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Disodium dimanganese(II) trioxalate dihydrate

Xin-Yang Huang^a and Yu-Ling Wang^{b*}

^aCollege of Electronics, Jiangxi University of Finance and Economy, Nanchang, Jiangxi 330013, People's Republic of China, and ^bCollege of Chemistry and Chemical Engineering, Jiangxi Normal University, Nanchang, Jiangxi 330022, People's Republic of China

Correspondence e-mail: ylwangchem@gmail.com

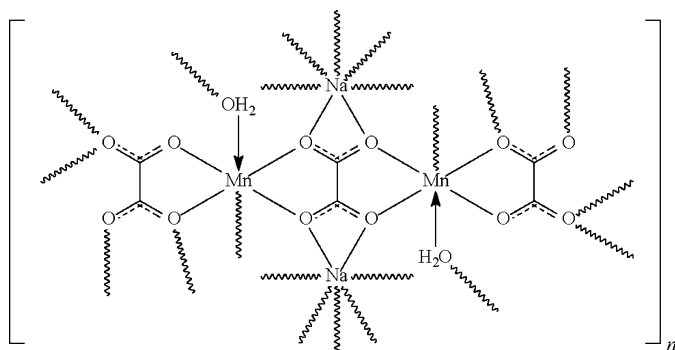
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Key indicators: single-crystal X-ray study; $T = 130$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.024; wR factor = 0.054; data-to-parameter ratio = 13.2.

In the crystal structure of the title compound, poly[di- μ_2 -aqua-di- μ_5 -oxalato- μ_4 -oxalato-disodiumdimanganese(II)], $[\text{Na}_2\text{Mn}_2(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})_2]_n$, one of the oxalate ions lies on an inversion centre. The Mn atom is six-coordinate and Na is seven-coordinate; two of the oxalate ions bridge in a μ_5 mode and the third in a μ_4 mode. The Mn atoms are bridged into a ladder motif; neighbouring ladders are bridged by the water molecules and Na atoms into a three-dimensional network structure. Water-oxalate hydrogen bonds exist in the structure.

Related literature

For related literature on metal oxalates, see: Bataille & Louër (1999); Castillo *et al.* (2001); Moulton & Zaworotko (2001); Naumov *et al.* (1995); Price *et al.* (2000); Wu *et al.* (2005); Yaghi *et al.* (1996).



Experimental

Crystal data

$[\text{Na}_2\text{Mn}_2(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})_2]$
 $M_r = 455.95$

Monoclinic, $P2_1/c$
 $a = 5.937$ (2) Å

$b = 15.785$ (6) Å
 $c = 7.167$ (3) Å
 $\beta = 100.416$ (4)°
 $V = 660.6$ (4) Å³
 $Z = 2$

Mo $K\alpha$ radiation
 $\mu = 2.06$ mm⁻¹
 $T = 130$ K
 $0.20 \times 0.18 \times 0.10$ mm

Data collection

Rigaku Mercury70 diffractometer
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku/MS, 2000)
 $T_{\min} = 0.684$, $T_{\max} = 0.821$

5047 measured reflections
 1514 independent reflections
 1415 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.054$
 $S = 1.03$
 1514 reflections
 115 parameters
 2 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.48$ e Å⁻³
 $\Delta\rho_{\min} = -0.33$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O7-H7A\cdots O2^i$	0.887 (10)	1.833 (11)	2.6877 (19)	161 (2)
$O7-H7B\cdots O3^{ii}$	0.889 (10)	1.947 (11)	2.8237 (19)	168 (2)

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

Data collection: *CrystalClear* (Rigaku/MS, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b) and *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2327).

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supplementary materials

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Disodium dimanganese(II) trioxalate dihydrate

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Comment

Carboxylate ligands have been extensively studied because of their versatile coordinating modes in the coordination chemistry (Moulton & Zaworotko, 2001; Yaghi *et al.*, 1996). Oxalate (ox) ligand is an important carboxylate ligand as it has a multiple coordinating modes, which together with the varied coordination geometry of metal ions has led to the generation of products containing one-dimensional chains, two-dimensional layers and three-dimensional frameworks (Castillo *et al.*, 2005; Naumov *et al.*, 1995; Bataille & Louër, 1999). The hydrothermal reaction of MnCl_2 with $\text{Na}_2(\text{ox})$ and oxalic acid yields the title complex, (I). We present its structure here.

