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Crystal structure of *catena*-poly[[tetraaquamanganese(II)]-μ-1,5-dihydroxynaphthalene-2,6-dicarboxylato]

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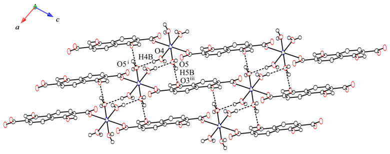
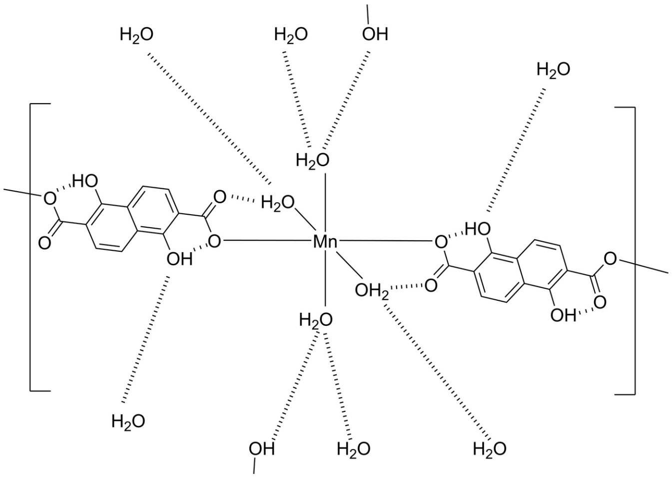
The title compound, $[Mn(H_2dondc)(H_2O)_4]_n$ or $[Mn(C_{12}H_6O_6)(H_2O)_4]_n$, was synthesized by the reaction of manganese(II) chloride ($MnCl_2$), 1,5-dihydroxynaphthalene-2,6-dicarboxylic acid (H_4dondc) and lithium hydroxide (LiOH). The asymmetric unit comprises half of an Mn^{II} ion, half of a 1,5-dihydroxynaphthalene-2,6-dicarboxylate dianion (H_2dondc^{2-}) and two water molecules. The Mn^{II} ion is located on a crystallographic inversion center and exhibits a six-coordinated MnO_6 octahedral geometry. The octahedron is comprised of two oxygen atoms from the two H_2dondc^{2-} ligands and four oxygen atoms from the water molecules. The carboxylate group and naphthalene moiety lie almost coplanar to each other and show a monodentate coordination to the Mn^{II} ion. The planar H_2dondc^{2-} ligands bridge Mn^{II} ions to form a one-dimensional chain along the diagonal direction of the *b* and *c* axes. In the crystal, there are two types of intra-chain hydrogen-bonding interactions. The first is between the phenolic hydroxyl groups and carboxylate groups. The phenolic hydroxyl groups of the ligand are protonated and act as intra-chain hydrogen-bonding donors to coordinated oxygen atoms of the carboxylate groups. The other is between coordinated water molecules and non-coordinated oxygen atoms of the carboxylate groups. The parallel chains are connected not only by inter-chain hydrogen-bonding interactions between coordinated water molecules and phenolic hydroxyl groups but also by inter-chain hydrogen-bonding interactions between coordinated water molecules to give two-dimensional networks. The chains are further connected by inter-chain π–π stacking interactions between the naphthalene moieties.



