Asian Journal of Chemistry Vol. 22, No. 8 (2010), 6622-6624

NOTE

Three-Dimensional Cd(II) Coordination Compound with α-Po Topology Framework

JIANMIN SHENG
Department of Medicine, Dezhou University, Shandong-253023, P.R. China
E-mail: dzjmsheng@163.com

The pyridinecarboxylato-bridged coordination polymer of cadmium(II) with the formula [Cd(pbc)$_2$] (Hpbc = 3-pyrid-3-ylbenzoic acid) has been synthesized by the hydrothermal method and characterized by X-ray single crystal diffraction. In compound [Cd(pbc)$_2$], the ligands act as bridging ligands exhibiting rich coordination modes to link metal ions. The pbc$^-$ groups bridge Cd(II) ions to an infinite 3D framework.

Key Words: Coordination polymer, Crystal structure, Cadmium(II).

The design and synthesis of metal-organic frameworks (MOFs) are of great current interest not only because of their potential applications in gas storage, ion exchange, luminescence, non-linear optics and catalysis, but also because of their intriguing variety of architectures and topologies[1-5]. The range and variety of self-assembled inorganic structures that can be constructed relies on suitable metal-ligand interactions and the various types of polymeric structures include 1-D, 2-D and 3-D network structures[6-8]. The most common strategy used to obtain coordination polymers is to employ appropriate bridging ligands capable of binding to several metal centers through direct bond formation. The pyridine-carboxylic ligand is one of the most widely used bridging ligands for designing polynuclear complexes with novel structural features. The versatility of this group is illustrated by the variety of its coordination modes when acting as a bridge.

Elemental analysis was carried out on a Carlo Erba 1106 full-automatic trace organic elemental analyzer. FT-IR spectra were recorded with a Bruker Equinox 55 FT-IR spectrometer in dry KBr pullet in the range of 4000-400 cm^{-1}.

Preparation of compounds [Cd(pbc)$_2$]: The mixture of Cd(OAc)$_2$·2H$_2$O (0.5 mmol, 0.133 g) , Hpbc (1 mmol, 0.199 g), NaOH (1 mmol, 0.04 g) and H$_2$O (12 mL) was heated in a 20 mL stainless steel reactor with a Teflon liner at 160 ºC for 120 h and then was cooled to room temperature at 2 ºC/h. Blue black crystals were obtained. Yield: 46 % (based on Cd). Anal. calcd. (%) for $C_{24}H_{16}CdN_2O_4$: C, 56.65; H, 3.17; N, 5.51. Found (%): C, 56.70; H, 3.13; N, 5.46. IR (KBr, ν_{max}, cm^{-1}): 1617, s; 1590, s; 1440, s; 1069, m; 834, m; 714, m; 638, m.

X-Crystallography: Suitable single crystals were selected under a polarizing microscope and fixed with epoxy cement on fine glass fibers which were mounted on a Bruker Smart 1000 CCD diffractometer with a MoK$_\alpha$ radiation (λ = 0.71073 Å) at 293(2) K. The hydrogen atoms bound to carbon were located by geometrically calculations. All non-hydrogen atoms were refined by full-matrix least-squares techniques. All calculations were performed by the SHELXTL 97 program[9]. Crystal data, intensity collection and structure refinement details are summarized in Table-1. Selected interatomic distances and bond angles are given in Table-2. CCDC:714869.

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE
REFINEMENT SUMMARY FOR CADMIUM(II) COMPLEX

Empirical formula	$C_{24}H_{16}N_2O_4Cd$	Z, Calculated density (mg/m^3)	4, 1.740
Formula weight	508.80	Absorption coefficient (mm^{-1})	1.160
Crystal system space group	Monoclinic, $P2_1/n$	F(000)	1016
Unit cell dimensions (Å)	a = 8.943(5) b = 10.494(5) c = 21.968 (5)	Limiting indices	$-11 \leq h \leq 7$ $-13 \leq k \leq 13$ $-29 \leq l \leq 28$
Volume (Å^3)	1942.8(15)	Largest diff. peak and hole (e/Å^3)	0.889 and -0.563
θ range for data collection	1.97-28.17	Reflections collected/unique	4689/4384
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0233$, $wR_2 = 0.0602$	R indices (all data)	$R_1 = 0.0255$, $wR_2 = 0.0616$