The asymmetric unit of (I) consists of one manganese(II) ion, one sodium(I) ion, one and half ox dianions, and one coordinated water molecule. As depicted in Fig. 1, the Mn atom is six-coordinated by four oxygen atoms from three dianionic ox ligands in a distorted square planar geometry, and two oxygen atoms from water molecule and ox ligand in the apical positions. The bond dimensions involving Mn are normal (Table 1), and are comparable to the values in related manganese (II) complexes (Wu *et al.*, 2005). The Na atom is seven-coordinated by seven O atom from four dianionic ox ligands, and one water molecule with the Na—O bond lengths varying from 2.302 (2)–2.712 (2) Å, which are comparable to the values in the $[\text{Na}_2\text{Co}_2(\text{ox})_3(\text{H}_2\text{O})_2]_n$ compound (Price *et al.*, 2000).

It is interesting that the coordinated water molecule displays a μ_2 coordinating mode bridging the Mn1 and Na1 atoms, which further bridge by a μ_2 carboxylate O atom to form a 4-membered NaMnO_2 ring with a Na \cdots Mn separation of 3.55 Å (Fig. 1). Two types of ox ligands are observed in this structure. One is located on an inversion centre with a coplanar conformation and bridges two Mn atoms and two Na atoms, in which each O atom exhibits a μ_2 coordinating fashion. The other displays a nonplanar conformation with the two carboxylate groups twisted with a dihedral angle of 19.8 (5)°. It bridges two Mn atoms and three Na atoms using its two monodentate O atoms, one μ_2 -O atom and one μ_3 -O atom. The Mn ions are linked by the ox ligands to form a one-dimensional ladder structure propagating along *a* axis, as shown in Fig. 2. The ladder is repeated by translation about every 5.9 Å along the *a* direction, comparable to the length of the *a* axis. The ladders are further connected by the Na ions and water molecules through the Na—O bonds to produce a three-dimensional structure, as shown in Fig. 3. The O—H \cdots O hydrogen bonds between the water molecules and oxalate O atoms are observed in the three-dimensional structure with a O \cdots O distances of 2.688 (2) and 2.824 (2) Å, respectively (Table 2).

Experimental

The title compound was synthesized by a hydrothermal method under autogenous pressure. A mixture of $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ (0.269 g, 1 mmol), $\text{Na}_2\text{C}_2\text{O}_4$ (0.268 g, 2 mmol), $\text{H}_2\text{C}_2\text{O}_4$ (0.180 g, 2 mmol), and 15 ml distilled water was stirred under ambient conditions. The final mixture was sealed in a 25 ml Teflon-lined steel autoclave and heated at 423 K for 3 days, and then cooled to room temperature. Colorless prism crystals of (I) were obtained, and these were recovered by filtration, washed with distilled water and dried in air (yield 32%). Analysis calculated for $\text{C}_6\text{H}_4\text{O}_{14}\text{Mn}_2\text{Na}_2$: C 15.81, H 0.88%; found: C 15.92, H 0.90%.

Refinement

The H atoms bonded to O atoms were visible in difference maps and refined with a *DFIX* restraint (*SHELXTL*; Sheldrick, 1997b) of O—H = 0.90 Å and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Figures

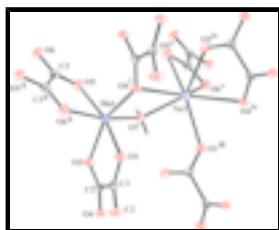


Fig. 1. ORTEP drawing of the title compound. Thermal ellipsoids are drawn at the 60% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $x + 1, y, z$; (ii) $-x + 2, -y + 1, -z + 2$; (iii) $x, -y + 1/2, z - 1/2$; (iv) $x + 1, -y + 1/2, z - 1/2$; (v) $-x + 2, -y + 1, -z + 1$.]

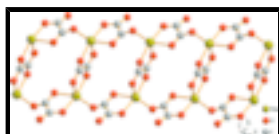


Fig. 2. A view of the one-dimensional $\text{Mn}_2(\text{ox})_3$ ladder-like structure.

