene to construct a new Co(II) coordination polymer.

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

Synthesis of Co(5-NO_2-ip)(bimb)]$_n$ (1): The mixtures of $CoCl_2 \cdot 6H_2O$ (0.5 mmol, 0.119 g), 5-NO_2-ip (0.5 mmol, 0.106 g), bimb (0.5 mmol, 0.119 g), 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: 43 % based on Co.). Elemental Anal. Calcd. (%) for $C_{22}H_{17}N_5O_6Co$: C, 52.19; H, 3.38; N, 13.83; found: C, 52.15; H, 3.39; N, 13.81.

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[9]. All the structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 using the program[10] SHEXL 97. 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 selected bond lengths and angles are listed in Table-1.

Crystal structure{Co(2,3-PDC) (bib)$_{1.5}$]·3H_2O}n (1): Single-crystal X-ray analysis shows that complex **1** exhibits a two-dimensional layer structure. The coordination environment of Co(II) ion is shown in Fig. 1. The fundamental unit of complex **1** consists of one Co ion, one 5-NO_2-ip and two halves of bimb ligands. Each Co(II) ion is coordinated by four carboxylate oxygen atoms and two nitrogen atoms from bimb ligands. Two such Co(II) are connected by two carboxylate groups (μ_2-η^1:η^1) of two different 5-NO_2-ip ligands to form dinculear unit with the Co···Co distance of 4.461 Å. The dinuclear units are linked by 5-NO_2-ip ligands to form one-dimensional chains (Fig. 2), which are further extended into a two-dimensional architecture, which can be simplified as a (4.4) sql topological net (Fig. 3).

TABLE-1
SELECTED BOND LENGTHS (Å)
AND ANGLES (°) FOR COMPLEXES **1**

Complex **1**			
Co(1)–O(1)	2.0979 (17)	Co(1)–O(4)^{i}	2.0230 (15)
Co(1)–N(1)	2.1157 (18)	Co(1)–O(3)^{ii}	2.0385 (14)
Co(1)–N(3)	2.1758 (18)	Co(1)–O(2)	2.3822 (16)
O(4)^{i}–Co(1)–O(3)^{ii}	101.95 (6)	O(4)^{i}–Co(1)–N(3)	87.26 (6)
O(4)^{i}–Co(1)–O(1)	160.12 (6)	O(3)^{ii}–Co(1)–N(3)	91.87 (6)
O(3)^{ii}–Co(1)–O(1)	96.38 (5)	O(1)–Co(1)–N(3)	84.50 (6)
O(4)^{i}–Co(1)–N(1)	97.36 (7)	N(1)–Co(1)–N(3)	170.18 (7)
O(3)^{ii}–Co(1)–N(1)	95.63 (6)	O(4)^{i}–Co(1)–O(2)	102.36 (6)
O(1)–Co(1)–N(1)	88.36 (7)	O(3)^{ii}–Co(1)–O(2)	154.20 (5)
O(1)–Co(1)–O(2)	58.47 (5)	N(3)–Co(1)–O(2)	80.80 (6)
N(1)–Co(1)–O(2)	89.72 (6)		

