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Crystal structure of poly[diaqua-bis(μ_2 -3-((1*H*-imidazol-1-yl)methyl)benzoato- $\kappa^2 N:O$)manganese(II)], $C_{22}H_{22}MnN_4O_6$

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Abstract

$C_{22}H_{22}MnN_4O_6$, monoclinic, $P2_1/n$, $a = 11.9331(7)$ Å, $b = 5.5962(3)$ Å, $c = 16.0671(9)$ Å, $\beta = 107.391(6)^\circ$, $Z = 2$, $V = 1023.92(11)$ Å³, $R_{gt}(F) = 0.046$, $wR_{ref}(F^2) = 0.055$, $T = 287$ K.

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A part of the polymeric crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

All chemicals were used without further purification. The title compound was prepared under hydrothermal conditions. A mixture of $Mn(OAc)_2 \cdot 4H_2O$ (24.5 mg, 0.1 mmol), 3-(1*H*-imidazol-1-ylmethyl)benzoic acid hydrochloride (11.3 mg, 0.05 mmol), NaOH (2.00 mg, 0.05 mmol) and 5 mL distilled water in a 25 mL Teflon-lined autoclave was kept under autogenous pressure at 353 K for 3 days. After cooling to room temperature at a rate of 5 K h^{−1}, yellow block crystals were collected by filtration and washed with distilled water (yield 67%, based on Mn).

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.32 × 0.26 × 0.21 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.70 mm ^{−1}
Diffractometer, scan mode:	SuperNova, ω -scans
θ_{max} , completeness:	25.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	5738, 1882, 0.036
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1653
$N(param)_{refined}$:	151
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3], OLEX2 [4]

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

Atom	x	y	z	U_{iso}^*/U_{eq}
Mn1	0.5000	1.0000	0.5000	0.0168(2)
O1	0.3663(2)	0.7120(4)	0.46752(16)	0.0376(6)
H1A	0.3919	0.5881	0.4979	0.056*
H1B	0.3063	0.7826	0.4738	0.056*
O2	0.6255(2)	0.7630(4)	0.46449(17)	0.0373(6)
O3	0.7902(2)	0.9809(4)	0.50252(18)	0.0423(7)
N1	1.0637(3)	0.6210(6)	0.14321(18)	0.0349(7)
N2	1.0832(2)	0.6085(5)	0.28382(18)	0.0305(7)
C1	0.7302(3)	0.8105(6)	0.4635(2)	0.0288(8)
C2	0.7828(3)	0.6403(6)	0.4122(2)	0.0269(7)
C3	0.7157(3)	0.4515(6)	0.3664(2)	0.0313(8)
H3	0.6436	0.4393	0.3635	0.038*
C4	0.7673(3)	0.2833(6)	0.3257(2)	0.0347(8)
H4	0.7267	0.1677	0.2980	0.042*
C5	0.8827(3)	0.3034(6)	0.3300(2)	0.0324(8)
H5	0.9144	0.1950	0.3075	0.039*
C6	0.9491(3)	0.4971(6)	0.3702(2)	0.0287(8)
C7	0.8988(3)	0.6636(6)	0.4120(2)	0.0277(7)
H7	0.9394	0.7816	0.4379	0.033*
C8	1.0749(3)	0.5223(7)	0.3687(2)	0.0345(9)
H8A	1.1108	0.6194	0.4084	0.041*
H8B	1.1089	0.3875	0.3800	0.041*
C9	1.1331(4)	0.8175(7)	0.2687(2)	0.0432(10)
H9	1.1653	0.9234	0.3061	0.052*
C10	1.1210(4)	0.8223(8)	0.1826(2)	0.0449(10)
H10	1.1454	0.9339	0.1565	0.054*
C11	1.0442(4)	0.4976(7)	0.2065(2)	0.0384(9)
H11	1.0106	0.3620	0.1995	0.046*

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Discussion

Coordination polymers have developed rapidly not only due to their esthetic topological structures, but also owing to their potential applications [5–7]. At present, many coordination polymers have been prepared by various organic ligands. Obviously, the design of suitable organic ligands and the reasonable selection of metal centers are crucial to the construction and structural tuning of the resulting complexes [8–10]. Organic ligands bearing imidazole and carboxylate groups separated by a $-\text{CH}_2-$ spacer can show versatile coordination modes, which makes it a useful linker to generate coordination polymers [11–13]. Of further interest, the 3-(1*H*-imidazol-1-ylmethyl)benzoate ligand remains largely unexplored hitherto in the field of coordination polymers.

In this work, we report a two-dimensional coordination polymer constructed from Mn(II) ions under hydrothermal conditions. The asymmetric unit of the crystal structure consists of half of a Mn(II) center, one bridging L^- anion and one coordinated water molecule. Each Mn(II) ion is in a distorted octahedral geometry finished by two carboxylate oxygen atoms and two imidazole nitrogen atoms from L^- anions and two water molecules. The distances of Mn–O bonds are 2.200(2), 2.218(2) Å and the distance of Mn–N bond is 2.299(3) Å. The bond angles about the Mn(II) centers range from 88.80(10) to 180°. These values match with previously reported similar Mn(II) coordination polymers [14, 15]. In the title complex, L^- anions connect Mn(II) ions to form an infinite two dimensional layer structure. In addition, there are three kinds of intermolecular $\text{OH}\cdots\text{O}$ hydrogen bonds with $\text{O}\cdots\text{O}$ distances of 2.864(4) and 2.686(4) Å, respectively. Interestingly, the two dimensional layer structure of the title compound is expanded into a three-dimensional supramolecular structure.

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