Mengyang Wang, Kaiqiang Yang, Yujiu Wang and Ying Ying*

Crystal structure of *catena*-poly[(bis(μ -1,1'-[(5-methoxy-2,4,6-trimethyl-1,3-phenylene)bis(methylene)]bis(1*H*-1,2,4-triazole)- κ^2 N:N')-bis(isothiocyanato- κ N)manganese(II)], C₃₄H₄₀MnN₁₄O₂S₂

Table 1: Data collection and handling.

Crystal:	Pink block
Size:	0.28 × 0.19 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.53 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	29.3°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7219, 4157, 0.031
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3521
$N(\text{param})_{\text{refined}}$:	245
Programs:	Olex2 [1], SHELX [2]

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Abstract

C₃₄H₄₀MnN₁₄O₂S₂, triclinic, $P\bar{1}$ (no. 2), $a = 9.1383(4)$ Å, $b = 9.5039(6)$ Å, $c = 10.5526(6)$ Å, $\alpha = 91.564(4)^\circ$, $\beta = 94.624(5)^\circ$, $\gamma = 91.737(4)^\circ$, $V = 912.68(9)$ Å³, $Z = 1$, $R_{\text{gt}}(F) = 0.0374$, $wR_{\text{ref}}(F^2) = 0.0910$, $T = 125$ K.

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The title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

KSCN (0.1 mmol, 10 mg) in the mixed solution of H₂O and CH₃OH ($v/v = 1:1$) (2 mL) is added to Mn(CH₃COO)₂·H₂O (0.2 mmol, 34.6 mg) in a mixed solution of H₂O and CH₃OH ($v/v = 1:1$) (2 mL). The mixture is stirred for half an hour, decanted off, and filtered. Then the filtrate is collected and

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	1.000000	0.500000	0.500000	0.01151(10)
S1	0.75900(5)	0.95034(5)	0.52586(5)	0.02566(13)
O1	0.32897(13)	0.30976(14)	−0.12975(13)	0.0220(3)
N1	0.90593(17)	0.37308(18)	−0.10954(16)	0.0263(4)
N2	0.88515(15)	0.25171(16)	−0.18419(15)	0.0192(3)
N3	0.97294(15)	0.40767(16)	−0.30998(15)	0.0193(3)
N4	0.62966(15)	0.24889(16)	0.34619(14)	0.0168(3)
N5	0.55416(15)	0.36057(17)	0.38993(16)	0.0226(4)
N6	0.79335(14)	0.39933(16)	0.43434(14)	0.0169(3)
N7	0.89603(16)	0.69012(17)	0.55495(16)	0.0223(3)
C1	0.95791(19)	0.4633(2)	−0.19032(19)	0.0248(4)
H1	0.982234	0.556830	−0.167593	0.030*
C2	0.92700(18)	0.2740(2)	−0.30097(18)	0.0197(4)
H2	0.924407	0.206059	−0.366313	0.024*
C3	0.81867(19)	0.1225(2)	−0.13748(18)	0.0211(4)
H3A	0.890470	0.076958	−0.081005	0.025*
H3B	0.790614	0.058087	−0.208821	0.025*
C4	0.68451(18)	0.15348(19)	−0.06700(17)	0.0175(4)
C5	0.56670(18)	0.21663(18)	−0.13287(17)	0.0168(4)
C6	0.44716(17)	0.24893(18)	−0.06507(17)	0.0171(4)
C7	0.44103(17)	0.21991(18)	0.06479(17)	0.0163(4)
C8	0.55914(17)	0.15386(18)	0.12807(17)	0.0160(4)
C9	0.68076(17)	0.11842(18)	0.06214(17)	0.0164(4)
C10	0.80660(18)	0.0403(2)	0.12740(18)	0.0213(4)
H10A	0.893149	0.100663	0.136514	0.032*
H10B	0.825151	−0.042030	0.077138	0.032*
H10C	0.781141	0.012663	0.209871	0.032*
C11	0.5646(2)	0.2511(2)	−0.27304(18)	0.0238(4)
H11A	0.613749	0.179476	−0.317545	0.036*

