

NOTE

Hydrothermal Synthesis and Crystal Structure of Cd(II) Coordination Polymer

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One new cadmium compound $\{[\text{Cd}(\text{L})] \cdot (\text{bip})\}_n \cdot (1)$ [H_2L = 5-hydroxyisophthalic acid and bip = 1,5-bis(2-methyl-imidazol-1-yl) pentane] has been successfully synthesized. Compound shows a two-dimensional frameworks. The bip ligands are filled the hole of 2D layer.

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

The rational design and construction of novel functional metal-organic frameworks is currently of great interest for the past decade due to their diverse topologies and potential applications in gas storage, magnetism, catalysis and luminescence¹⁻⁴. Although the rapid progress in metal-organic frameworks has been made, it is also a great challenge to rationally prepare and control the structures and composition of target products in crystal engineering because of the difficult prediction of either the composition or the structure of the reaction product.

All reagent and solvents employed were commercially available and used as received without further purification.

Preparation of compound: A mixture of 5-hydroxyisophthalic acid (1 mmol), $\text{Cd}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ (1 mmol), 1,5-bis(2-methyl-imidazol-1-yl) pentane (1 mmol) and distilled water (15 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 160 °C for 96 h, followed by slow cooling to room temperature. Yellow crystals of the compound formed.

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 $\text{MoK}\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$) 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 program⁵. The crystallographic data and experimental details of structural analyses for coordination polymers are summarized in Table-1. Selected bond and angle parameters are listed in Table-2. CCDC: 862871. The molecular structure of Cd(II) coordination polymer at 30 % probability displacement ellipsoids is given in Fig. 1.

Structure description: Single-crystal X-ray analyses revealed that the compounds **1** crystallizes in *orthorhombic* the Pccn group. The Cd1 atom is six-coordination with a distorted octahedral coordination geometry define by six oxygen atom. The Cd-O lengths are ranging from 2.2416(14) to 2.5038(14) Å. In compound, the carboxylate groups adopt two coordinated modes: *bis*-chelating and monodentate modes, which lead to form a two-dimensional layer structure and 1,5-bis(2-methyl-imidazol-1-yl) pentane ligands are filled in the hole (Fig. 2).

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

Empirical formula	$\text{C}_{38}\text{H}_{30}\text{N}_4\text{O}_8\text{Cd}_2$	Z, Calculated density (mg/m^3)	1,1.629
Formula weight	2827.88	Absorption coefficient (mm^{-1})	0.824
Crystal system space group	Monoclinic, Cc	F(000)	1440
Unit cell dimensions	a = 14.3898 (6) Å b = 14.5914 (6) Å c = 13.8173 (6) Å	Limiting indices	-17 ≤ h ≤ 18 -18 ≤ k ≤ 17 -17 ≤ l ≤ 11
Volume (Å ³)	2881.8 (2)	Largest diff. peak and hole ($e/\text{Å}^3$)	0.595 and -0.626
θ Range for data collection	1.99-27.50	Goodness-of-fit on F ²	1.057
Final R indices [I > 2σ(I)]	R ₁ = 0.0253 wR ₂ = 0.0669	R indices (all data)	R ₁ = 0.0269, wR ₂ = 0.0680

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

Cd1-O4 ⁱ	2.2416 (14)	Cd1-O1 ⁱⁱⁱ	2.3117 (14)
Cd1-O4 ⁱⁱ	2.2416 (14)	Cd1-O2 ⁱⁱⁱ	2.5038 (14)
Cd1-O1a	2.3117 (14)	Cd1-O2a	2.5038 (14)
O4 ⁱ -Cd1-O4 ⁱⁱ	102.69 (8)	O4 ⁱⁱ -Cd1-O1 ⁱⁱⁱ	127.85 (5)
O4 ⁱ -Cd1-O1a	127.85 (5)	O1a-Cd1-O1 ⁱⁱⁱ	125.85 (7)
O4 ⁱⁱ -Cd1-O1a	87.42 (5)	O4 ⁱ -Cd1-O2 ⁱⁱⁱ	139.16 (5)
O4 ⁱ -Cd1-O1 ⁱⁱⁱ	87.42 (5)	O4 ⁱⁱ -Cd1-O2 ⁱⁱⁱ	92.44 (5)

Symmetry codes: (i) $-x+1/2, y+1/2, -z+1/2$; (ii) $x-1/2, y+1/2, z$; (iii) $-x, y, -z+1/2$

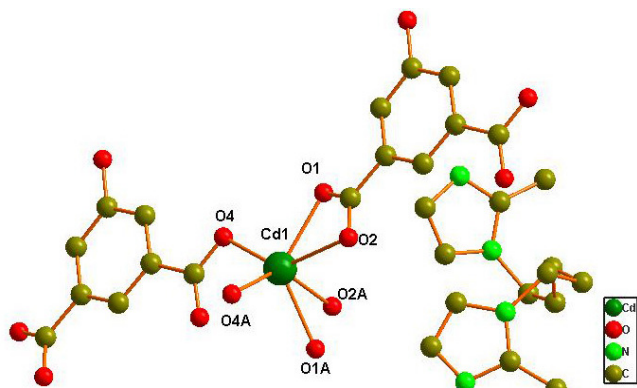


Fig. 1. Molecular structure of the title compound at 30 % probability displacement ellipsoids

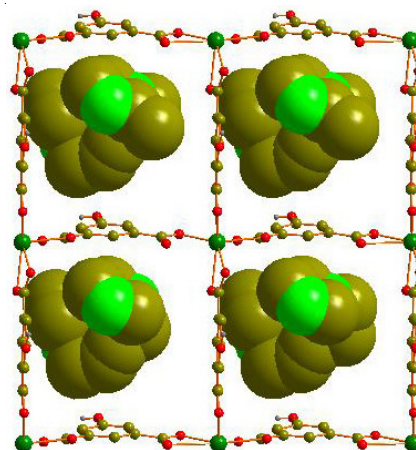


Fig. 2. 2D layer structure of compound and the bip ligands filled in the hole

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