NOTE

Hydrothermal Synthesis and Crystal Structure of A New 1D Chain Mn(II) Coordination Polymer

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One new Mn(II) compound $\{[\text{Mn}(\text{L})(\text{H}_2\text{O})]\cdot 2\text{H}_2\text{O}\}_n$ (H_2L = 5-methylisophthalic acid) has been successfully synthesized. Compound shows a one-dimensional chain. The carboxylate group in compound adopt two coordination modes viz., *bis*-chelating and *bis*-monodentate modes.

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

The rational design and construction of novel functional metal-organic frameworks (MOFs) 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-methylisophthalic acid (1 mmol), $\text{Mn}(\text{OAc})_2\cdot 2\text{H}_2\text{O}$ (1 mmol), *bis*(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 (Fig. 1).

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

Fig. 1. Molecular structure of $\{[\text{Mn}(\text{L})(\text{H}_2\text{O})]\cdot 2\text{H}_2\text{O}\}_n$ at 30 % probability displacement ellipsoids

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 program⁵. The

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

Empirical formula	$\text{C}_9\text{H}_{11}\text{O}_7\text{Mn}$	Z, Calculated density (mg/m^3)	2, 1.839
Formula weight	286.12	Absorption coefficient (mm^{-1})	1.299
Crystal system space group	Triclinic, P-1	$F_{(000)}$	292
Unit cell dimensions	$a = 7.752(5)$ Å, $b = 8.606(5)$ Å, $c = 8.702(5)$ Å	Limiting indices	$-6 \leq h \leq 9$, $-6 \leq k \leq 10$, $-10 \leq l \leq 10$
Volume ($\text{\AA}^3$)	516.8(2)	Largest diff. peak and hole ($\text{e}/\text{\AA}^3$)	0.841 and -0.491
θ range for data collection	2.41-25.00	Goodness-of-fit on F^2	1.090
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0341$ $wR_2 = 0.1060$	R indices (all data)	$R_1 = 0.0348$, $wR_2 = 0.1073$

Fig. 2

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.

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) $-x, y, -z+1/2$.

Structure description: In $\{[\text{Mn}(\text{L})(\text{H}_2\text{O})]\cdot 2\text{H}_2\text{O}\}_n$, Mn(II) atom is coordinated to five oxygen atoms from three L ligands and one oxygen atom from coordination water molecule. In compound the carboxylate groups adopt two coordinated modes: *bis*-chelating and *bis*-monodentate modes, which further connect the Mn atoms to form a one-dimensional chains (Fig. 2).

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