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NOTE

Hydrothermal Synthesis and Crystal Structure of Aqua-*bis*[(1,3-di(4-pyridyl)propane)dithiocyanato]manganese(II), $Mn(C_{13}H_{14}N_2)_2(CNS)_2$

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One new manganese complex formed by $Mn(OAc)_2{\cdot}4H_2O$, thiophene-3,4-dicarboxylic acid and bpp [1,3-di(4-pyridyl)propane] is reported. Compound shows a one-dimensional framework. The 1D supramolecular structure is formed *via* hydrogen bonding connection.

Keywords: Coordination polymer, Crystal structure, Manganese(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 Mn $(OAc)_2.4H_2O$ (0.25 mmol), thiophene-3,4-dicarboxylic acid (0.25 mmol) and bpp [1,3-di(4-pyridyl)propane], (0.25 mmol), KOH (0.25 mmol) and distilled water (8 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 393 K for 48 h, followed by slow cooling to room temperature. Yellow 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: 958012. The molecular structure of title compound is shown in Fig. 1.

X-ray diffraction analysis revealed that the fundamental building unit consists of dithiocyanato and bpp (bpp = 1,3-di(4-pyridyl)-propane) as bridging ligands to construct a new coordination polymer. The asymmetric unit of the title structure

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

Empirical formula	$C_{56}H_{56}Mn_2N_{12}S_4$	Z, Calculated density (mg/m^3)	4, 1.270
Formula weight	1135.25	Absorption coefficient (mm^{-1})	0.612
Crystal system space group	Monoclinic, P2 (1)/n	F(000)	2360
Unit cell dimensions	a = 18.959(3) Å	Limiting indices	-22 ≤ h ≤ 22
	b = 16.596(2) Å		-16 ≤ k ≤ 20
	c = 20.796(3) Å		-25 ≤ l ≤ 21
Volume (Å^3)	5937.7(14)	Largest diff. peak and hole (e/Å^3)	0.449 and- 0.365
θ range for data collection	2.27-25.50	Goodness-of-fit on F^2	0.998
Final R indices [I>2σ(I)]	R_1 = 0.0741 wR_2 = 0.1606	R indices (all data)	R_1 = 0.2128, wR_2 = 0.2210

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

Mn1-N9	2.181 (6)	Mn1-N7	2.283 (5)
Mn1-N10	2.195 (6)	Mn1-N6(ii)	2.298 (5)
Mn1-N5	2.277 (5)	Mn1-N8(i)	2.292 (5)
N9-Mn1-N10	177.3(2)	N10-Mn1-N7	91.5 (2)
N9-Mn1-N5	91.0 (2)	N7-Mn1-N5	177.48 (19)
N9-Mn1-N7	90.9 (2)	N10-Mn1-N8(i)	89.07 (19)
N10-Mn1-N5	86.52 (19)	N9-Mn1-N6(ii)	91.4 (2)

Symmetry codes: (i) –x + 5/2,y-1/2,-z + 1/2 (ii) –x + 3/2,y + 1/2,-z + /2

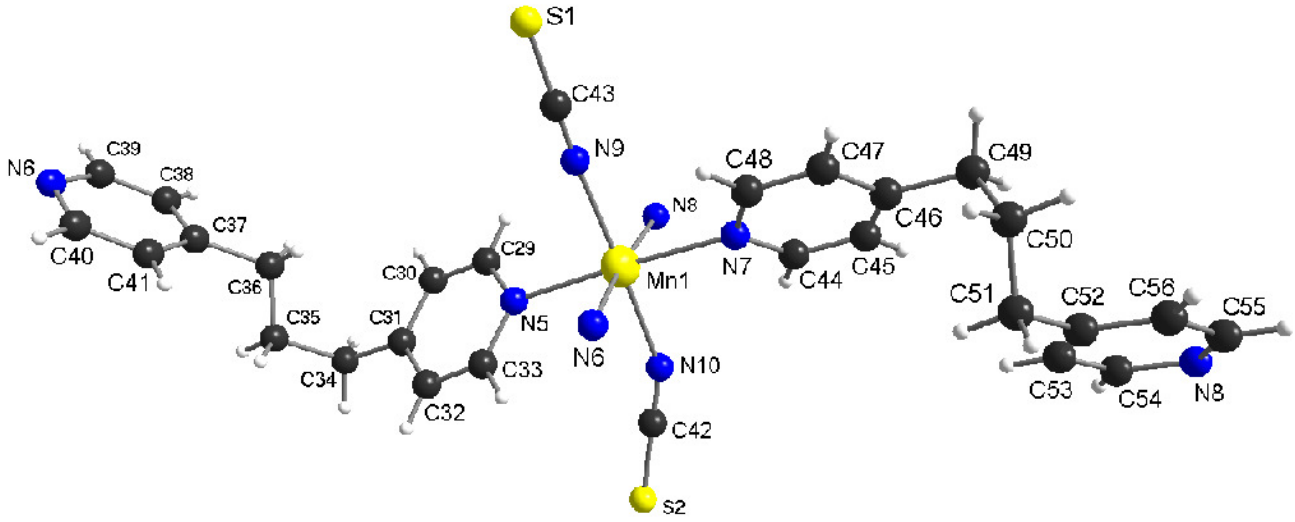

Fig. 1. Molecular structure of the title compound at 30 % probability displacement ellipsoids

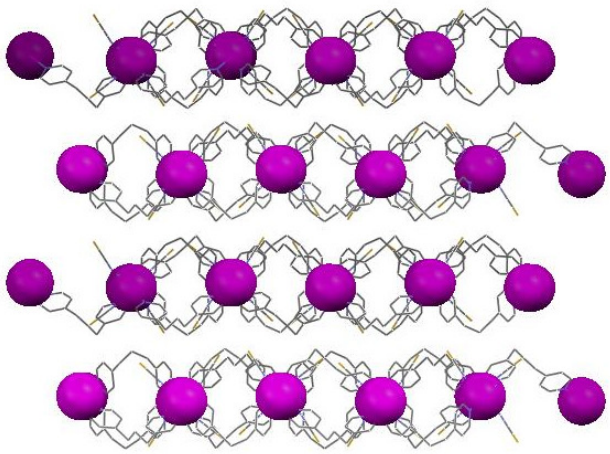

Fig. 2. 1D structure formed *via* hydrogen bonding interactions

contains one Mn(II) ion, two dithiocyanato and two bpp molecules. The manganese atom is six-coordinated [MnN6] in a distorted octahedral manner, and two nitrogen atoms (N9 and N10) from two dithiocyanato ligands. The Mn-N bond lengths are 2.181(6) Å and 2.195(6) Å, and two nitrogen atoms (N5 and N7) from two bpp molecules. The Mn-N bond lengths are 2.277(5) Å and 2.283(5) Å. The chains are further assembled by the intermolecular hydrogen bonding interaction leading to the formation of a 1D framework. (Fig. 2).

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