TABLE-2
SELECTED BOND LENGTHS (Å) AND ANGLES (°) FOR COMPLEXE

Cd(1)-O(1)	2.247(14)	Cd(1)-O(2)$^{\#1}$	2.315(16)
Cd(1)-O(3)	2.563(18)	Cd(1)-O(4)	2.309(16)
Cd(1)-N(1)$^{\#2}$	2.318(16)	Cd(1)-N(2)$^{\#3}$	2.349(17)
O(1)-Cd(1)-N(2)$^{\#3}$	86.85(6)	O(4)-Cd(1)-N(2)$^{\#3}$	85.34(7)
O(2)$^{\#1}$-Cd(1)-N(2)$^{\#3}$	80.23(6)	N(1)$^{\#2}$-Cd(1)-N(2)$^{\#3}$	161.86(5)
O(1)-Cd(1)-O(3)	143.94(5)	O(4)-Cd(1)-O(3)	53.54(5)
O(2)$^{\#1}$-Cd(1)-O(3)	108.01(5)	N(1)$^{\#2}$-Cd(1)-O(3)	86.83(5)

Structure description: The complex crystallizes in monoclinic system space group $P2_1/c$, each Cd(II) ion is coordinated by four O atoms [Cd-O = 2.247-2.563 Å] and two N atoms [Cd(1)-N(1) = 2.318(2) Å and Cd(1) -N (2) = 2.349(2) Å] which come from five different pbc$^-$ ligands to form a octahedral geometry. The Cd-O and Cd-N bond lengths agree well with published results for related complexes and bond angles of O(N)-Cd-O(N) are from 53.54-161.86°. Four O atoms formed the equatorial plane and two N occupy the two axial sites (Fig. 1). The ligands have two coordination modes. One acts as a diconnector to link two Cd(II) centers (μ_2-N, O, O) which is shown that O_{COO^-} chelates with Cd bidentately and the other corresponds to a triconnector that link three Cd(II) centers (μ_3-N, O, O) which is shown that O_{COO^-} adopts a *bis*-monodentate *syn*-antibridging mode to construct a binuclear octahedral $[Cd_2C_2O_4]$ SBU, with non-bonding Cd···Cd distances of 4.553 Å. The SBUs are further interconnected through different pbc$^-$ ligands, thereby generating a 3D extended network which is composed of six-connected nodes (Fig. 2).

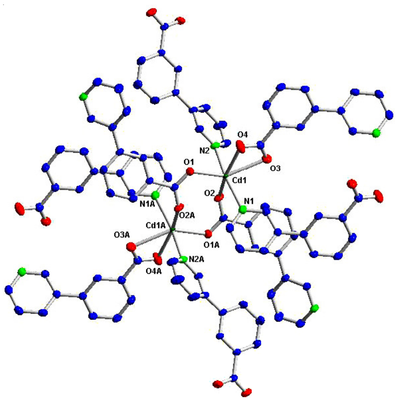

Fig. 1. A perspective view of dinuclear Cd(II) crystal structure

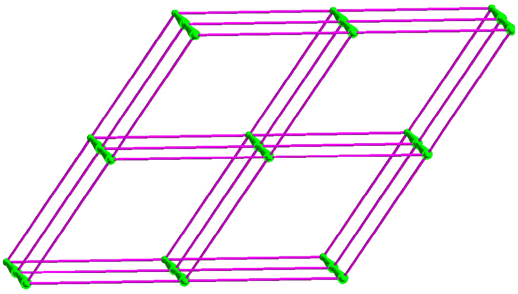

Fig. 2. Topological representation of the structure of compound leading to a 41263 topology

REFERENCES

1. G.F. Swiegers and T.J. Malefetse, *Chem. Rev*., **100**, 3483 (2000).
2. J. Yang, J.F. Ma, Y.Y. Liu and S.R. Batten, *Cryst. Eng. Commun*., **11**, 151 (2009).
3. B. Moulton and M.J. Zaworotko, *Chem. Rev*., **101**, 1629 (2001).
4. Q.R. Fang, G.S. Zhu, M. Xue, Z.P. Wang, J.Y. Sun and S.L. Qiu, *Cryst. Growth Des*., **8**, 319 (2008).
5. J. Pang, E.J.P. Marcotte, C. Seward, R.S. Brown and S.N. Wang, *Angew. Chem. Int. Ed*., **40**, 4042 (2001).
6. C. Wu, A. Hu, L. Zhang and W. Lin, *J. Am. Chem. Soc*., **127**, 8940 (2005).
7. S.R. Batten and R. Robson, *Angew. Chem. Int. Ed*., **37**, 1460 (1998).
8. X.H. Bu, M.L. Tong, H.C. Chang, S. Kitagawa and S.R. Batten, *Angew. Chem. Int. Ed*., **43**, 192 (2004).
9. G.M. Sheldrick, Shelxtl NT Version 5.1. Program for Solution and Refinement of Crystal Structures, University of Göttingen, Germany (1997).

(*Received*: 6 February 2010; *Accepted*: 22 May 2010) AJC-8742