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catena-Poly[[[diaquamanganese(II)]-μ-oxalato] monohydrate]

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.001 Å
R factor = 0.020
wR factor = 0.054
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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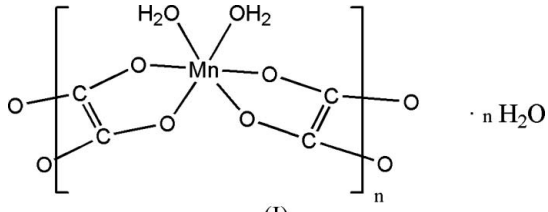
In the title compound, $\{[Mn(C_2O_4)(H_2O)_2]\cdot H_2O\}_n$, the octahedrally coordinated Mn atom, lying on a twofold rotation axis, is bonded to four carboxyl O atoms from oxalate groups and two O atoms from two water molecules. By means of the bridging oxalate ligand, the title compound exhibits a one-dimensional chain structure. The crystal packing is stabilized by hydrogen bonds of the type O—H···O(oxalate).

Comment

The oxalate dianion is well known as a bridging ligand and its coordination compounds have potential magnetic behavior (Verdaguer, 2001). Many of its bi-, tri-, tetranuclear, one-, two- and three-dimensional network compounds have been reported (Huizing *et al.*, 1977; Gleizes *et al.*, 1992; Sanada *et al.*, 1998).



(I)

We report here the crystal structure of one such compound, *catena*-poly[[[diaquamanganese(II)]-μ-oxalato] monohydrate], (I), composed of one-dimensional chains stabilized by hydrogen-bonding interactions. Each Mn^{II} atom has a distorted octahedral coordination comprising four O atoms (O1, O1*a*, O3*b* and O3*d*) from oxalate groups and two O atoms from two water molecules. The O2*a*—Mn1—O2 angle is 84.71 (5)°. The other important angles O1—Mn1—O3*b*, O2*a*–Mn1—O1, O2*a*—Mn1—O1*a* and O1*a*—Mn1—O3*b* are

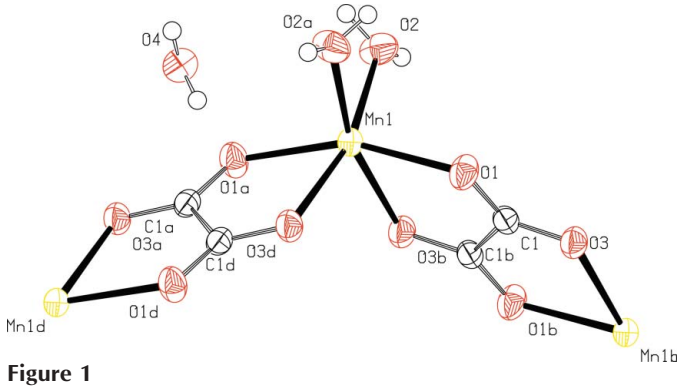


Figure 1
A view of the molecular structure of (I), showing labelling of 50% probability ellipsoids [Symmetry codes: (*a*) $\frac{1}{2}-x, 1-y, z$; (*b*) $-x, 1-y, z$; (*d*) $\frac{1}{2}+x, y, z$.]

90.57 (3), 92.09 (3), 103.84 (4) and 75.04 (3)°, respectively. The crystal packing involves O—H···O(oxalate) hydrogen bonds, resulting in a stable layered structure (Table 2 and Fig. 2).

Experimental

$MnCO_3$ (0.115 g, 1 mmol) was added to a solution of oxalic acid (0.216 g, 2 mmol) in water (15 ml) and the reaction mixture was stirred for 1 h at 323 K. After filtration, the pale-yellow solution was allowed to stand at room temperature. Pale-yellow needle-like crystals were formed by slow evaporation of the solvent at room temperature over approximately 15 d.

Crystal data

$[Mn(C_2O_4)(H_2O)_2]\cdot H_2O$
M_r = 197.01
Orthorhombic, *Pcca*
a = 9.7660 (9) Å
b = 6.6155 (6) Å
c = 10.5192 (10) Å
V = 679.61 (11) Å^3
Z = 4
D_x = 1.926 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2752 reflections
θ = 3.1–28.2°
μ = 1.93 mm^{-1}
T = 292 (2) K
Block, pale yellow
0.40 × 0.36 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.474, T_{max} = 0.654
3698 measured reflections
824 independent reflections
781 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 28.3°
$h = -13 \rightarrow 11$
$k = -8 \rightarrow 6$
$l = -12 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.054
S = 1.07
824 reflections
57 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2 + 0.0879P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0119 (16)

Table 1
Selected bond lengths (Å).

Mn1—O2	2.1561 (9)	Mn1—O3	2.2080 (8)
Mn1—O1	2.1862 (8)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O3^{i}	0.83 (2)	2.03 (2)	2.8234 (12)	160 (3)
O2—H2B···O4^{i}	0.83 (2)	1.87 (2)	2.6913 (12)	171 (2)
O4—H4A···O1	0.79 (2)	2.01 (2)	2.7554 (11)	159 (2)

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

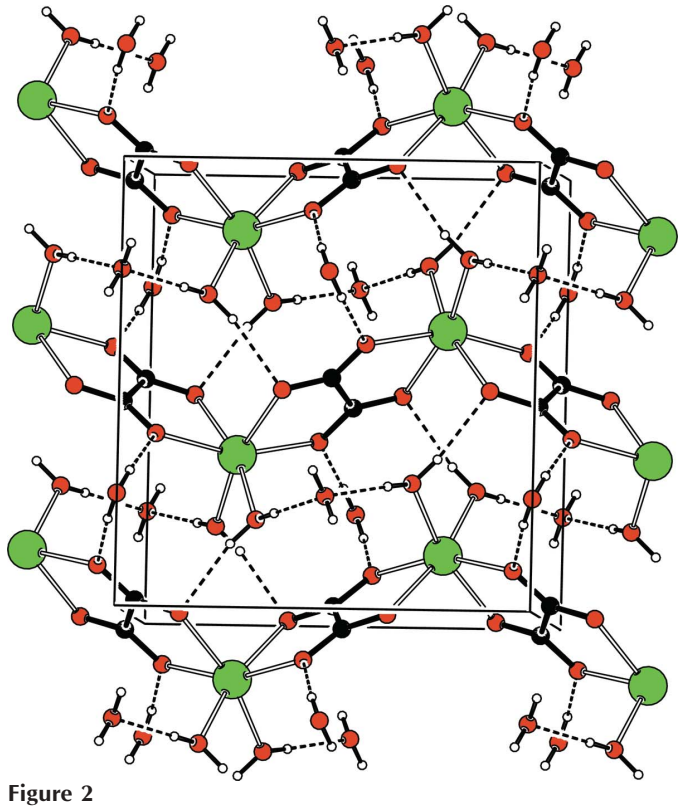


Figure 2
A view, approximately along the b axis, of the layered structure of the title compound. Hydrogen bonds are shown as dashed lines.

The H atoms of the water molecules were located in difference maps and were refined with restrained O—H distances.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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