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NOTE

Synthesis and Crystal Structure of a New Cd(II) Coordination Polymer Based on Phthalic Acid and *bis*(imidazole)

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One new coordination polymer $[Cd_2(PAA)_2(bib)]_n$ (H_2PAA= phthalic acid and bib= 4,4'-*bis* (2-methylimidazol-1-ylmethyl)biphenyl) has been synthesized by the hydrothermal method and characterized by X-ray single crystal diffraction. In compound $[Cd_2(PAA)_2(bib)]_n$, the phthalic acid ligand acts as bridging ligands exhibiting two coordination modes to link metal ions: *bis*-monodentate and bidentate chelating/bridging modes. The carboxylic groups bridge Cd(II) ions to an infinite 1D framework. The 4,4'-*bis* (2-methylimidazol-1-ylmethyl)biphenyl) ligands coordinate to two Cd(II) centers to give rise to a two-dimensional net.

Key Words: Coordination polymer, Crystal structure.

Crystal engineering of supramolecular metal-organic frameworks has recently attracted considerable interest due to their potential applications as functional materials in molecular magnetism, catalysis, gas sorption and luminescence[1-3]. The construction of metal-organic frameworks mainly depends on the nature of the organic and metal ions, which is a key strategy for the building metal-organic frameworks (MOFs). Therefore, a considerable number of transition metal compounds using carboxylate ligands have been reported during the last decade because the carboxylate ligands can adopt a variety of coordination modes and result in diverse multidimensional frameworks[4-6]. Most studies have been focused on the rigid carboxylate ligands[7,8]. In this paper, carboxylate ligand (phthalic acid) and 4,4'-*bis*(2-methylimidazol-1-ylmethyl)-biphenyl) (bib) to construct a new Cd(II) coordination polymer are reported.

Preparation of compounds $[Cd_2(PAA)_2(bib)]_n$: A mixture of phthalic acid (H_2PAA)(1 mmol), $Cd(OAc)_2{\cdot}2H_2O$ (1 mmol), 4,4'-*bis* (2-methylimidazol-1-ylmethyl)biphenyl) (1 mmol), NaOH (2 mmol) and distilled water (15 mL) was heated to 160 ºC for 96 h in a 25 mL stainless steel reactor with a Teflon liner, followed by slow cooling to room temperature. Colourless crystals for compound $[Cd_2(PAA)_2(bib)]_n$ were obtained in 57 % yield (based on Cd).

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_α radiation ($\lambda = 0.71073$ 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.

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

Empirical formula	$C_{38}H_{30}N_4O_8Cd_2$	Z, Calculated density (mg/m^3)	1,1.734
Formula weight	895.46	Absorption coefficient(mm^{-1})	1.300
Crystal system space group	Triclinic, P-1	F(000)	446
Unit cell dimensions	a =7.435(4) Å b =10.003(6) Å c =12.4318 (7) Å	Limiting indices	-7 ≤ h ≤ 9 -12 ≤ k ≤ 12 -15 ≤ l ≤ 15
Volume (Å^3)	887.76(8)	Largest diff. peak and hole (e/Å^3)	0.334 and-0.359
θ range for data collection	1.65-26.25	Reflections collected/unique	4902/3403
Final R indices [I>2σ (I)]	R_1=0.0224, wR_2=0.0575	R indices (all data)	R_1 = 0.0244, wR_2 = 0.0592

Structure description: The local coordination geometry of polymer $[Cd_2(PAA)_2(bib)]_n$ with atomic numbering scheme in depicted in Fig. 1. It is shown that the asymmetry unit of

the molecule consists of one Cd(II) ion, four coordinated phthalic acid and one coordinated 4,4'-*bis* (2-methylimidazol-1-ylmethyl)biphenyl). The Cd(II) ion is surrounded by five oxygen atoms and one nitrogen atom. The bond lengths and bond angles are given in Table-1 in compound 1, the phthalic acid ligand adopts bis-mondentate and bisdentate chelating/ bridging modes, which lead to form a one-dimensional chain (Fig. 2). The adjacent chains are interacted into two-dimensional (4,4) layer by 4,4'-*bis* (2-methylimidazol-1-ylmethyl)biphenyl) ligands (Fig. 3).