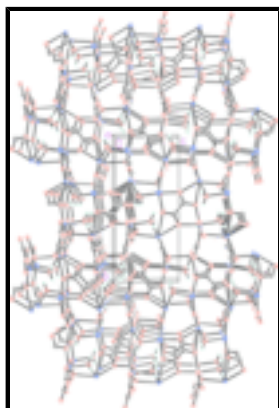


Fig. 3. A perspective view of the three-dimensional structure of (I) (viewed down the a axis).

poly[di- μ_2 -aqua-di- μ_5 -oxalato- μ_4 -oxalato-disodiumdimanganese(II)],

Crystal data

$[\text{Na}_2\text{Mn}_2(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})_2]$

$M_r = 455.95$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 5.937\ (2)\ \text{\AA}$

$b = 15.785\ (6)\ \text{\AA}$

$c = 7.167\ (3)\ \text{\AA}$

$\beta = 100.416\ (4)^\circ$

$V = 660.6\ (4)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 448$

$D_x = 2.292\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2218 reflections

$\theta = 2.6\text{--}27.5^\circ$

$\mu = 2.06\ \text{mm}^{-1}$

$T = 130\ \text{K}$

Prism, white

$0.20 \times 0.18 \times 0.10\ \text{mm}$

Data collection

Rigaku Mercury70 diffractometer	$R_{\text{int}} = 0.022$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 27.5^\circ$
Monochromator: graphite	$\theta_{\text{min}} = 2.6^\circ$
$T = 130$ K	$h = -7 \rightarrow 7$
ω scans	$k = -20 \rightarrow 17$
Absorption correction: multi-scan (CrystalClear; Rigaku/MSO, 2000)	$l = -9 \rightarrow 7$
$T_{\text{min}} = 0.684$, $T_{\text{max}} = 0.821$	Standard reflections: .;
5047 measured reflections	every . reflections
1514 independent reflections	intensity decay: .
1415 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.024$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0234P)^2 + 0.5936P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
1514 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
115 parameters	$\Delta\rho_{\text{max}} = 0.48 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\text{min}} = -0.33 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Na1	0.96700 (12)	0.32021 (4)	0.29951 (10)	0.01170 (16)

supplementary materials

Mn1	0.77063 (4)	0.396970 (16)	0.70734 (4)	0.00868 (9)
O1	0.6514 (2)	0.27044 (7)	0.73592 (18)	0.0122 (3)
O2	0.3505 (2)	0.19589 (8)	0.7916 (2)	0.0153 (3)
O3	0.3964 (2)	0.41196 (8)	0.71439 (18)	0.0121 (3)
O4	0.0795 (2)	0.33091 (8)	0.66136 (18)	0.0126 (3)
O5	0.8909 (2)	0.52445 (8)	0.76226 (18)	0.0128 (3)
O6	1.0935 (2)	0.60435 (8)	0.98897 (19)	0.0140 (3)
O7	0.6836 (2)	0.41824 (8)	0.40310 (18)	0.0111 (3)
H7A	0.556 (3)	0.3905 (12)	0.357 (3)	0.017*
H7B	0.676 (4)	0.4710 (8)	0.359 (3)	0.017*
C1	0.4430 (3)	0.26164 (11)	0.7476 (2)	0.0101 (3)
C2	0.2918 (3)	0.34261 (11)	0.7036 (2)	0.0095 (3)
C3	0.9948 (3)	0.53706 (11)	0.9280 (3)	0.0106 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0084 (3)	0.0128 (3)	0.0139 (3)	-0.0002 (3)	0.0021 (3)	0.0015 (3)
Mn1	0.00639 (14)	0.00773 (14)	0.01170 (14)	-0.00048 (9)	0.00103 (10)	-0.00016 (10)
O1	0.0066 (6)	0.0100 (6)	0.0203 (6)	-0.0002 (5)	0.0029 (5)	0.0017 (5)
O2	0.0094 (6)	0.0102 (6)	0.0262 (7)	-0.0014 (5)	0.0029 (5)	0.0042 (5)
O3	0.0088 (6)	0.0099 (6)	0.0177 (7)	0.0003 (5)	0.0024 (5)	0.0010 (5)
O4	0.0060 (6)	0.0142 (6)	0.0172 (6)	0.0008 (5)	0.0014 (5)	-0.0007 (5)
O5	0.0151 (7)	0.0101 (6)	0.0124 (6)	-0.0015 (5)	0.0000 (5)	0.0013 (5)
O6	0.0187 (7)	0.0098 (6)	0.0128 (6)	-0.0045 (5)	0.0008 (5)	0.0009 (5)
O7	0.0092 (6)	0.0096 (6)	0.0138 (6)	-0.0012 (5)	0.0001 (5)	0.0009 (5)
C1	0.0091 (8)	0.0091 (8)	0.0119 (8)	-0.0004 (6)	0.0010 (7)	-0.0007 (6)
C2	0.0082 (8)	0.0121 (8)	0.0087 (8)	0.0010 (6)	0.0026 (6)	-0.0002 (6)
C3	0.0094 (8)	0.0095 (8)	0.0132 (8)	0.0000 (6)	0.0030 (7)	0.0010 (7)

