Asian Journal of Chemistry; Vol. 27, No. 2 (2015), 767-768

ASIAN JOURNAL OF CHEMISTRY

http://dx.doi.org/10.14233/ajchem.2015.16912

NOTE

Hydrothermal Synthesis and Crystal Structure of *bis*-(1,10-Phenanthroline) 3-Hydroxy-thiophene-2,5-dicarboxylate Cadmium(II) Tetrahydrate [$Cd(C_{30}H_{20}N_4SO_6)_4(H_2O)NO_3$]

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Received: 23 December 2013; *Accepted*: 20 February 2014; *Published online*: 10 January 2015; AJC-16664

One new cadmium compound using $Cd(OAc)_2.2H_2O$, 3-Hydroxy-thiophene-2,5- dicarboxylic acid and bpp ([1,10] Phenanthroline) has been successfully synthesized. Compound shows a one-dimensional framework. The 1D supramolecular structure is formed *via* hydrogen bonding connection.

Keywords: Coordination polymer, Crystal structure, Cadmium(II).

Metal organic frameworks (MOFs) have received much attention in the field of crystal engineering and supramolecular chemistry because of their diverse structures and promising applications in functional materials such as luminescent materials, gas adsorption and magnetism[1-4]. Hydrogen bonds are well suited for the design of polymeric arrangement and crystal engineering because of their important directional interactions and because they can interlink 1-D, or 3-D structures into higher-dimensionality systems[5,6].

All the reagent and solvents employed were commercially available and used as received without further purification.

General procedure: A mixture of $Cd(OAc)_2.2H_2O$ (0.1 mmol, 0.0267 g), 3-Hydroxy-thiophene-2,5- dicarboxylic acid (0.25 mmol, 0.043 g), {[1,10]phenanthroline (0.25 mmol, 0.050 g)} and distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 403 K for 5 days, followed by slow cooling to room temperature. Colourless crystals of the compound formed.

Detection method: Diffraction intensity data of the single crystal of the five compounds were collected 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. All the structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 using the program SHEXL 97[7]. 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. The 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. CCDC: 960958.

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

Empirical formula	$C_{30}H_{28}O_{13}N_5SCd$
Formula weight	811.03
Crystal system space group	Monoclinic, P2(1) /n
Unit cell dimensions	a = 14.112(7) Å; b = 15.866(8) Å c = 14.704(7) Å
Volume (Å^3)	3284(3)
θ range for data collection	2.44 -25.50
Final R indices [I>2σ(I)]	R_1 = 0.0537; wR_2 = 0.1292
Z, Calculated density (mg/m^3)	4, 1.641
Absorption coefficient (mm^{-1})	0.803
F(000)	1644
Limiting indices	$-14 \le h \le 17$; $-19 \le k \le 17$ $-17 \le l \le 6$
Largest diff. peak and hole (e/Å^3)	0.753 and-0.675
Goodness-of-fit on F^2	1.015
R indices (all data)	R_1 = 0.0917; wR_2 = 0.1536

X-ray diffraction analysis revealed that the fundamental building unit consists of 3-hydroxy-thiophene-2,5-dicarboxylate and bpp (bpp = [1,10]phenanthroline) as bridging ligands to construct a new coordination polymer. The asymmetric unit of the title structure contains one Cd (II) ion, one 3-hydroxy-

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

Cd(1)-O(3)	2.248(4)	Cd(1)-N(5)	2.331(6)
Cd(1)-O(1)	2.315(4)	Cd(1)-N(2)	2.386(5)
Cd(1)-N(4)	2.327(6)	Cd(1)-N(3)	2.398(5)
N(4)-Cd(1)-N(2)	104.4(2)	O(1)-Cd(1)-N(2)	90.35(17)
N(5)-Cd(1)-N(2)	159.26(16)	O(3)-Cd(1)-N(2)	86.34(15)
O(3)-Cd(1)-N(3)	155.54(15)	N(4)-Cd(1)-N(5)	71.9(2)
O(1)-Cd(1)-N(3)	83.48(16)	O(1)-Cd(1)-N(5)	89.0(2)
O(8)-N(1)-O(9)	154(5)	O(3)-Cd(1)-N(5)	114.40(16)
N(4)-Cd(1)-N(3)	87.65(17)	O(1)-Cd(1)-N(4)	159.0(2)
N(5)-Cd(1)-N(3)	89.71(17)	O(3)-Cd(1)-N(4)	103.24(18)
N(2)-Cd(1)-N(3)	69.63(15)	O(3)-Cd(1)-O(1)	92.41(16)

