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NOTE

Hydrothermal Synthesis and Crystal Structure of *bis*-(1,10-Phenanthroline)cobalt(II) Thiophene-2,3-dicarboxylate

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One new cobalt compound with $Co(NO_3)_2{\cdot}6H_2O$, thiophene-2,3-dicarboxylic acid and 1,10-phenanthroline (1,10-phen) has been successfully synthesized. Compound shows a one-dimensional framework. The 3D supramolecular structure is formed *via* hydrogen bonding connection.

Keywords: Coordination polymer, Crystal structure, Cobalt(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 reagent and solvents employed were commercially available and used as received without further purification.

General procedure: A mixture of $Co(NO_3)_2{\cdot}6H_2O$ (0.15 mmol), thiophene-2,3-dicarboxylic acid (0.15 mmol) and 1,10-phenanthroline (1,10-phen) (0.35 mmol) and distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 403 K for 36 h, followed by slow cooling to room temperature. Red crystals of the compound formed (Fig. 1).

Detection method: Diffraction intensity data of the single crystal of the five compounds were collected on a Bruker SMART APEX-II CCD diffractometer equipped with a graphite monochromated MoK_α radiation ($\lambda = 0.71073$ 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.

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COBALT(II) COMPLEX

Empirical formula	$C_{36}H_{40}N_4O_{17}S_2Co$
Formula weight	923.77
Crystal system space group	Monoclinic, C2/c
Unit cell dimensions	a=16.699(7) Å; b=22.687(10) Å c=13.017(6) Å
Volume (Å^3)	4045(3)
θ range for data collection	2.62-25.50
Final R indices [I>2σ(I)]	R_1= 0.0511; wR_2= 0.1063
Z, calculated density (mg/m^3)	4, 1.517
Absorption coefficient (mm^{-1})	0.608
F(000)	1916
Limiting indices	-20≤h≤20; -27≤k≤27; -15≤l≤15
Largest diff. peak and hole (e/Å^3)	0.520 and -0.486
Goodness-of -fit on F^2	1.031
R indices (all data)	R_1= 0.0806, wR_2= 0.1215

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

Co(1)-N(1)	2.141(2)	Co(1)-O(5)	2.065(2)
Co(1)-N(2)	2.152(3)	Co(1)-N(2)#1	2.152(3)
O(5)#1-Co(1)-O(5)	85.92(14)	N(1)-Co(1)-N(2)	76.90(10)
O(5)#1-Co(1)-N(1)	93.93(10)	N(1)#1-Co(1)-N(2)	93.49(10)
O(5)-Co(1)-N(1)	97.01(10)	O(5)#1-Co(1)-N(2)#1	87.31(10)
O(5)#1-Co(1)-N(1)#1	97.01(10)	O(5)-Co(1)-N(2)#1	167.86(9)
O(5)-Co(1)-N(1)#1	93.93(10)	N(1)-Co(1)-N(2)#1	93.49(10)
N(1)-Co(1)-N(1)#1	165.03(14)	N(1)#1-Co(1)-N(2)#1	76.90(10)
O(5)#1-Co(1)-N(2)	167.86(9)	N(2)-Co(1)-N(2)#1	101.02(14)
O(5)-Co(1)-N(2)	87.31(10)	C(6)-N(2)-Co(1)	114.1(2)

Symmetry codes: #1 –x + 1, y, -z + 3/2

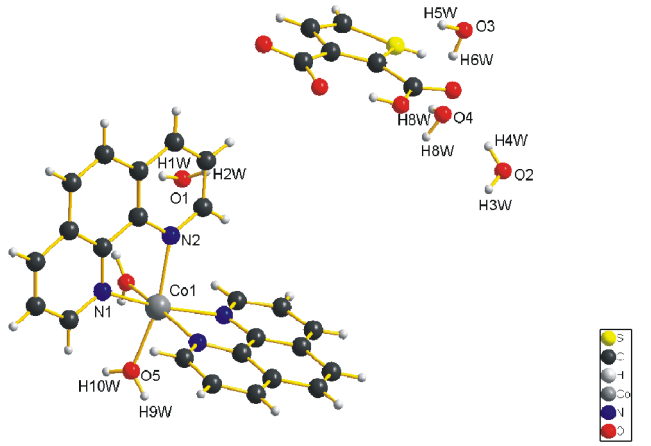

Fig. 1. Molecular structure of cobalt(II) complex at 30 % probability displacement ellipsoids

X-ray diffraction analysis revealed that the fundamental building unit consists of Co(II) ion and 1,10-phenanthroline (1,10-phen) as bridging ligands to construct a new coordination polymer. The asymmetric unit of the title structure contains one Co(II) ion, one thiophene-2,3-dicarboxylate and two 1,10-phen molecules. The Cobalt atom is six-coordinated in a distorted octahedral manner and two nitrogen atoms (N1 and N2) from two 1,10-phenanthroline ligands. The Co-N bond lengths are 2.141 (2) Å, 2.152 (3) Å, respectively. In addition, the carboxylic and the carboxylate group as well as the water molecule. Some are listed as follows: O(5)-H (10W)···O (1)#2, [O···O = 2.676(4)\%A, O-H···O = 167.9\%]; O(7)-H(7)···O(6), [O···O = 2.446(3)\%A, O--H...O = 175.1\%]; O(5)-H(9W)···O(9)#3, [O···O = 2.704 (3)\%A, O-H···O = 172.1\%]; O(4)-H(8W)···O(7), [O···O = 3.059(6)\%A, O-H···O = 171.9\%]; O(2)-H(4W)···O(8), [O···O = 2.814(4)\%A, O-H···O = 178.2\%]; O(3)-H(5W)···O(2)#4, [O···O = 2.723(4)\%A, O--H···O = 179.2\%]; O(2)-H(3W)···O(6)#1, [O···O = 2.857(4)\%A, O-H···O = 151.8\%]. Symmetry codes: #1 -x + 1, y, -z + 3/2; #2 x, -y + 2, z + 1/2; #3 x-1/2, y + 1/2, z; #4 x + 1/2, -y + 1/2, z + 1/2. The chains are further assembled by the intermolecular hydrogen bonding interaction leading to the formation of a 3D framework (Fig.2).

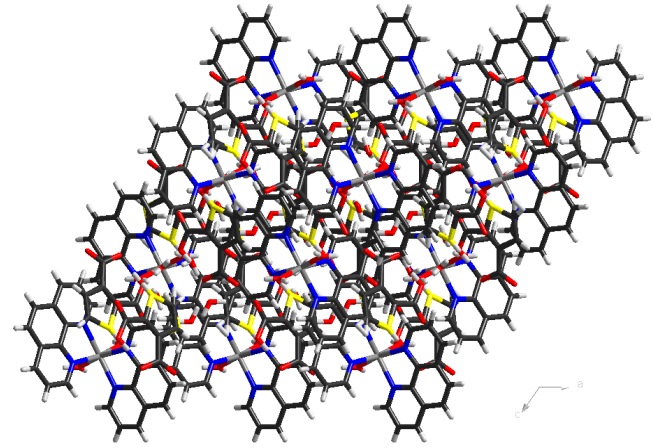

Fig. 2. 3D Structure formed *via* hydrogen bonding interactions

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