Asian Journal of Chemistry; Vol. 25, No. 14 (2013), 8233-8234

ASIAN JOURNAL OF CHEMISTRY

http://dx.doi.org/10.14233/ajchem.2013.15085

NOTE

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

BO SHEN and XIANJIANG LI*

Shandong Shengli Co. Ltd., Jinan 250101, Shandong Province, P.R. China

*Corresponding author: E-mail: whyull@yeah.net

(*Received*: 3 January 2013; *Accepted*: 12 August 2013) AJC-13919

One new Mn(II) compound $\{[Mn(L)(H_2O)]\cdot 2H_2O\}_n$ (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 luminescence[1-4]. 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), $Mn(OAc)_2\cdot 2H_2O$ (1 mmol), *bis*(1 mmol) and distilled water (15 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 160 ºC 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

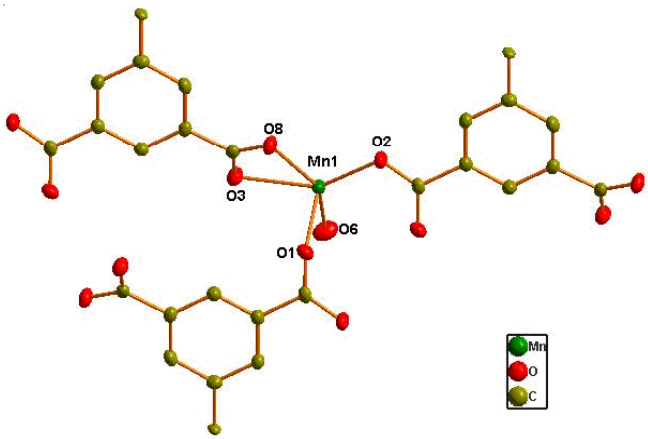

Fig. 1. Molecular structure of $\{[Mn(L)(H_2O)]\cdot 2H_2O\}_n$ at 30 % probability displacement ellipsoids

1000 CCD diffractometer with a MoK_α 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[5]. The

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

Empirical formula	$C_9H_{11}O_7Mn$	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	$-6 \le h \le 9$, $-6 \le k \le 10$, $-10 \le l \le 10$
Volume (Å^3)	516.8(2)	Largest diff. peak and hole (e/Å^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

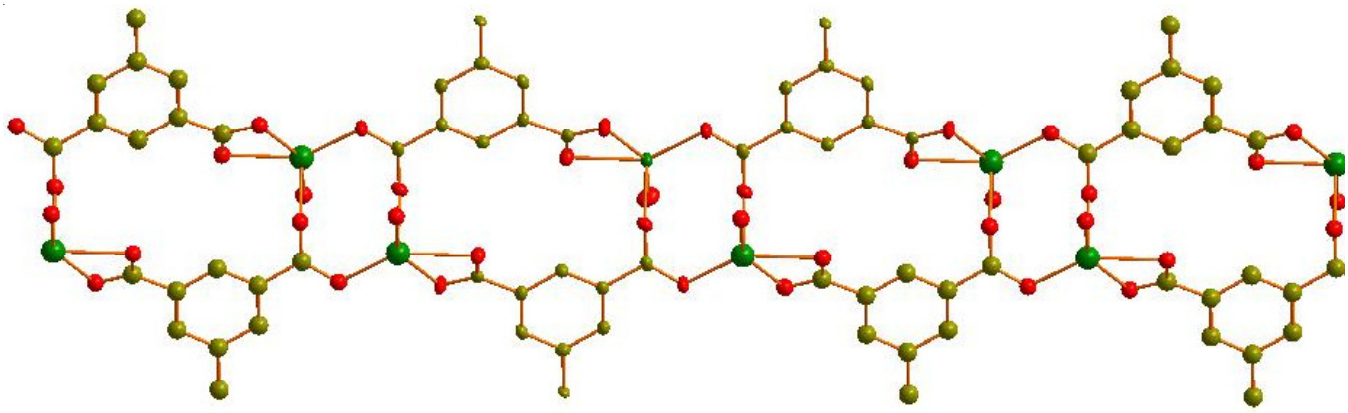

Fig. 2

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 $\{[Mn(L)(H_2O)]\cdot 2H_2O\}_n$, 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).

REFERENCES

1. M.D. Ward, *Cood. Chem. Rev*. **251**, 1663 (2007).
2. Q. Chen, J.B. Lin, W.Xue, M.H. Zeng and X.M. Chen, *Inorg. Chem*., **50**, 2321 (2011).
3. R.Q. Zou, R.Q. Zhong, M. Du, D.S. Pandey and Q. Xu, *Cryst. Growth Des*., **8**, 452 (2008).
4. Y. Wu, B.-H. Yang, M. Li, C.-A. Tian and L.-G. Qiu, *Asian J. Chem.,* **24**, 4044 (2012).
5. G.M. Sheldrick, SHELXTL97, Program for the Refinement of Crystal Structure, University of Gottingen, Germany (1997).