Geometric parameters (\AA , $^\circ$)

Na1—O2 ⁱ	2.3021 (17)	O2—Na1 ^{vii}	2.3021 (17)
Na1—O1 ⁱⁱ	2.3359 (15)	O3—C2	1.254 (2)
Na1—O6 ⁱⁱⁱ	2.3565 (16)	O4—C2	1.256 (2)
Na1—O7	2.4958 (16)	O4—Mn1 ^{viii}	2.1856 (14)
Na1—O4 ^{iv}	2.5638 (17)	O4—Na1 ^{viii}	2.5638 (17)
Na1—O5 ⁱⁱⁱ	2.6561 (16)	O4—Na1 ^{vii}	2.7121 (16)
Na1—O4 ⁱ	2.7121 (16)	O5—C3	1.251 (2)
Na1—C3 ⁱⁱⁱ	2.814 (2)	O5—Na1 ⁱⁱⁱ	2.6561 (16)
Mn1—O1	2.1411 (14)	O6—C3	1.253 (2)
Mn1—O5	2.1477 (14)	O6—Mn1 ^v	2.1803 (15)
Mn1—O7	2.1740 (15)	O6—Na1 ⁱⁱⁱ	2.3565 (16)
Mn1—O6 ^v	2.1803 (15)	O7—H7B	0.889 (10)
Mn1—O4 ^{iv}	2.1856 (14)	O7—H7A	0.887 (10)
Mn1—O3	2.2444 (15)	C1—C2	1.561 (2)

O1—C1	1.263 (2)	C3—C3 ^v	1.554 (3)
O1—Na1 ^{vi}	2.3359 (15)	C3—Na1 ⁱⁱⁱ	2.814 (2)
O2—C1	1.241 (2)		
O2 ⁱ —Na1—O1 ⁱⁱ	133.60 (6)	C1—O1—Mn1	116.98 (11)
O2 ⁱ —Na1—O6 ⁱⁱⁱ	91.64 (5)	C1—O1—Na1 ^{vi}	132.89 (11)
O1 ⁱⁱ —Na1—O6 ⁱⁱⁱ	98.56 (5)	Mn1—O1—Na1 ^{vi}	108.83 (6)
O2 ⁱ —Na1—O7	143.02 (5)	C1—O2—Na1 ^{vii}	125.70 (12)
O1 ⁱⁱ —Na1—O7	82.97 (5)	C2—O3—Mn1	112.82 (11)
O6 ⁱⁱⁱ —Na1—O7	86.77 (5)	C2—O4—Mn1 ^{viii}	136.59 (12)
O2 ⁱ —Na1—O4 ^{iv}	87.38 (5)	C2—O4—Na1 ^{viii}	108.68 (11)
O1 ⁱⁱ —Na1—O4 ^{iv}	106.90 (5)	Mn1 ^{viii} —O4—Na1 ^{viii}	96.42 (5)
O6 ⁱⁱⁱ —Na1—O4 ^{iv}	145.55 (5)	C2—O4—Na1 ^{vii}	110.12 (11)
O7—Na1—O4 ^{iv}	74.01 (5)	Mn1 ^{viii} —O4—Na1 ^{vii}	95.50 (5)
O2 ⁱ —Na1—O5 ⁱⁱⁱ	75.66 (5)	Na1 ^{viii} —O4—Na1 ^{vii}	105.96 (5)