1. Chemical context

Metal–organic frameworks (MOFs) or coordination polymers (CPs) are compounds composed of metal ions and organic ligands that are connected by coordination bonds and form networks of different dimensionalities (one-dimensional, two-dimensional or three-dimensiona) in a crystal structure. These materials have received significant attention due to their diverse structures, and their physical and chemical applications, including magnetism, conductivity, gas sorption and catalytic activity (Kurmoo, 2009; Kurmoo *et al.*, 1995; Zhong *et al.*, 2023; Nakatani *et al.*, 1990; Kitagawa *et al.*, 2004). Multitopic organic ligands such as polypyridines, polyamines and polycarboxylates are often used in the synthesis of these materials. Among these ligands, the benzenedicarboxylate ligand (bdc^{2-} dianion) and its analogues are well-known bridging ligands that yield functional materials (Kurmoo, 2009; Furukawa *et al.*, 2010). We have reported on electrode materials that use bdc^{2-} dianion analogues (Ogihara *et al.*, 2014, 2021, 2023; Yasuda & Ogihara, 2014) and magnetic materials that involve polycarboxylate in which the number of carboxylate groups and the distances between carboxylate groups systematically vary (Kumagai *et al.*, 2001, 2002; Kurmoo *et al.*, 2001, 2003). We also reported a series of two-dimensional (2D) layered compounds that employ R_4-benzenedicarboxylate (R_4-bdc^{2-}; R = H, F, Cl, and Br) as a bridging ligand and M^{II} ions (M^{II} = Mn, Co, Zn, and Cu). The structures and water adsorption-desorption properties are tuned by altering the halogen atoms attached to the benzene ring or metal ions used in these compounds (Kumagai *et al.*, 2012, 2021). 1,5-Dihydroxynaphthalene-2,6-dicarboxylic acid (H_4dondc) is also a dicarboxylate analogue, in which phenolic hydroxyl groups are introduced within the naphthalene backbone. The H_4dondc ligand can give four available charges (1− to 4−) depending on the deprotonation state, and MOFs with the 4− state of the ligand, where both the carboxyl groups and phenolic hydroxyl groups are deprotonated, were synthesized at high temperature using solvothermal reactions or microwaves to give honeycomb-type pores with open metal sites (Yeon *et al.*, 2015; Dietzel *et al.*, 2020). We have previously reported the first structural characterization of $\{[Co(H_2dondc)(H_2O)_4]\cdot 2DMF\}_n$ (DMF = *N*,*N*′-dimethylformamide, CCDC reference: 2421049, RURSIK), in which the ligand acts as a 2− anion (Kumagai *et al.*, 2025). Here, we have focused on the use of H_2dondc^{2-} in the synthesis of an Mn^{II}–H_2dondc^{2-} dianion system under ambient conditions and report on the single-crystal structure of $[Mn(H_2dondc)(H_2O)_4]_n$.



2. Structural commentary

The title compound, $[[Mn(H_2dondc)(H_2O)_4]_n$, consists of an Mn^{II} ion, H_2dondc^{2-} and four water molecules. The Mn^{II} ion lies on a crystallographic inversion center and its asymmetric unit consists of half of an Mn^{II} ion, half of a H_2dondc^{2-} ligand and two water molecules. The characteristic point of the structure is a three-dimensional (3D) hydrogen-bonding network that consists of one-dimensional (1D) coordination chains built up by MnO_6 octahedra bridged by H_2dondc^{2-} ligands and inter-chain O—H···O hydrogen bonding and π–π stacking interactions of the naphthalene moieties. We have reported a similar compound, $\{[Co(H_2dondc)(H_2O)_4]\cdot 2DMF\}_n$, in which DMF (dimethylformamide) molecules are included in the crystal (Kumagai *et al.*, 2025). Here we describe the structure of $[Mn(H_2dondc)(H_2O)_4]_n$ and the differences between this structure and $\{[Co(H_2dondc)(H_2O)_4]\cdot 2DMF\}_n$. Comparisons of selected bond distances, angles and hydrogen-bonding geometry are summarized in the supporting information. Fig. 1 shows the one-dimensional chain structure of $[Mn(H_2dondc)(H_2O)_4]_n$ with the numbering scheme. The Mn^{II} ion occupies a crystallographic inversion center; therefore, octahedron is formed and each pair of H_2dondc^{2-} ligands and water molecules coordinate *trans* positions to each other. The Mn—O1 (carboxylate) bond length [2.1310 (13) Å] in $[Mn(H_2dondc)(H_2O)_4]$ is shorter than the Mn—O4 and Mn—O5 (H_2O) bond lengths [2.1521 (16) Å and 2.2335 (15) Å, respectively], which is indicative of a slightly elongated octahedral geometry along the Mn—O5 bond. The ligands bridge the octahedral Mn^{II} ions to form a linear chain along the diagonal direction of the *b* and *c* axes. The Mn···Mn separation defined by Mn–H_2dondc^{2-}–Mn connectivity within the chain is 13.22 (5) Å, which is similar to that for the Co compound [13.27 (3) Å; Kumagai *et al.*, 2025). The carboxylate group exhibits a monodentate coordination to the Mn^{II} ion and the phenolic hydroxyl groups show no coordination bonding to the Mn^{II} ion, giving the 2− anion. The phenolic hydroxyl groups show intra-chain hydrogen-bonding interactions with the coordinated oxygen atoms of the carboxylate groups. The non-coordinated oxygen atom of the carboxylate group (O2) shows intra-chain hydrogen-bonding interactions with coordinated water molecules (O4) at an O···O distance of 2.756 (2) Å. The oxygen atoms of the carboxylate groups act as intra-chain hydrogen-bond acceptors, and the coordinated water molecules and phenolic hydroxyl groups act as intra-chain hydrogen-bond donors. These structural features are similar to those of the previously reported Co^{II} compound (Kumagai *et al.*, 2025). The difference between the structures of the title and Co^{II} compounds is the planarity between the