Symmetry codes: (i) x–1, y, z; (ii) –x + 2, –y, –z + 1

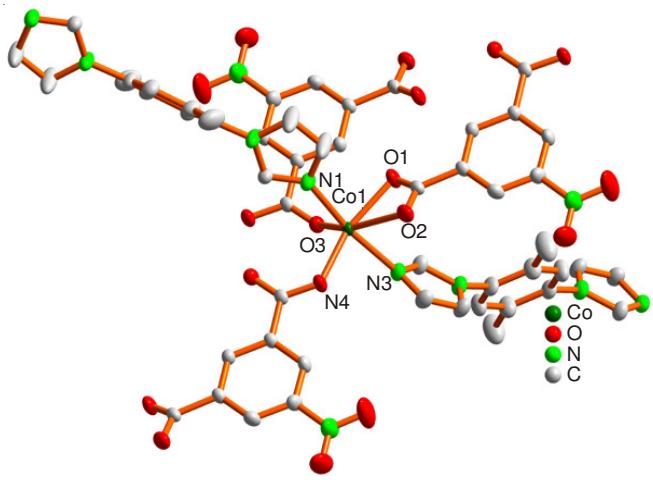

Fig. 1. Coordination environment for Co(II) ion

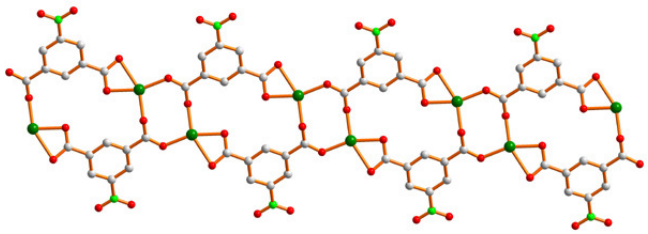

Fig. 2. One-dimensional (1D) chain formed by 5-NO_2-ip ligands and Co(II) ions

As depicted in Fig. 4 the -CH_3 from imidazole ring and carboxylate oxygen atoms form multipoint hydrogen bonds. The 2D layers aren interconnected *via* the hydrogen bonds to form a 3D supramolecular structure, with a H(8A)···O(6) # distance of 2.46 Å (symmetry code: x, -1 + y, z) and a H(8A)···O(8) # distance of 2.46 Å (symmetry code: x, -1 + y, z) (Fig. 4).

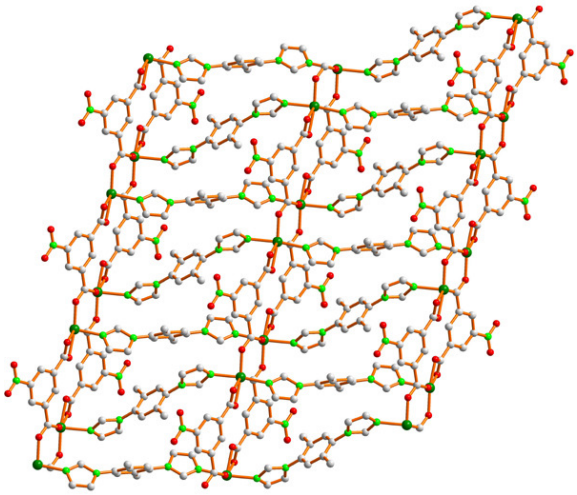

Fig. 3. Two-dimensional (2D) layer for complex **1**

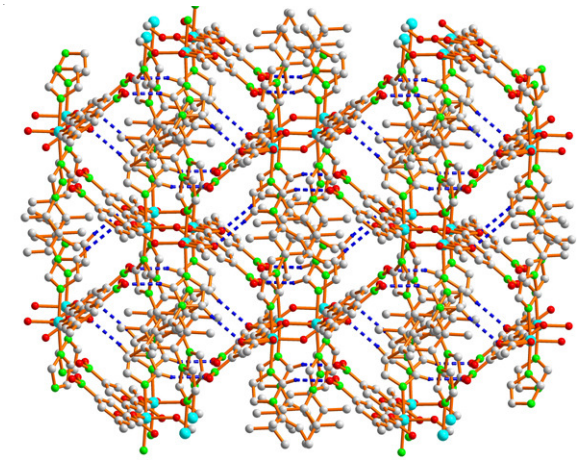

Fig. 4. Three-dimensional (3D) supramolecular structure for complex **1**

REFERENCES

1. P.J. Hagrman, D. Hagrman and J. Zubieta, *Angew. Chem. Int. Ed.*, **38**, 2638 (1999).
2. S. Kitagawa, R. Kitaura and S.-i. Noro, *Angew. Chem. Int. Ed.*, **43**, 2334 (2004).
3. M. Eddaoudi, J. Kim, N. Rosi, D. Vodak, J. Wachter, M. O'Keefe and O.M. Yaghi, *Science*, **295**, 469 (2002).
4. B. Zhao, H.-L. Gao, X.-Y. Chen, P. Cheng, W. Shi, D.-Z. Liao, S.-P. Yan and Z.-H. Jiang, *Chem. Eur. J.*, **12**, 149 (2005).
5. L.J. Charbonniere, R. Ziessel, M. Montalti, L. Prodi, N. Zaccheroni, C. Boehme and G. Wipff, *J. Am. Chem. Soc.*, **124**, 7779 (2002).
6. T. Gunnlaugsson, J.P. Leonard, K. Senechal and A.J. Harte, *J. Am. Chem. Soc.*, **125**, 12062 (2003).
7. J.-P. Zhang and X.-M. Chen, *Chem. Commun.*, 1689 (2006).
8. Y.-F. Zhou, M.-C. Hong and X.-T. Wu, *Chem. Commun.*, 135 (2006).
9. A.X.S. Bruker, SAINT Software Reference Manual, Madison, WI, (1998).
10. G.M. Sheldrick, SHELXTL NT Version 5.1. Program for Solution and Refinement of Crystal Structures, University of Göttingen, Germany (1997).