*Corresponding author: Ying Ying, Jiangxi Province Key Laboratory of Tumor Pathogens and Molecular Pathology and Department of Pathology, Schools of Basic Medical Sciences, Nanchang University, Nanchang, Jiangxi, China, e-mail: ying_ying666@126.com

Mengyang Wang: Joint Programme of Nanchang University of London, Nanchang University, Nanchang, Jiangxi, China

Kaiqiang Yang and Yujiu Wang: Department of Cardiac Surgery, Binzhou Medical University Hospital, Binzhou Medical University, Binzhou, Shandong, China

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H11B	0.613929	0.340604	−0.281510	0.036*
H11C	0.464719	0.255130	−0.308435	0.036*
C12	0.3383(2)	0.4627(2)	−0.1237(2)	0.0269(4)
H12A	0.431134	0.494593	−0.150835	0.040*
H12B	0.329835	0.495514	−0.037806	0.040*
H12C	0.260203	0.499082	−0.178351	0.040*
C13	0.30863(18)	0.2609(2)	0.13202(19)	0.0224(4)
H13A	0.232688	0.289280	0.070715	0.034*
H13B	0.335324	0.337601	0.191229	0.034*
H13C	0.273541	0.181794	0.176941	0.034*
C14	0.55640(18)	0.12995(19)	0.27025(17)	0.0175(4)
H14A	0.455378	0.119346	0.291377	0.021*
H14B	0.605666	0.043645	0.291287	0.021*
C15	0.77092(18)	0.27455(19)	0.37310(17)	0.0172(4)
H15	0.844631	0.214658	0.352548	0.021*
C16	0.65747(18)	0.4477(2)	0.44239(18)	0.0217(4)
H16	0.638642	0.533627	0.481004	0.026*
C17	0.83923(17)	0.79840(19)	0.54292(17)	0.0170(4)

is added dropwise to a tube. The ascorbic acid (0.05 mmol, 8.8 mg) in mixed solution of H₂O and CH₃OH (*v/v* = 1:1) (2 mL) is slowly added. Then 1,1'-(5-methoxy-2,4,6-trimethyl-1,3-phenylene)bis(methylene)]bis(1*H*-1,2,4-triazole) (btmtmb; 0.1 mmol, 31 mg) in 4 mL of CH₃OH is added dropwise. The light pink block crystals of the title compound are obtained after two weeks at room temperature. Yield: 43% based on Mn.

Experimental details

H atoms bonded to C atoms from organic ligands were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, with *U*_{iso}(H) = 1.2 times *U*_{eq}(C).

Comment

Coordination polymers (CPs) have attracted much attention not only due to their structural and topology but also because of their possible applications as molecule-based functional materials in many fields such as sensors and magnetism [3, 4]. Since most of the structures and properties of CPs are significantly influenced by the ligands, the selection of suitable ligands in the construction of CPs is one of the most important areas in coordination polymers. The 1,2,4-triazole and its derivatives are widely used in the synthesis of CPs with fascinating magnetic properties [5]. On the other hand, manganese has been shown great potential in the construction of manganese coordination compounds, which has been exemplified by the famous {Mn₁₂} single-molecule magnet [6, 7]. In this study, we choose Mn(II) ions as the metal

nodes and the 1,3-bis-(1,2,4-triazol-1-ylmethyl)-5-methoxy-2,4,6-trimethyl-benzene (btmtmb) ligands as the organic connectors to build a new Mn(II)-coordination polymer.

The single-crystal X-ray study reveals that the title complex shows a one-dimensional chain structure. The asymmetric unit includes a half Mn²⁺ ion, one btmtmb ligand and one SCN[−] ligand. Further structural analysis showed that the Mn²⁺ ion is six-coordinated by two nitrogen atoms from SCN[−] and four nitrogen atoms from four crystallographically dependent btmtmb ligands. Two SCN[−] ions occupy the axial positions, and the equatorial plane is defined by four nitrogen atoms from btmtmb ligands. The Mn(II) ions are linked via btmtmb ligands to form the Mn₂(btmtmb)₂ basic structural units, which are further assembled into a chain. Consecutive chains are further packed into three-dimensional supramolecular structure through interlayer π–π interactions between symmetry-related planes (distance: 3.605 Å). The structure of the title compound has a similar configuration with the recently reported Fe(II)-complex [8].

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