O1 ⁱⁱ —Na1—O5 ⁱⁱⁱ	143.19 (5)	C3—O5—Mn1	114.42 (11)
O6 ⁱⁱⁱ —Na1—O5 ⁱⁱⁱ	52.40 (4)	C3—O5—Na1 ⁱⁱⁱ	83.95 (10)
O7—Na1—O5 ⁱⁱⁱ	74.26 (5)	Mn1—O5—Na1 ⁱⁱⁱ	159.97 (6)
O4 ^{iv} —Na1—O5 ⁱⁱⁱ	94.32 (4)	C3—O6—Mn1 ^v	113.92 (11)
O2 ⁱ —Na1—O4 ⁱ	65.42 (4)	C3—O6—Na1 ⁱⁱⁱ	97.75 (11)
O1 ⁱⁱ —Na1—O4 ⁱ	68.39 (5)	Mn1 ^v —O6—Na1 ⁱⁱⁱ	148.30 (6)
O6 ⁱⁱⁱ —Na1—O4 ⁱ	97.62 (5)	Mn1—O7—Na1	98.73 (5)
O7—Na1—O4 ⁱ	151.36 (5)	Mn1—O7—H7B	119.2 (15)
O4 ^{iv} —Na1—O4 ⁱ	113.01 (4)	Na1—O7—H7B	118.0 (15)
O5 ⁱⁱⁱ —Na1—O4 ⁱ	130.13 (5)	Mn1—O7—H7A	109.3 (15)
O1—Mn1—O5	163.98 (5)	Na1—O7—H7A	99.2 (15)
O1—Mn1—O7	102.55 (5)	H7B—O7—H7A	110 (2)
O5—Mn1—O7	92.86 (5)	O2—C1—O1	126.34 (16)
O1—Mn1—O6 ^v	87.97 (5)	O2—C1—C2	118.12 (16)
O5—Mn1—O6 ^v	77.01 (5)	O1—C1—C2	115.54 (15)
O7—Mn1—O6 ^v	168.70 (5)	O3—C2—O4	127.40 (16)
O1—Mn1—O4 ^{iv}	82.54 (5)	O3—C2—C1	116.24 (15)
O5—Mn1—O4 ^{iv}	102.38 (5)	O4—C2—C1	116.36 (15)
O7—Mn1—O4 ^{iv}	88.64 (5)	O5—C3—O6	125.80 (16)
O6 ^v —Mn1—O4 ^{iv}	88.67 (5)	O5—C3—C3 ^v	117.67 (19)
O1—Mn1—O3	75.55 (5)	O6—C3—C3 ^v	116.52 (19)
O5—Mn1—O3	101.24 (5)	O5—C3—Na1 ⁱⁱⁱ	69.81 (10)
O7—Mn1—O3	87.11 (5)	O6—C3—Na1 ⁱⁱⁱ	56.07 (9)
O6 ^v —Mn1—O3	99.66 (5)	C3 ^v —C3—Na1 ⁱⁱⁱ	171.83 (16)
O4 ^{iv} —Mn1—O3	156.18 (5)		
O2 ⁱ —Na1—Mn1—O1	-109.75 (6)	O6 ^v —Mn1—O1—C1	98.97 (13)
O1 ⁱⁱ —Na1—Mn1—O1	34.66 (4)	O4 ^{iv} —Mn1—O1—C1	-172.11 (13)

