Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[triaqua(butane-1,2,3,4-tetracarboxylato)dimanganese(II)] monohydrate]

Ling Wu

Jilin Agriculture Engineering Polytechnic College, Siping 136000, People's Republic of China
Correspondence e-mail: jlliangshizhuangke@yahoo.com.cn

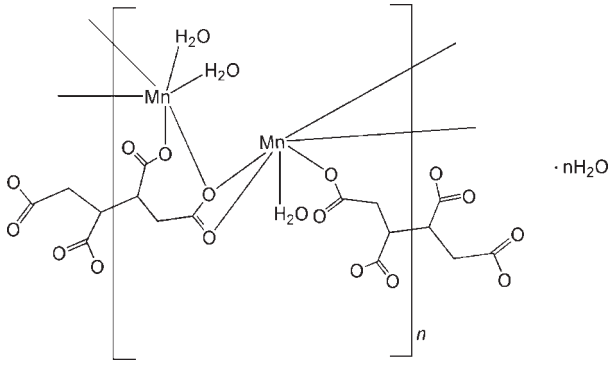
Received 19 October 2009; accepted 19 October 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.106; data-to-parameter ratio = 13.4.

The asymmetric unit of the title Mn^{II} coordination polymer, $\{[Mn_2(C_8H_6O_8)(H_2O)_3]\cdot H_2O\}_n$, contains two crystallographically independent Mn^{II} cations, two half butane-1,2,3,4-tetracarboxylato anions, each lying on a centre of inversion, and four water molecules. The Mn^{II} cation has a distorted octahedral coordination environment. One Mn centre is coordinated by four carboxylate O atoms from two different anions and two water O atoms. The other Mn centre is coordinated by five carboxylate O atoms from four different anions and one water O atom. One water molecule does not coordinate to a Mn centre. The crystal packing is stabilized by several O—H···O hydrogen bonds, forming a three-dimensional framework.

Related literature

For multicarboxylate ligands in the construction of coordination polymers, see: Yang *et al.* (2008). For butane-1,2,3,4-tetracarboxylic acid in coordination chemistry, see: Liu *et al.* (2008).



Experimental

Crystal data

$[Mn_2(C_8H_6O_8)(H_2O)_3]\cdot H_2O$
M_r = 824.14
Monoclinic, $P2_1/n$
a = 8.1962 (4) Å
b = 12.3291 (7) Å
c = 12.9758 (6) Å
β = 97.760 (5)°
V = 1299.22 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.01 mm^{-1}
T = 293 K
0.33 × 0.21 × 0.17 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.764, T_{max} = 0.852
7085 measured reflections
3031 independent reflections
1990 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.106
S = 0.88
3031 reflections
227 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2W—HW22···O6^{i}	0.843 (10)	2.46 (5)	2.998 (4)	122 (4)
O2W—HW22···O4W	0.843 (10)	2.39 (4)	2.985 (10)	128 (4)
O3W—HW31···O4^{ii}	0.850 (10)	2.075 (19)	2.874 (4)	156 (4)
O4W—HW41···O1^{ii}	0.86 (12)	2.43 (14)	3.091 (12)	133 (16)
O4W—HW42···O6^{iii}	0.85 (13)	2.58 (14)	3.124 (11)	123 (14)
O1W—HW11···O7^{iv}	0.850 (10)	2.098 (11)	2.944 (4)	173 (4)
O1W—HW12···O3^{ii}	0.854 (10)	2.39 (4)	2.935 (4)	123 (3)
O2W—HW21···O2^{iii}	0.845 (10)	1.919 (18)	2.731 (4)	161 (4)
O3W—HW32···O2W^{v}	0.849 (10)	2.333 (17)	3.155 (5)	163 (5)

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+2, -y+1, -z+2$; (v) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The author thanks Jilin Agriculture Engineering Polytechnic College for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5105).

References

Bruker (1997). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, Y.-Y., Ma, J.-F., Yang, J., Ma, J.-C. & Su, Z.-M. (2008). *CrystEngComm*, **10**, 894–904.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yang, J., Ma, J.-F., Batten, S. R. & Su, Z.-M. (2008). *Chem. Commun.* pp. 2233–2235.

supplementary materials

Acta Cryst. (2009). E**65**, m1425 [**doi:10.1107/S1600536809042998**]

Poly[[triaqua(butane-1,2,3,4-tetracarboxylato)dimanganese(II)] monohydrate]

L. Wu

Comment

So far, the multicarboxylate ligands, such as 1,2,3-benzenedicarboxylic acid, 1,2,4-benzenedicarboxylic acid and 1,3,5-benzenedicarboxylic acid, are widely used to construct the coordination polymers with interesting properties (Yang *et al.* 2008). In this regard, butane-1,2,3,4-tetracarboxylatic acid (H_4L) is also a good ligand in coordination chemistry due to its strong coordination ability and versatile coordination modes, so much attention has been paid to it in recent years (Liu *et al.* 2008). In this contribution, H_4L was selected as a bridging ligand, and a new manganese coordination polymer, namely $[Mn_2(L)(H_2O)_3]\cdot H_2O$ (**I**).