TABLE-2
SELECTED BOND LENGTHS(Å) AND ANGLES (º) FOR Ni(II) COMPLEX

Cd(1)-N(1)	2.1992(18)	Cd(1)-O(2)^{ii}	2.3021(17)
Cd(1)-O(1)	2.2022(17)	Cd(1)-O(3A)^{ii}	2.4144(16)
Cd(1)-O(3)^{i}	2.2294(16)		
N(1)-Cd1-O(1)	121.74(8)	O(1)-Cd(1)-O(2)^{ii}	94.56(7)
N(1)-Cd(1)-O(3)^{i}	132.35(7)	O(3)^{i}-Cd(1)-O(2)^{ii}	114.44(6)
O(1)-Cd(1)-O(3)^{i}	85.24(6)	N(1)-Cd(1)-O(3A)^{ii}	87.87(6)
N(1)-Cd(1)-O(2)^{ii}	102.53(6)	O(1)-Cd(1)-O(3A)^{ii}	150.36(8)

Symmetry codes: (i) *x*-1, *y*, *z*; (ii) -*x*+1, -*y*, -*z*+1

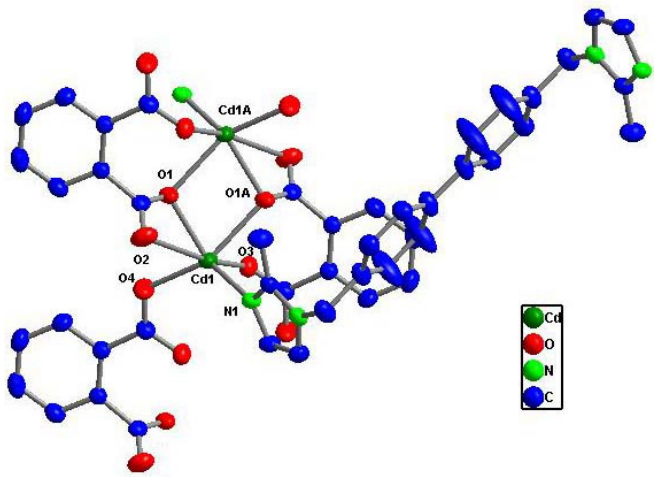

Fig. 1. Molecular structure of the title compound [$Cd_2(PAA)_2$(bib)]

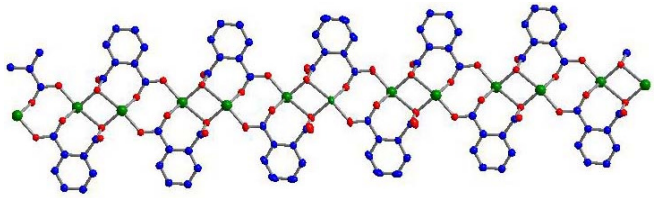

Fig. 2. One dimensional zigzag chain formed *via* phthalic ligands

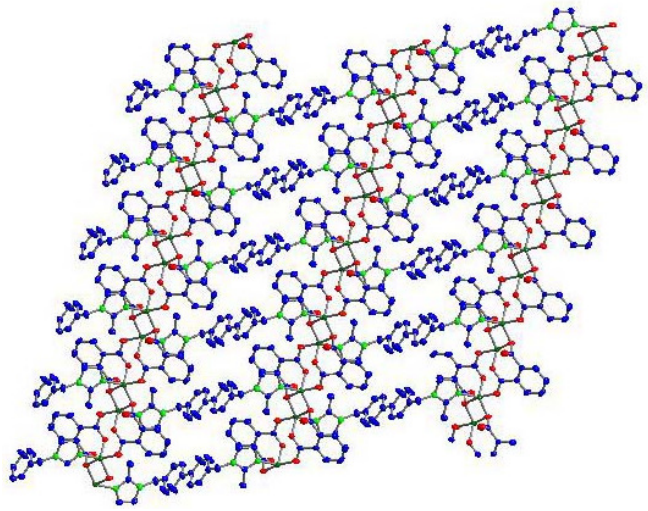

Fig. 3. Two dimensional layer net for the compound [$Cd_2(PAA)_2$(bib)]

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