supplementary materials

O6 ⁱⁱⁱ —Na1—Mn1—O1	134.71 (6)	O3—Mn1—O1—C1	-1.55 (12)
O7—Na1—Mn1—O1	113.12 (6)	Na1—Mn1—O1—C1	-126.08 (12)
O4 ^{iv} —Na1—Mn1—O1	-83.84 (6)	Na1 ^{vi} —Mn1—O1—C1	168.66 (16)
O5 ⁱⁱⁱ —Na1—Mn1—O1	177.87 (5)	O5—Mn1—O1—Na1 ^{vi}	-89.89 (18)
O4 ⁱ —Na1—Mn1—O1	-22.03 (6)	O7—Mn1—O1—Na1 ^{vi}	106.15 (6)
C3 ⁱⁱⁱ —Na1—Mn1—O1	157.62 (5)	O6 ^v —Mn1—O1—Na1 ^{vi}	-69.69 (6)
Mn1 ⁱⁱ —Na1—Mn1—O1	6.34 (4)	O4 ^{iv} —Mn1—O1—Na1 ^{vi}	19.23 (6)
Na1 ⁱⁱ —Na1—Mn1—O1	38.17 (7)	O3—Mn1—O1—Na1 ^{vi}	-170.21 (7)
Na1 ^{vi} —Na1—Mn1—O1	-35.49 (4)	Na1—Mn1—O1—Na1 ^{vi}	65.25 (5)
O2 ⁱ —Na1—Mn1—O5	63.21 (6)	O1—Mn1—O3—C2	-9.55 (11)
O1 ⁱⁱ —Na1—Mn1—O5	-152.38 (5)	O5—Mn1—O3—C2	-173.45 (12)
O6 ⁱⁱⁱ —Na1—Mn1—O5	-52.33 (6)	O7—Mn1—O3—C2	94.20 (12)
O7—Na1—Mn1—O5	-73.92 (6)	O6 ^v —Mn1—O3—C2	-94.91 (12)
O4 ^{iv} —Na1—Mn1—O5	89.12 (6)	O4 ^{iv} —Mn1—O3—C2	14.2 (2)
O5 ⁱⁱⁱ —Na1—Mn1—O5	-9.17 (7)	Na1—Mn1—O3—C2	65.79 (12)
O4 ⁱ —Na1—Mn1—O5	150.93 (6)	Na1 ^{vi} —Mn1—O3—C2	-15.96 (12)
C3 ⁱⁱⁱ —Na1—Mn1—O5	-29.42 (6)	O1—Mn1—O5—C3	26.3 (3)
Mn1 ⁱⁱ —Na1—Mn1—O5	179.31 (4)	O7—Mn1—O5—C3	-169.35 (12)
Na1 ⁱⁱ —Na1—Mn1—O5	-148.87 (7)	O6 ^v —Mn1—O5—C3	5.57 (12)
Na1 ^{vi} —Na1—Mn1—O5	137.47 (4)	O4 ^{iv} —Mn1—O5—C3	-80.12 (13)
O2 ⁱ —Na1—Mn1—O7	137.13 (7)	O3—Mn1—O5—C3	103.03 (13)
O1 ⁱⁱ —Na1—Mn1—O7	-78.46 (6)	Na1—Mn1—O5—C3	-127.40 (12)
O6 ⁱⁱⁱ —Na1—Mn1—O7	21.58 (6)	Na1 ^{vi} —Mn1—O5—C3	-43.73 (15)
O4 ^{iv} —Na1—Mn1—O7	163.03 (7)	O1—Mn1—O5—Na1 ⁱⁱⁱ	-178.56 (14)
O5 ⁱⁱⁱ —Na1—Mn1—O7	64.74 (6)	O7—Mn1—O5—Na1 ⁱⁱⁱ	-14.22 (19)
O4 ⁱ —Na1—Mn1—O7	-135.15 (8)	O6 ^v —Mn1—O5—Na1 ⁱⁱⁱ	160.70 (19)
C3 ⁱⁱⁱ —Na1—Mn1—O7	44.50 (6)	O4 ^{iv} —Mn1—O5—Na1 ⁱⁱⁱ	75.01 (19)
Mn1 ⁱⁱ —Na1—Mn1—O7	-106.78 (6)	O3—Mn1—O5—Na1 ⁱⁱⁱ	-101.84 (18)
Na1 ⁱⁱ —Na1—Mn1—O7	-74.95 (8)	Na1—Mn1—O5—Na1 ⁱⁱⁱ	27.73 (19)
Na1 ^{vi} —Na1—Mn1—O7	-148.61 (5)	Na1 ^{vi} —Mn1—O5—Na1 ⁱⁱⁱ	111.40 (17)
O2 ⁱ —Na1—Mn1—O6 ^v	-26.93 (7)	O1—Mn1—O7—Na1	-69.96 (6)
O1 ⁱⁱ —Na1—Mn1—O6 ^v	117.49 (6)	O5—Mn1—O7—Na1	114.42 (6)
O6 ⁱⁱⁱ —Na1—Mn1—O6 ^v	-142.47 (8)	O6 ^v —Mn1—O7—Na1	88.3 (3)
O7—Na1—Mn1—O6 ^v	-164.05 (7)	O4 ^{iv} —Mn1—O7—Na1	12.09 (5)
O4 ^{iv} —Na1—Mn1—O6 ^v	-1.02 (7)	O3—Mn1—O7—Na1	-144.46 (5)
O5 ⁱⁱⁱ —Na1—Mn1—O6 ^v	-99.31 (6)	Na1 ^{vi} —Mn1—O7—Na1	-31.69 (5)
O4 ⁱ —Na1—Mn1—O6 ^v	60.79 (7)	O2 ⁱ —Na1—O7—Mn1	-73.35 (10)
C3 ⁱⁱⁱ —Na1—Mn1—O6 ^v	-119.56 (6)	O1 ⁱⁱ —Na1—O7—Mn1	99.18 (5)
Mn1 ⁱⁱ —Na1—Mn1—O6 ^v	89.17 (6)	O6 ⁱⁱⁱ —Na1—O7—Mn1	-161.78 (5)
Na1 ⁱⁱ —Na1—Mn1—O6 ^v	121.00 (7)	O4 ^{iv} —Na1—O7—Mn1	-10.70 (4)
Na1 ^{vi} —Na1—Mn1—O6 ^v	47.34 (5)	O5 ⁱⁱⁱ —Na1—O7—Mn1	-110.03 (5)