As shown in Fig. 1, the asymmetric unit of **(I)** contains two crystallographically Mn^{II} cation, two half *L* anions and four water molecules. The *L* ligand ligand is at an inversion center. Each Mn^{II} cation has a distorted octahedral coordination environment. Mn1 is coordinated by four carboxylate O atoms from two different *L* anions and two water O atoms. Mn2 is coordinated by five carboxylate O atoms from three different *L* anions and one water O atom. The *L* ligands bridging the neighboring Mn^{II} centers to form a complicated three-dimensional framework structure of **(I)** (Fig. 2). The hydrogen-bonding interactions between the water molecules and the carboxylate O atoms further stabilize the three-dimensional framework structure of **(I)**.

Experimental

A mixture of $Mn(NO_3)_2.6H_2O$ (0.10 mmol), H_4L (0.05 mmol) and water (12 ml) was sealed in a Teflon reactor (15 ml), which was heated at 140 °C for 3 days and then gradually cooled to room temperature. Purple crystals of **(I)** were isolated (yield 64% based on Mn).

Refinement

H atoms bonded to C atom were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H)=1.2U_{eq}$(carrier). The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H = 0.85±0.01 Å and H···H = 1.35±0.01 Å; their temperature factors were tied to those of parent atoms by a factor of 1.5.

Figures

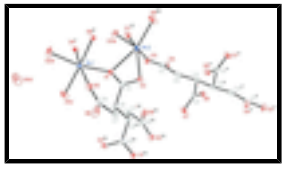


Fig. 1. A view of the local coordination of the Mn^{II} cations in **(I)**, showing the atom-numbering scheme. Displacement ellipsoids at the 30% probability level (symmetry operations i: 2.5-*x*, *y*-0.5, 1.5-*z*; ii: *x*-0.5, 1.5-*y*, *z*-0.5; iii: 1.5-*x*, *y*+0.5, 1.5-*z*; iv: 2-*x*, 1-*y*, 2-*z*); v: 2-*x*, 2-*y*, 2-*z*).

catena-Poly[triaqua[bis[manganese(II)]]-butane-1,2,3,4-tetracarboxylato] hydrate

Crystal data

$[Mn_2(C_8H_6O_8)(H_2O)_3]\cdot H_2O$	$F_{000} = 832$
$M_r = 824.14$	$D_x = 2.107$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 3031 reflections
$a = 8.1962$ (4) Å	$\theta = 3.0$–$29.1°$
$b = 12.3291$ (7) Å	$\mu = 2.01$ mm^{-1}
$c = 12.9758$ (6) Å	$T = 293$ K
$\beta = 97.760$ (5)°	Block, colorless
$V = 1299.22$ (11) Å^3	0.33 × 0.21 × 0.17 mm
$Z = 2$	

