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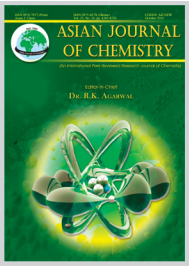

NOTE

Synthesis and Crystal Structure of a Two-Dimensional Zn(II) Coordination Polymer

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A new coordination polymer $[Zn_2(PAA)_2(bib)]_n$ (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 $[Zn_2(PAA)_2(bib)]_n$, the phthalic acid acts as bridging ligands exhibiting two coordination modes to link metal ions: *bis*-monodentate and monoatomic bridging modes. The carboxylic groups bridge Zn(II) ions to an infinite one-dimensional framework. 4,4'-*Bis*(2-methylimidazol-1-ylmethyl)biphenyl) ligands coordinate to two Zn(II) centers to give rise to a two-dimensional net.

Key Words: Coordination polymer, Crystal structure.

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, nonlinear 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 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.

Physical measurements: 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 $[Zn_2(PAA)_2(bib)]_n$: A mixture of phthalic acid (H_2PAA) (0.166 g, 1 mmol), $Zn(OAc)_2{\cdot}2H_2O$ (0.216 g, 1 mmol), 4,4'-*bis*(2-methylimidazol-1-ylmethyl)biphenyl) (bib) (0.342 g, 1 mmol), NaOH (0.08 g, 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 $[Zn_2(PAA)_2(bib)]_n$ were obtained in 44 % yield (based on Zn). Elemental Anal. calcd. (%) for $C_{38}H_{30}N_4O_8Zn_2$: C,62.01; H, 4.11; N, 7.61. Found: C, 61.94; H, 4.15; N, 7.66. IR: 1627 s, 1475 s, 1366 m, 1257 m, 1115 m, 964 w, 817 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_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 CCDC: 825948.

Structure description: The local coordination geometry of polymer $[Zn_2(PAA)_2(bib)]_n$ with atomic numbering scheme is depicted in Fig. 1. It is shown that the asymmetry unit of the molecule consists of one zinc(II) ion, four coordinated 1,2-PAA and one coordinated bib ligand. The Zn(II) ion is surrounded by four oxygens and one nitrogen atom. The bond lengths and bond angles are given in Table-1 and the bond lengths of Zn-O and Zn-O are in the reliable ranges. In compound **1**, the 1,2-PAA ligand adopts *bis*-mondentate and monoatomic bridging modes, which lead to form a one-dimensional chain (Fig. 2.). The adjacent chains are interacted into two-dimensional (4,4) layer by bib ligands (Fig. 3).

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

Empirical formula	$C_{38}H_{30}Zn_2N_4O_8$	Z, Calculated density (mg/m^3)	1,1.584
Formula weight	801.40	Absorption coefficient (mm^{-1})	1.489
Crystal system space group	Triclinic, P-1	F (000)	410
Unit cell dimensions	a = 7.047(8) Å b = 10.0041(11) Å c = 12.2534 (13) Å	Limiting indices	-8 ≤ h ≤ 8 -8 ≤ k ≤ 11 -14 ≤ l ≤ 14
Volume (Å^3)	840.35(16)	Largest diff. peak and hole (e/Å^3)	0.334 and- 0.359
θ range for data collection	1.67-24.99	Reflections collected / unique	4337/2911
Final R indices [I > 2 sigma(I)]	R_1 = 0.0267, wR_2 = 0.0747	R indices (all data)	R_1 = 0.0284, wR_2 = 0.0760

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

Bond	(º)
Zn(1)—O(3A)^i	1.9591(14)
Zn(1)—N(1)	1.9907(17)
Zn(1)—O(1)	2.0193(15)
O(3A)^i—Zn(1)—N(1)	129.92(7)
O(3A)^i—Zn(1)—O(1)	115.85(6)
N(1)—Zn(1)—O(1)	106.92(7)
O(3)^i—Zn(1)—O(2)^{ii}	91.99(6)
Zn(1)—O(2)^{ii}	2.0323(16)
Zn(1)—O(3)	2.4476(15)
N(1)—Zn(1)—O(2)^{ii}	109.80(7)
O(1)—Zn(1)—O(2)^{ii}	94.64(6)
O(3A)^i—Zn(1)—O(3)	74.30(6)
N(1)—Zn(1)—O(3)	90.42(6)

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

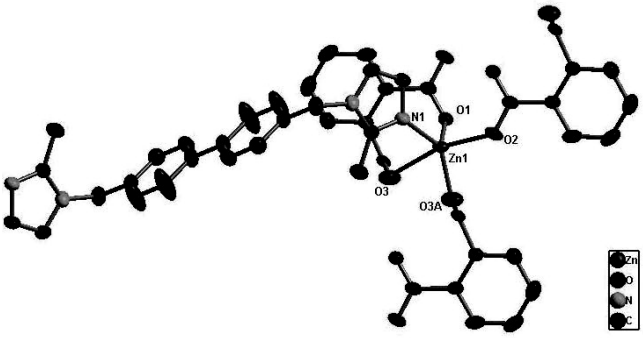

Fig. 1. Molecular structure of the title compound [$Zn_2(PAA)_2$(bib)] with the atom labeling scheme. Displacement ellipsoids are drawn at the 50 % probalility level

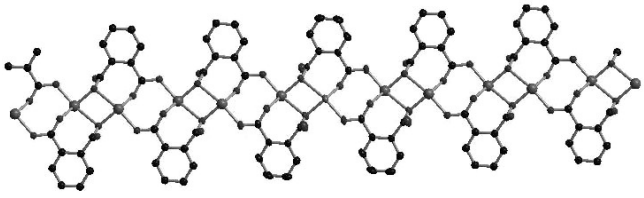

Fig. 2. One dimensional zigzag chain formed *via* phthalic ligands

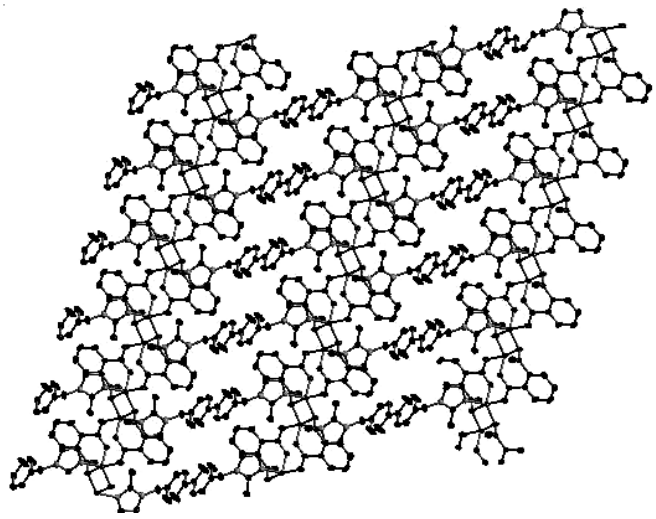

Fig. 3. Two dimensional layer net for the compound [$Zn_2(PAA)_2$(bib)]

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