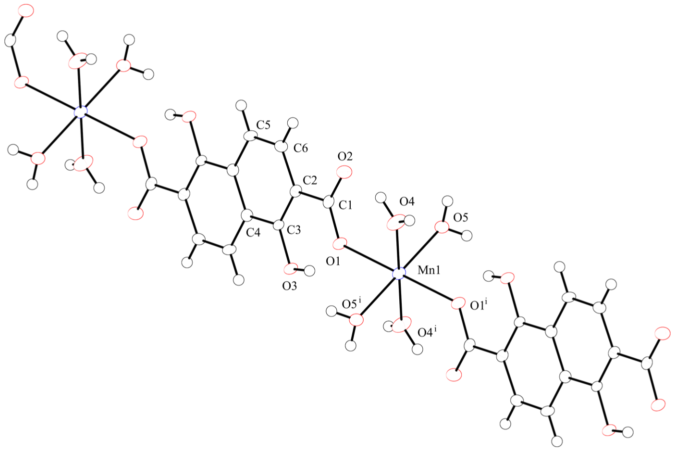


Figure 1
The one-dimensional chain structure of the title compound with the atom-labeling scheme and 50% probability displacement ellipsoids. Hydrogen atoms are omitted for clarity. [Symmetry code: (i) $-x + 1, -y + 2, -z + 2$.]

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O4—H4$A\cdots$O2	0.88 (3)	2.02 (3)	2.756 (2)	141 (3)
O4—H4$B\cdots$O5$^{\rm i}$	0.79 (3)	2.04 (3)	2.814 (2)	169 (3)
O3—H3$\cdots$O1	0.79 (3)	1.75 (3)	2.480 (2)	153 (3)
O5—H5$A\cdots$O2$^{\rm ii}$	0.80 (3)	1.88 (3)	2.664 (2)	168 (3)
O5—H5$B\cdots$O3$^{\rm iii}$	0.71 (3)	2.13 (3)	2.798 (2)	157 (3)

Symmetry codes: (i) $-x+2, -y, -z+1$; (ii) $x, y-1, z$; (iii) $x+1, y, z$.

carboxylate group and naphthalene ring. While the carboxylate group and the naphthalene ring are almost coplanar with an C6—C2—C1—O1 torsion angle of 179.77 (17)° in $[\mathrm{Mn(H_2dondc)(H_2O)_4}]_n$, the Co$^{\rm II}$ compound shows a slightly tilted geometry with a torsion angle of 171.94 (11)°.

