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NOTE

A New Zinc(II) Coordination Polymer with Two-Dimensional *sql* Topology Based on Asymmetrically Tricarboxylate and Nitrogen-Containing Ligand

LIPING XU

Department of Chemistry Engineering, Zibo Vocational Institute, Shandong 255314, P.R. China

Corresponding author: E-mail: dzjmsheng@163.com

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A new coordination polymer {[Zn(Hbtc)(bpmp)$_{0.5}$]·H_2O_n} (**1**) [H_3btc=biphenyl-3,4',5- tricarboxylate and bpmp=1,4-*bis*(4-pyridylmethyl)-piperazine] has been obtained under hydrothermal conditions. Complex {[Zn(Hbtc) (bpmp)$_{0.5}$]·H_2O_n} (**1**), is triclinic, space group P-1 with a = 8.189 (5) Å, b = 8.919 (5) Å, c = 15.998 (5) Å, β = 90.622 (5)°V =1050.9 (9) Å^3, Z = 2, M_r = 501.78, D_c = 1.586g/cm^3, F(000) = 516 and μ = 1.22 mm^{-1}. The final refinement gave R = 0.0483 and wR = 0.1187 for 2390 reflections with I > 2σ (I). X-ray diffraction analysis reveals that complex **1** shows a two-dimensional (4,4) *sql* layer.

Keywords: Zinc(II), Coordination polymer, Topology.

In recent years , the study of design and construction of coordination polymers *via* careful selection of metal ions and organic ligands has attracted much attention due to their structural diversity and the potential applications in adsorption, magnetism, separation[1-4], catalysis, optics, *etc*. Generally, structures and properties of coordination polymers are affected by many factors, mainly including the organic ligands with suitable functional groups and molecular skeletons, nature of the metal ions and reaction conditions such as temperature, pH value, solvent, *etc*[5,6].

In this paper, we used the asymmetrically tricarboxylate and pyridyl-containing ligands to construct a new Zn(II) coordination polymer.

All the reagents and solvents employed were commercially available and used without further purification. Elemental analysis was carried out on a Vario ELIII elemental analyzer. or. FT-IR spectra were recorded with a Bruker Equinox 55 FT-IR spectrometer as a dry KBr pellet in the 4000-400 cm^{-1} range.

Preparation of {[Zn(Hbtc)(bpmp)$_{0.5}$]·H_2O_n} (1): The starting materials were biphenyl-3,4',5- tricarboxylate (H_3btc) (0.143 g, 0.5 mmol), 1,4-*bis*(4-pyridylmethy) piperazine (bmpm) (0.105 g, 0.5 mmol), (0.145 g, 0.5 mmol), NaOH (0.04 g, 1 mmol) and H_2O (15 mL). Colorless crystals of complex **1** were collected in 45 % yield based on Zn. Anal. Calcd. for: C, 50.27; H, 2.61; N, 5.58. Found: C, 50.24; H, 2.63; N, 5.61. IR (KBr, ν_{max}, cm^{-1}): 1620 (s), 1530 (s), 1503 (s), 1437 (s), 1347 (m), 1263 (m), 1217 (m), 1179 (w), 1047 (m), 955 (w), 836 (m), 797 (m).

X-ray crystallography: Single crystal X-ray diffraction analyses of complex **1** was carried out on a Bruker SMART APEXII CCD diffractometer equipped with a graphite monochromated MoK_α radiation (λ = 0.71073 Å) by using a ω-scan mode. Empirical absorption correction was applied using the SADABS programs[7]. All the structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 using the program SHEXL 97[8]. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were located by geometrically calculations and their positions and thermal parameters were fixed during the structure refinement.

Single-crystal X-ray diffraction analysis reveals that the asymmetric unit of complex **1** consists of one crystallographically independent Zn(II) ion, one Hbtc^{2-}, half of bmpm ligand and one lattice water molecule. The center Zn(II) atom is in a tetrahedral coordination environment having three Zn-O bond with carboxylate groups[1.939(3)-2.113(3)Å] (Fig. 1) and one Zn-N bond from pyridyl ligand [Zn(1)-N(1)= 2.048 (4) Å]. The Hbtc^{2-} ligands adopt μ_1-η^1:η^0 and μ_2-η^1:η^1 coordination mode. The μ_2-η^1:η^1 carboxylate groups connected Zn(II) ions to form a dinuclear Zn(II) unit with the Zn-Zn distance of 4.266 Å. The dinuclear Zn(II) units connect by Hbtc^{2-} ligand to form a one-dimensional chains (Fig. 2). The 1D chains are further connected by bmpm ligands to construct two-dimensional layer structure (Fig. 3).