thiophene-2,5-dicarboxylate and two bpp molecules (Fig. 1). Cadmium atom is six-coordinated in a distorted octahedral manner and four nitrogen atoms (N2, N3, N4 and N5) from two [1,10]phenanthroline ligands. The Cd-N bond lengths are 2.386(5) Å, 2.398(5) Å, 2.327(6) Å and 2.331(6) Å, respectively and two oxygen atoms (O1 and O3), The Cd-O bond lengths are 2.315(4) Å and 2.248(4) Å, respectively. In addition, Some hydrogen bonds are listed as follows: O(6)-H(6)...O(5), [O...O = 2.709(7)\%A, O--H...O = 138.9\%]; O(1)-H(2W)...O(13), [O...O = 2.833(12)\%A, O--H...O = 172.4\%]; O(1)-H(1W)...O(12)#1, [O...O = 2.683(7)\%A, O--H...O = 178.4\%]. Symmetry codes: #1 -x + 1,-y,-z + 1. The chains are further assembled by the intermolecular hydrogen bonding interaction leading to the formation of a 1D framework (Fig. 2).

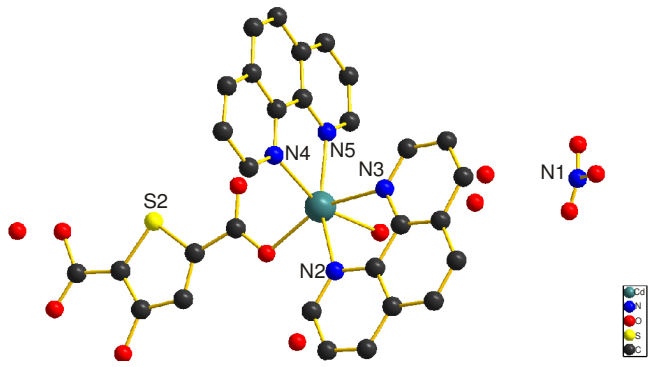

Fig. 1. Molecular structure of the title compound at 30 % probability displacement ellipsoids

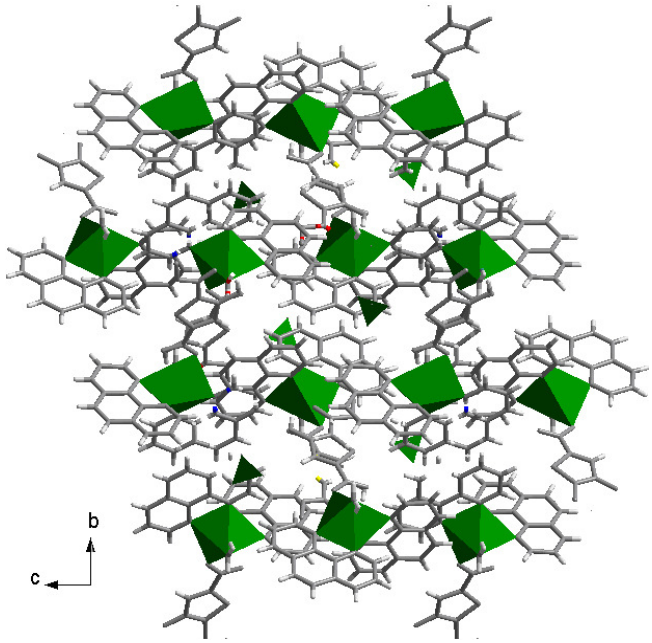

Fig. 2. 1D structure formed *via* hydrogen bonding interactions

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