3. Supramolecular features

The coordinated water molecules of the title compound play important roles in forming intra- and inter-chain hydrogen-bonding interactions that yield a hydrogen-bonding network in the crystal structure (Table 1). The chains are hydrogen bonded both in the direction of naphthalene ring stacking and in the planar direction of the naphthalene rings to form a three-dimensional network. Fig. 2 shows the two-dimensional inter-chain hydrogen-bonding network in the planar direction of the naphthalene rings. The non-coordinated oxygen atoms (O2$^{\rm ii}$) of the carboxylate groups hydrogen bond to coordinated water molecules (O5) of the adjacent chain at a distance of 2.664 (2) Å. O2 acts as a hydrogen-bond acceptor and the coordinated water molecule acts as a hydrogen-bond donor. This two-dimensional hydrogen-bonding network is similar to that of the previously reported Co$^{\rm II}$ complex (Kumagai *et al.*, 2025). Coordinated water molecules (O4) show inter-chain hydrogen-bonding interactions at a distance of 2.814 (2) Å between the coordinated water molecules of adjacent chains (O5) in the direction of naphthalene ring stacking, as shown in Fig. 3. The water molecules also act as hydrogen-bond donors (O4) and as hydrogen-bond acceptors (O5). The coordinated water molecules (O5) form two types of inter-chain hydrogen-bonding interactions in the direction of the naphthalene ring stacking. One is a hydrogen-bonding interaction with a water molecule of an adjacent chain [O4$\cdots$O5$^{\rm i}$ = 2.814 (2) Å; symmetry code as in Table 1] and the other is a hydrogen bond with a phenolic hydroxyl group in a neighboring chain [O5$\cdots$O3$^{\rm iii}$ = 2.798 (2) Å; symmetry code as in Table 1]. Water molecules (O5) act not only as hydrogen-bond acceptors toward other water molecules but also as hydrogen-bond donors to phenolic hydroxyl groups. The almost planar naphthalene moieties are stacked along the crystallographic *a*-axis direction in the crystal, with shortest centroid$\cdots$centroid distances between the naphthalene rings and C$\cdots$C distances of 3.7345 (13) and 3.378 (3) Å, respectively. These distances are indicative of π–π stacking interactions between the naphthalene moieties. The one-dimensional chains thereby form a three-dimensional network through hydrogen bonding and π–π stacking interactions. The difference between $[\mathrm{Mn(H_2dondc)(H_2O)_4}]_n$ and the Co$^{\rm II}$ compound is the absence of DMF molecules between the chains in the crystal structure (Kumagai *et al.*, 2025). The presence of DMF molecules between the chains prevents π–π stacking between the naphthalene moieties; the naphthalene moieties of the Co$^{\rm II}$ compound showed C—H$\cdots\pi$ interactions between DMF molecules and the naphthalene rings rather than the π–π stacking observed in the title compound. This result suggests that the inter-chain interactions can be controlled by the solvent in the crystal.

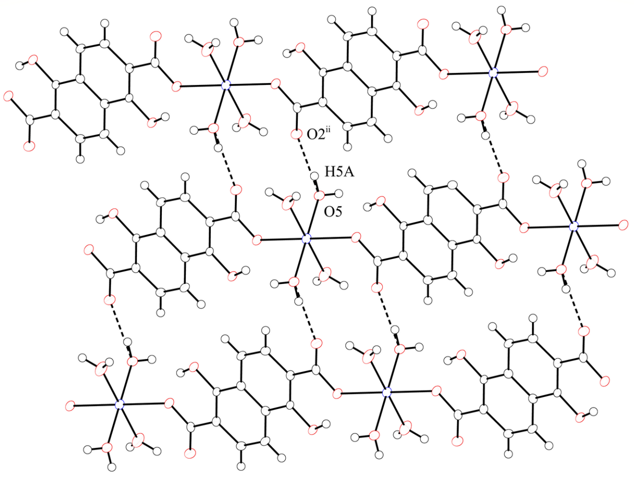


Figure 2
View of the two-dimensional hydrogen-bonding network in the planar direction of the naphthalene rings. Hydrogen-bonding interactions are shown as dashed lines.