O2 ⁱ —Na1—Mn1—O4 ^{iv}	-25.91 (6)	O4 ⁱ —Na1—O7—Mn1	98.19 (10)
O1 ⁱⁱ —Na1—Mn1—O4 ^{iv}	118.50 (6)	C3 ⁱⁱⁱ —Na1—O7—Mn1	-136.63 (6)
O6 ⁱⁱⁱ —Na1—Mn1—O4 ^{iv}	-141.45 (7)	Mn1 ⁱⁱ —Na1—O7—Mn1	88.85 (5)
O7—Na1—Mn1—O4 ^{iv}	-163.03 (7)	Na1 ⁱⁱ —Na1—O7—Mn1	150.99 (4)
O5 ⁱⁱⁱ —Na1—Mn1—O4 ^{iv}	-98.29 (6)	Na1 ^{vi} —Na1—O7—Mn1	25.32 (4)
O4 ⁱ —Na1—Mn1—O4 ^{iv}	61.81 (6)	Na1 ^{vii} —O2—C1—O1	-177.19 (13)
C3 ⁱⁱⁱ —Na1—Mn1—O4 ^{iv}	-118.54 (6)	Na1 ^{vii} —O2—C1—C2	3.4 (2)
Mn1 ⁱⁱ —Na1—Mn1—O4 ^{iv}	90.19 (5)	Mn1—O1—C1—O2	-168.96 (14)
Na1 ⁱⁱ —Na1—Mn1—O4 ^{iv}	122.01 (9)	Na1 ^{vi} —O1—C1—O2	-3.7 (3)
Na1 ^{vi} —Na1—Mn1—O4 ^{iv}	48.36 (5)	Mn1—O1—C1—C2	10.45 (19)
O2 ⁱ —Na1—Mn1—O3	-179.73 (6)	Na1 ^{vi} —O1—C1—C2	175.74 (11)
O1 ⁱⁱ —Na1—Mn1—O3	-35.32 (5)	Mn1—O3—C2—O4	-162.51 (15)
O6 ⁱⁱⁱ —Na1—Mn1—O3	64.72 (6)	Mn1—O3—C2—C1	17.43 (18)
O7—Na1—Mn1—O3	43.14 (6)	Mn1 ^{viii} —O4—C2—O3	-34.9 (3)
O4 ^{iv} —Na1—Mn1—O3	-153.83 (6)	Na1 ^{viii} —O4—C2—O3	87.01 (19)
O5 ⁱⁱⁱ —Na1—Mn1—O3	107.88 (5)	Na1 ^{vii} —O4—C2—O3	-157.33 (15)
O4 ⁱ —Na1—Mn1—O3	-92.01 (6)	Mn1 ^{viii} —O4—C2—C1	145.13 (13)
C3 ⁱⁱⁱ —Na1—Mn1—O3	87.64 (6)	Na1 ^{viii} —O4—C2—C1	-92.93 (14)
Mn1 ⁱⁱ —Na1—Mn1—O3	-63.64 (4)	Na1 ^{vii} —O4—C2—C1	22.73 (17)
Na1 ⁱⁱ —Na1—Mn1—O3	-31.81 (8)	O2—C1—C2—O3	159.90 (16)
Na1 ^{vi} —Na1—Mn1—O3	-105.47 (4)	O1—C1—C2—O3	-19.6 (2)
O2 ⁱ —Na1—Mn1—Na1 ^{vi}	-74.26 (5)	O2—C1—C2—O4	-20.2 (2)
O1 ⁱⁱ —Na1—Mn1—Na1 ^{vi}	70.15 (4)	O1—C1—C2—O4	160.39 (15)
O6 ⁱⁱⁱ —Na1—Mn1—Na1 ^{vi}	170.19 (4)	Mn1—O5—C3—O6	174.76 (15)
O7—Na1—Mn1—Na1 ^{vi}	148.61 (5)	Na1 ⁱⁱⁱ —O5—C3—O6	3.09 (18)
O4 ^{iv} —Na1—Mn1—Na1 ^{vi}	-48.36 (5)	Mn1—O5—C3—C3 ^v	-4.7 (2)
O5 ⁱⁱⁱ —Na1—Mn1—Na1 ^{vi}	-146.65 (3)	Na1 ⁱⁱⁱ —O5—C3—C3 ^v	-176.4 (2)
O4 ⁱ —Na1—Mn1—Na1 ^{vi}	13.46 (6)	Mn1—O5—C3—Na1 ⁱⁱⁱ	171.67 (9)
C3 ⁱⁱⁱ —Na1—Mn1—Na1 ^{vi}	-166.89 (4)	Mn1 ^v —O6—C3—O5	175.21 (15)
Mn1 ⁱⁱ —Na1—Mn1—Na1 ^{vi}	41.83 (3)	Na1 ⁱⁱⁱ —O6—C3—O5	-3.5 (2)
Na1 ⁱⁱ —Na1—Mn1—Na1 ^{vi}	73.66 (7)	Mn1 ^v —O6—C3—C3 ^v	-5.3 (2)
O5—Mn1—O1—C1	78.8 (2)	Na1 ⁱⁱⁱ —O6—C3—C3 ^v	176.00 (18)
O7—Mn1—O1—C1	-85.19 (13)	Mn1 ^v —O6—C3—Na1 ⁱⁱⁱ	178.71 (12)

