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Crystal structure of poly[diaqua-bis(μ_2 -1-(4-(1*H*-imidazol-1-yl)benzyl)-1*H*-1,2,4-triazole- κ^2 N:N')manganese(II)] terephthalate tetrahydrate, $\text{MnC}_{32}\text{H}_{38}\text{N}_{10}\text{O}_{10}$

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Abstract

$\text{MnC}_{32}\text{H}_{38}\text{N}_{10}\text{O}_{10}$, triclinic, $P\bar{1}$ (no. 2), $a = 8.508(2)$ Å, $b = 8.659(3)$ Å, $c = 12.755(4)$ Å, $\alpha = 71.120(10)^\circ$, $\beta = 84.432(16)^\circ$, $\gamma = 88.133(16)^\circ$, $V = 885.0(5)$ Å³, $Z = 1$, $R_{\text{gt}}(F) = 0.0371$, $wR_{\text{ref}}(F^2) = 0.1040$, $T = 223(2)$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A 20 mL H_2O solution of $\text{MnSO}_4 \cdot \text{H}_2\text{O}$ (0.5 mmol) and terephthalic acid (0.5 mmol) was added to one leg of an H-shaped-tube, and a 20 mL EtOH solution of 1-(imidazo-1-yl)-4-(1,2,4-triazol-1-ylmethyl)benzene (itmb) (0.50 mmol) was added to the other leg of the tube. After two weeks colorless crystals were obtained.

Experimental details

All H atoms were included in calculated positions and refined as riding atoms, with $\text{C}-\text{H} = 0.94$ Å, $\text{O}-\text{H} = 0.84-0.88$ Å, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for all other H atoms.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.60 \times 0.50 \times 0.40$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.44 mm^{-1}
Diffractometer, scan mode:	Rigaku Saturn, ω
θ_{max} , completeness:	27.5° , 98%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	8006, 3949, 0.029
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2978
$N(\text{param})_{\text{refined}}$:	254
Programs:	Bruker [1], SHELX [2], Olex2 [3]

Comment

Coordination polymers have been paid great interest because of their fascinating topologies and interesting properties for potential applications as functional materials such as photocatalysis, luminescence, magnetism and molecular sensors in the last two decades [4–8]. The organic ligands, which have their differences in size, flexibility, coordination ability, number of carboxylate groups, positions of the carboxylate groups and so on, are important in the design of frameworks [9–11]. In addition, triazol based ligands [12, 13] are known to be connectors for the propagation of coordination networks.

In this paper, we select terephthalic acid to react with Mn(II) ions and 1-(imidazo-1-yl)-4-(1,2,4-triazol-1-ylmethyl)benzene (itmb) to obtain a new coordination polymer. The structure of the title compound is isomorphous to previously reported Mn(II) complex constructed by phthalic acid and itmb [13]. The asymmetric structure unit of the title complex consists of one half Mn^{2+} ion, one 1-(imidazo-1-yl)-4-(1,2,4-triazol-1-ylmethyl)benzene (itmb), three water molecules and one half terephthalate anion. Each Mn(II) atom is coordinated by four nitrogen atoms from four different itmb ligands and two oxygen atoms from two water molecules to furnish a $[\text{MnN}_4\text{O}_2]$ six-coordinate distorted octahedral geometry. The Mn–O bond lengths are 2.1765(13) Å, and the Mn–N distances are 2.2421(16), and 2.2857(16) Å, both of which are in the normal range. The bond angles around the Mn(II) are in the ranges of $84.10(6)-180^\circ$. The Mn(II) atoms are connected by four itmb ligands and two H_2O to form a one-dimensional coordination polymer. Moreover, the coordinated water molecules, the solvated water molecules and carboxyl O atoms form hydrogen bonding interactions

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
C1	0.4203(2)	0.3323(3)	0.26336(15)	0.0333(4)
H1	0.5227	0.3557	0.2756	0.040*
C2	0.2134(2)	0.3178(3)	0.18399(16)	0.0412(5)
H2	0.1440	0.3300	0.1288	0.049*
C3	0.1771(2)	0.2442(3)	0.29357(16)	0.0436(5)
H3	0.0802	0.1959	0.3284	0.052*
C4	0.3292(2)	0.1908(2)	0.46125(14)	0.0306(4)
C5	0.2611(2)	0.0440(3)	0.52483(16)	0.0415(5)
H5	0.2032	−0.0151	0.4915	0.050*
C6	0.2779(2)	−0.0164(3)	0.63767(16)	0.0407(5)
H6	0.2313	−0.1166	0.6808	0.049*
C7	0.3635(2)	0.0705(2)	0.68767(15)	0.0297(4)
C8	0.4323(3)	0.2156(3)	0.62241(16)	0.0430(5)
H8	0.4923	0.2740	0.6550	0.052*
C9	0.4150(3)	0.2772(3)	0.50920(16)	0.0431(5)
H9	0.4615	0.3773	0.4658	0.052*
C10	0.3743(2)	−0.0011(3)	0.81189(15)	0.0357(5)
H10A	0.2673	−0.0218	0.8494	0.043*
H10B	0.4294	−0.1062	0.8276	0.043*
C11	0.3978(2)	0.2042(2)	0.91127(15)	0.0317(4)
H11	0.2895	0.2187	0.9284	0.038*
C12	0.6435(2)	0.2203(3)	0.89542(17)	0.0399(5)
H12	0.7457	0.2532	0.9009	0.048*
C13	0.9344(2)	0.3788(3)	0.59136(15)	0.0421(5)
H13	0.8884	0.2959	0.6532	0.050*
C14	0.8786(2)	0.4082(3)	0.48753(16)	0.0424(5)
H14	0.7959	0.3442	0.4801	0.051*
C15	0.9433(2)	0.5299(2)	0.39554(14)	0.0307(4)
C16	0.8815(2)	0.5597(3)	0.28257(15)	0.0339(4)
Mn1	0.5000	0.5000	0.0000	0.02654(13)
N1	0.36640(18)	0.3725(2)	0.16435(12)	0.0328(4)
N2	0.31033(18)	0.2534(2)	0.34464(12)	0.0324(4)
N3	0.51191(17)	0.28054(19)	0.93707(12)	0.0316(4)
N4	0.45660(17)	0.10407(19)	0.85784(12)	0.0289(3)
N5	0.61733(18)	0.1124(2)	0.84675(14)	0.0401(4)
O1	0.71948(14)	0.43760(18)	0.07881(10)	0.0401(4)
H1A	0.7315	0.4601	0.1388	0.063*
H1B	0.7967	0.3885	0.0565	0.063*
O2	0.78341(17)	0.4613(2)	0.27467(11)	0.0479(4)
O3	0.93376(17)	0.68320(19)	0.20438(11)	0.0464(4)
O4	1.0392(2)	0.9929(2)	0.16473(17)	0.0656(5)
H4A	1.0061	0.8938	0.1746	0.063*
H4B	1.1382	0.9916	0.1675	0.063*
O5	1.03764(18)	0.7194(2)	−0.00873(13)	0.0499(4)
H5A	1.0194	0.8165	−0.0539	0.063*
H5B	0.9934	0.6930	0.0589	0.063*

with $d(\text{O} \cdots \text{O}) = 2.676\text{--}2.745$ Å. Through hydrogen bonds complexes and water molecules are interlinked to form the three-dimensional network.

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