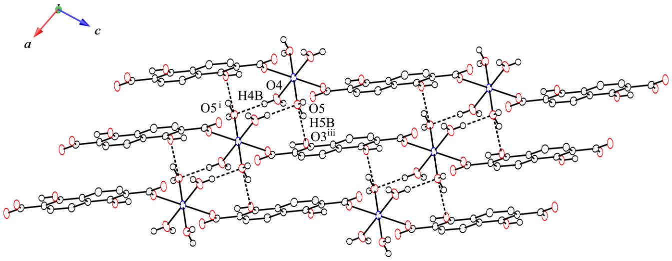


Figure 3
View of the two-dimensional hydrogen-bonding network in the direction of the naphthalene ring stacking. Hydrogen bonds are shown as dashed lines. Hydrogen atoms of the naphthalene rings are omitted for clarity.

4. Database survey

We have previously reported the structure of $\{[\mathrm{Co(H_2dondc)(H_2O)_4}]\cdot 2\mathrm{DMF}\}_n$ and a database survey using the Sci Finder database and Web of Science concerning H$_2$dondc^{2-} and Co$^{\rm II}$ (Kumagai *et al.*, 2025). This time a similar survey for H$_2$dondc^{2-} and Mn$^{\rm II}$ ion was conducted that resulted in no complete matches. The structures of metal complexes composed of an Mn$^{\rm II}$ ion and a dondc^{4-} ligand that form a three-dimensional network consisting of hexagonal channels have been reported (CADYOZ and CADYUF; Dietzel *et al.*, 2020).

5. Synthesis and crystallization

Manganese(II) chloride hexahydrate (0.39 g, 2.00 mmol) was dissolved in ethanol (20 mL). Lithium hydroxide (0.09 g, 4.00 mmol) and H_4dondc (0.24 g, 2.00 mmol) were dissolved in a mixture of water (10 mL) and DMF (10 mL). The Mn^{II} solution was poured into the mixture without stirring at room temperature. Single crystals were formed not only the interface of the solutions but also elsewhere due to the gradual diffusion of the solutions. Yellow crystals were obtained and one of these crystals was used for single-crystal X-ray crystallography analysis.

6. Refinement

The crystal data, data collection, and structure refinement details are summarized in Table 2. Hydrogen atoms attached to the phenolic hydroxy group and water molecules were extracted from difference-Fourier maps and refined isotropically. Other hydrogen atoms were placed in idealized positions (C—H = 0.95 Å) and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Mn(C_{12}H_6O_6)(H_2O)_4]$
M_r	373.17
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, b, c (Å)	5.2046 (3), 7.0001 (6), 9.8126 (8)
α, β, γ (°)	100.730 (7), 101.431 (6), 96.098 (6)
V (Å^3)	340.46 (5)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.03
Crystal size (mm)	0.13 × 0.07 × 0.05
Data collection	
Diffractometer	XtaLAB Synergy R, DW system, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2025)
T_{min}, T_{max}	0.698, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3959, 1563, 1373
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.088, 1.05
No. of reflections	1563
No. of parameters	126
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.48, −0.36

Computer programs: *CrysAlis PRO* (Rigaku OD, 2025), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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supporting information

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Crystal structure of *catena*-poly[[tetraaquamanganese(II)]-μ-1,5-dihydroxy-naphthalene-2,6-dicarboxylato]

Hitoshi Kumagai and Nobuhiro Ogihara

Computing details

catena-Poly[[tetraaquamanganese(II)]-μ-1,5-dihydroxynaphthalene-\ 2,6-dicarboxylato]

Crystal data

$[Mn(C_{12}H_6O_6)(H_2O)_4]$
M_r = 373.17
Triclinic, $P\overline{1}$
a = 5.2046 (3) Å
b = 7.0001 (6) Å
c = 9.8126 (8) Å
α = 100.730 (7)°
β = 101.431 (6)°
γ = 96.098 (6)°
V = 340.46 (5) Å^3
Z = 1
F(000) = 191
D_x = 1.820 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2369 reflections
θ = 3.0–30.5°
μ = 1.03 mm^{-1}
T = 150 K
Plate, clear yellow
0.13 × 0.07 × 0.05 mm