Symmetry codes: (i) $x+1, -y+1/2, z-1/2$; (ii) $x, -y+1/2, z-1/2$; (iii) $-x+2, -y+1, -z+1$; (iv) $x+1, y, z$; (v) $-x+2, -y+1, -z+2$; (vi) $x, -y+1/2, z+1/2$; (vii) $x-1, -y+1/2, z+1/2$; (viii) $x-1, y, z$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O7—H7A \cdots O2 ⁱⁱ	0.887 (10)	1.833 (11)	2.6877 (19)	161 (2)
O7—H7B \cdots O3 ^{ix}	0.889 (10)	1.947 (11)	2.8237 (19)	168 (2)

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

Fig. 1

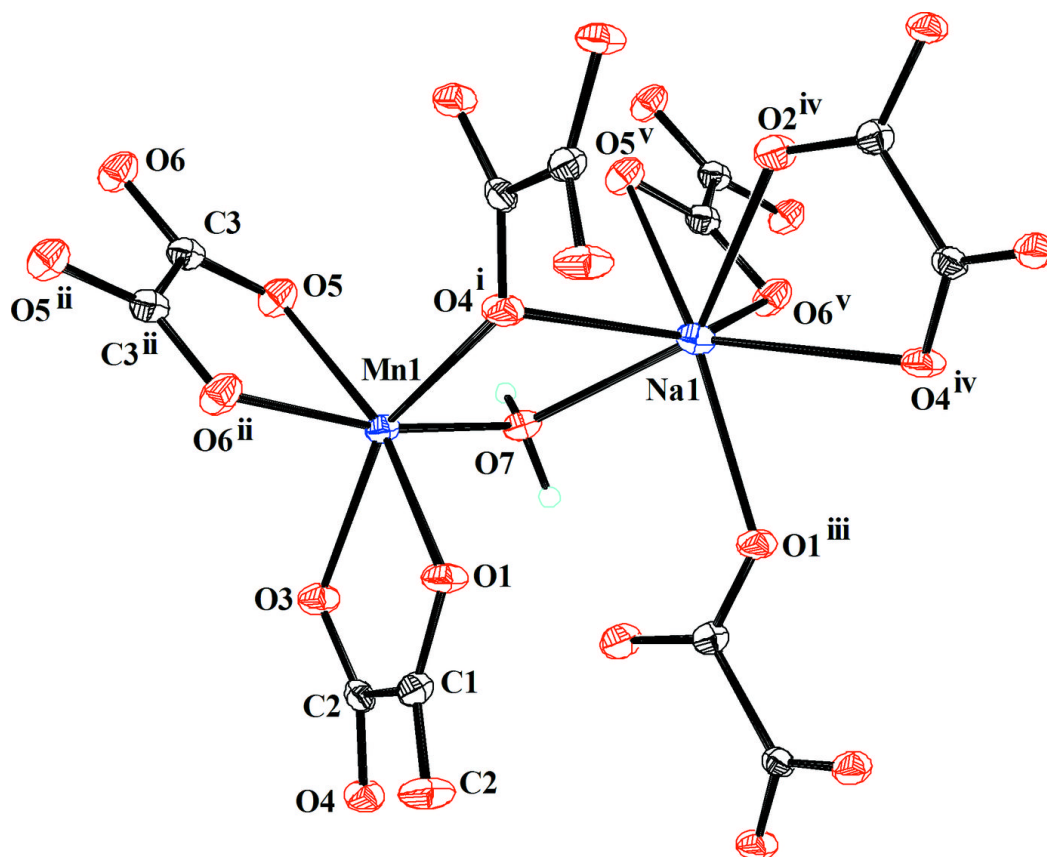


Fig. 3