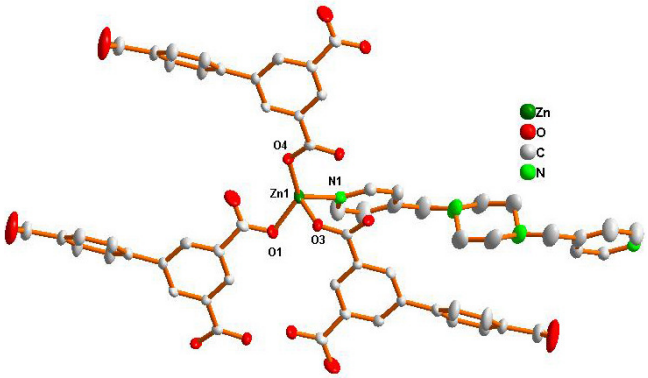

Fig. 1. A local coordination geometry of central Zn(II) atom

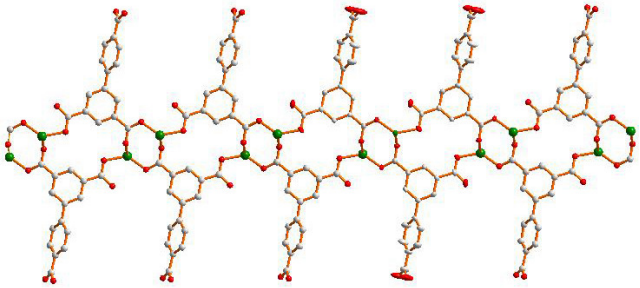

Fig. 2. 1D chain constructed by $Hbtc^{2-}$ and Zn(II) ions

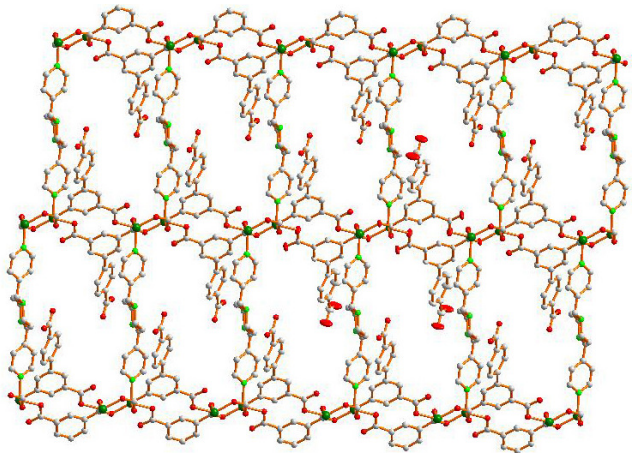

Fig. 3. 2D layer structure for complex **1**

REFERENCES

1. M. O'Keeffe and O.M. Yaghi, *Chem. Rev*., **112**, 675 (2012).
2. G.P. Yang, L. Hou, X.J. Luan, B. Wu and Y.Y. Wang, *Chem. Soc. Rev*., **41**, 6992 (2012).
3. S.L. Cai, S.R. Zheng, J. Fan, J.B. Tan, T.T. Xiao and W.G.J. Zhang, *Solid State Chem*., **184**, 3172 (2011).
4. J. Xu, Z. Su, M.S. Chen, S.S. Chen and W.Y. Sun, *Inorg. Chim. Acta*, **362**, 4002 (2009).
5. S.L. Huang, L. Zhang, Y.J. Lin and G.X. Jin, *Cryst. Eng. Comm*., **15**, 78 (2012).
6. Z.L. Chen, X.L. Liu, C.B. Zhang, Z. Zhang and F.P. Liang, *Dalton Trans*., **40**, 1911 (2011).
11. SAINT Software Reference Manual; Bruker AXS: Madison, WI (1998).
12. G.M. Sheldrick, SHELXTL NT, version 5.1; Program for Solution and Refinement of Crystal Structures, University of Göttingen, Germany (1997).