Data collection

XtaLAB Synergy R, DW system, HyPix diffractometer
Radiation source: Rotating-anode X-ray tube, Rigaku (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2025)
T_{min} = 0.698, T_{max} = 1.000
3959 measured reflections
1563 independent reflections
1373 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 27.5°, θ_{min} = 2.2°
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 8$
$l = -12 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.088
S = 1.05
1563 reflections
126 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Mn1	0.500000	0.000000	0.500000	0.01475 (16)
O5	0.7619 (3)	−0.1558 (2)	0.63695 (17)	0.0171 (3)
O1	0.4392 (3)	0.18483 (19)	0.68599 (15)	0.0165 (3)
O2	0.5957 (3)	0.4855 (2)	0.66930 (15)	0.0192 (3)
O3	0.1314 (3)	0.1263 (2)	0.84218 (16)	0.0159 (3)
O4	0.8266 (3)	0.2198 (2)	0.50602 (19)	0.0255 (4)
C2	0.2981 (4)	0.4521 (3)	0.8231 (2)	0.0134 (4)
C4	−0.0062 (4)	0.3969 (3)	0.9786 (2)	0.0132 (4)
C1	0.4570 (4)	0.3746 (3)	0.7202 (2)	0.0143 (4)
C6	0.3040 (4)	0.6571 (3)	0.8679 (2)	0.0148 (4)
H6	0.408213	0.744971	0.830212	0.018*
C3	0.1441 (4)	0.3249 (3)	0.8791 (2)	0.0121 (4)
C5	0.1639 (4)	0.7320 (3)	0.9640 (2)	0.0154 (4)
H5	0.171912	0.870198	0.992500	0.018*
H4A	0.825 (6)	0.336 (4)	0.557 (3)	0.050 (9)*
H4B	0.947 (5)	0.218 (4)	0.469 (3)	0.028 (7)*
H3	0.225 (5)	0.107 (4)	0.788 (3)	0.030 (7)*
H5A	0.713 (6)	−0.256 (4)	0.659 (3)	0.047 (9)*
H5B	0.836 (6)	−0.097 (4)	0.703 (3)	0.037 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0180 (2)	0.0118 (2)	0.0157 (3)	0.00224 (17)	0.00881 (17)	0.00079 (17)
O5	0.0203 (8)	0.0137 (8)	0.0179 (9)	0.0009 (6)	0.0063 (7)	0.0036 (7)
O1	0.0225 (7)	0.0108 (7)	0.0181 (8)	0.0025 (6)	0.0119 (6)	0.0004 (6)
O2	0.0262 (8)	0.0142 (7)	0.0225 (8)	0.0040 (6)	0.0162 (6)	0.0046 (6)
O3	0.0226 (8)	0.0098 (7)	0.0178 (8)	0.0024 (6)	0.0126 (6)	0.0010 (6)
O4	0.0237 (9)	0.0190 (9)	0.0346 (10)	−0.0009 (7)	0.0189 (8)	−0.0030 (7)
C2	0.0167 (9)	0.0121 (9)	0.0121 (10)	0.0038 (7)	0.0056 (7)	0.0009 (7)
C4	0.0151 (9)	0.0135 (10)	0.0120 (10)	0.0034 (8)	0.0048 (7)	0.0028 (7)
C1	0.0177 (9)	0.0136 (10)	0.0107 (10)	0.0027 (8)	0.0025 (8)	0.0005 (7)
C6	0.0187 (10)	0.0118 (9)	0.0149 (10)	0.0012 (8)	0.0059 (8)	0.0041 (8)
C3	0.0167 (9)	0.0085 (9)	0.0102 (9)	0.0029 (7)	0.0019 (7)	0.0006 (7)
C5	0.0213 (10)	0.0090 (9)	0.0170 (10)	0.0037 (8)	0.0065 (8)	0.0023 (8)

Geometric parameters (Å, º)

Mn1—O5	2.2335 (15)	O4—H4A	0.88 (3)
Mn1—O5^{i}	2.2335 (15)	O4—H4B	0.79 (3)
Mn1—O1^{i}	2.1310 (13)	C2—C1	1.490 (3)
Mn1—O1	2.1310 (13)	C2—C6	1.416 (3)
Mn1—O4	2.1521 (16)	C2—C3	1.394 (3)
Mn1—O4^{i}	2.1521 (16)	C4—C4^{ii}	1.417 (4)
O5—H5A	0.80 (3)	C4—C3	1.422 (3)
O5—H5B	0.71 (3)	C4—C5^{ii}	1.421 (3)
O1—C1	1.297 (2)	C6—H6	0.9500
O2—C1	1.241 (2)	C6—C5	1.365 (3)
O3—C3	1.361 (2)	C5—H5	0.9500
O3—H3	0.79 (3)		

O5—Mn1—O5^{i}	180.0	Mn1—O4—H4B	132.8 (19)
O1^{i}—Mn1—O5^{i}	89.70 (5)	H4A—O4—H4B	112 (3)
O1—Mn1—O5^{i}	90.30 (5)	C6—C2—C1	120.58 (17)
O1^{i}—Mn1—O5	90.30 (5)	C3—C2—C1	120.88 (17)
O1—Mn1—O5	89.70 (5)	C3—C2—C6	118.53 (18)
O1^{i}—Mn1—O1	180.0	C4^{ii}—C4—C3	118.3 (2)
O1^{i}—Mn1—O4	92.89 (6)	C4^{ii}—C4—C5^{ii}	120.0 (2)
O1—Mn1—O4^{i}	92.89 (6)	C5^{ii}—C4—C3	121.77 (17)
O1^{i}—Mn1—O4^{i}	87.11 (6)	O1—C1—C2	116.00 (17)
O1—Mn1—O4	87.11 (6)	O2—C1—O1	122.15 (18)
O4—Mn1—O5^{i}	88.22 (6)	O2—C1—C2	121.85 (17)
O4^{i}—Mn1—O5	88.22 (6)	C2—C6—H6	119.1
O4—Mn1—O5	91.78 (6)	C5—C6—C2	121.73 (18)
O4^{i}—Mn1—O5^{i}	91.78 (6)	C5—C6—H6	119.1
O4—Mn1—O4^{i}	180.0	O3—C3—C2	121.77 (17)
Mn1—O5—H5A	124 (2)	O3—C3—C4	116.76 (17)
Mn1—O5—H5B	116 (2)	C2—C3—C4	121.47 (17)
H5A—O5—H5B	102 (3)	C4^{ii}—C5—H5	120.0
C1—O1—Mn1	130.36 (12)	C6—C5—C4^{ii}	120.04 (18)
C3—O3—H3	106.0 (18)	C6—C5—H5	120.0
Mn1—O4—H4A	115 (2)		

Mn1—O1—C1—O2	−24.2 (3)	C6—C2—C1—O2	−1.0 (3)
Mn1—O1—C1—C2	155.01 (13)	C6—C2—C3—O3	−179.21 (17)
C2—C6—C5—C4^{ii}	−0.2 (3)	C6—C2—C3—C4	0.4 (3)
C4^{ii}—C4—C3—O3	178.9 (2)	C3—C2—C1—O1	0.9 (3)
C4^{ii}—C4—C3—C2	−0.7 (3)	C3—C2—C1—O2	−179.87 (18)
C1—C2—C6—C5	−178.81 (19)	C3—C2—C6—C5	0.1 (3)
C1—C2—C3—O3	−0.3 (3)	C5^{ii}—C4—C3—O3	−0.5 (3)
C1—C2—C3—C4	179.27 (17)	C5^{ii}—C4—C3—C2	179.88 (18)
C6—C2—C1—O1	179.77 (17)		

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x, -y+1, -z+2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O2	0.88 (3)	2.02 (3)	2.756 (2)	141 (3)
O4—H4*B*···O5^{iii}	0.79 (3)	2.04 (3)	2.814 (2)	169 (3)
O3—H3···O1	0.79 (3)	1.75 (3)	2.480 (2)	153 (3)
O5—H5*A*···O2^{iv}	0.80 (3)	1.88 (3)	2.664 (2)	168 (3)
O5—H5*B*···O3^{v}	0.71 (3)	2.13 (3)	2.798 (2)	157 (3)

Symmetry codes: (iii) $-x+2, -y, -z+1$; (iv) $x, y-1, z$; (v) $x+1, y, z$.