Data collection

Bruker APEX CCD area-detector diffractometer	3031 independent reflections
Radiation source: fine-focus sealed tube	1990 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.040$
$T = 293$ K	$\theta_{max} = 29.1°$
ω scans	$\theta_{min} = 3.0°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11\rightarrow7$
$T_{min} = 0.764$, $T_{max} = 0.852$	$k = -12\rightarrow15$
7085 measured reflections	$l = -17\rightarrow17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.106$	$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.88$	$(\Delta/\sigma)_{max} < 0.001$
3031 reflections	$\Delta\rho_{max} = 0.63$ e Å^{-3}
227 parameters	$\Delta\rho_{min} = -0.83$ e Å^{-3}
12 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.1879 (4)	0.8429 (3)	0.8558 (3)	0.0198 (8)
C2	1.0480 (4)	0.8783 (3)	0.9135 (3)	0.0271 (9)
H2A	1.0241	0.8197	0.9590	0.033*
H2B	0.9507	0.8893	0.8630	0.033*
C3	1.0781 (4)	0.9804 (3)	0.9778 (3)	0.0205 (7)
H3	1.1109	1.0378	0.9325	0.025*
C4	1.2178 (4)	0.9664 (3)	1.0691 (3)	0.0193 (8)
C5	0.9481 (4)	0.5441 (3)	0.8594 (3)	0.0193 (8)
C6	0.9556 (4)	0.4695 (3)	0.9522 (2)	0.0220 (8)
H6	1.0203	0.4052	0.9395	0.026*
C7	0.7837 (5)	0.4336 (3)	0.9692 (3)	0.0306 (9)
H7A	0.7915	0.3939	1.0343	0.037*
H7B	0.7172	0.4976	0.9760	0.037*
C8	0.6978 (5)	0.3639 (3)	0.8845 (3)	0.0275 (9)
O1	1.0249 (3)	0.5178 (2)	0.78555 (18)	0.0248 (6)
O2	0.8740 (3)	0.6329 (2)	0.85773 (19)	0.0263 (6)
O1W	1.0570 (4)	0.2456 (3)	0.8215 (3)	0.0391 (8)
O3	1.1646 (3)	0.7613 (2)	0.7983 (2)	0.0287 (6)
O2W	0.9047 (4)	0.2290 (3)	0.5915 (3)	0.0425 (8)
HW22	0.969 (4)	0.181 (3)	0.575 (4)	0.064*
O4	1.3228 (3)	0.8944 (2)	0.87012 (19)	0.0253 (6)
O3W	1.1264 (4)	0.6245 (3)	0.6096 (2)	0.0357 (7)
HW31	1.129 (6)	0.5569 (10)	0.597 (3)	0.054*
O5	0.7513 (3)	0.3496 (2)	0.7980 (2)	0.0317 (7)
O4W	1.0955 (15)	0.0359 (7)	0.6785 (11)	0.192 (4)
HW41	1.181 (13)	0.011 (12)	0.654 (14)	0.288*
HW42	1.06 (2)	−0.021 (8)	0.705 (14)	0.288*
O6	0.5696 (4)	0.3186 (3)	0.9039 (3)	0.0458 (9)
O7	1.2229 (3)	0.8806 (2)	1.12238 (19)	0.0268 (6)
O8	1.3177 (3)	1.0437 (2)	1.08580 (19)	0.0253 (6)
Mn1	0.96260 (7)	0.36380 (5)	0.70273 (4)	0.02057 (16)
Mn2	0.95382 (6)	0.68692 (4)	0.70684 (4)	0.01775 (15)
HW11	0.979 (4)	0.205 (3)	0.835 (4)	0.064 (18)*

HW12	1.129 (4)	0.203 (3)	0.802 (4)	0.065 (18)*
HW21	0.812 (2)	0.198 (3)	0.592 (4)	0.041 (14)*
HW32	1.102 (6)	0.654 (3)	0.5505 (18)	0.063 (18)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0179 (17)	0.025 (2)	0.0152 (16)	0.0031 (16)	−0.0039 (14)	0.0026 (15)
C2	0.0181 (18)	0.032 (2)	0.0288 (19)	0.0020 (17)	−0.0043 (16)	−0.0103 (17)
C3	0.0188 (17)	0.0238 (19)	0.0173 (16)	0.0020 (16)	−0.0032 (14)	−0.0006 (15)
C4	0.0162 (16)	0.023 (2)	0.0180 (16)	0.0050 (16)	−0.0016 (14)	−0.0002 (16)
C5	0.0191 (17)	0.021 (2)	0.0153 (16)	−0.0061 (16)	−0.0080 (14)	−0.0003 (14)
C6	0.0279 (18)	0.0190 (19)	0.0169 (16)	−0.0047 (17)	−0.0054 (15)	−0.0017 (15)
C7	0.035 (2)	0.030 (2)	0.0261 (19)	−0.010 (2)	−0.0026 (17)	0.0011 (18)
C8	0.026 (2)	0.017 (2)	0.036 (2)	0.0032 (17)	−0.0059 (18)	−0.0048 (17)
O1	0.0317 (14)	0.0231 (14)	0.0188 (12)	−0.0017 (12)	0.0005 (11)	−0.0016 (11)
O2	0.0284 (14)	0.0264 (16)	0.0232 (13)	0.0014 (12)	0.0005 (11)	0.0024 (12)
O1W	0.0288 (16)	0.0375 (19)	0.0508 (19)	0.0121 (16)	0.0045 (15)	0.0166 (16)
O3	0.0197 (13)	0.0327 (16)	0.0328 (14)	−0.0037 (12)	0.0006 (11)	−0.0140 (13)
O2W	0.0367 (17)	0.0322 (18)	0.061 (2)	−0.0119 (15)	0.0148 (16)	−0.0229 (16)
O4	0.0191 (12)	0.0246 (15)	0.0323 (14)	−0.0045 (11)	0.0040 (11)	−0.0093 (12)
O3W	0.0359 (17)	0.0418 (19)	0.0312 (16)	−0.0032 (15)	0.0116 (14)	−0.0101 (14)
O5	0.0291 (15)	0.0325 (17)	0.0296 (15)	0.0015 (13)	−0.0098 (12)	−0.0031 (13)
O4W	0.179 (9)	0.162 (8)	0.243 (11)	0.014 (6)	0.060 (8)	0.014 (8)
O6	0.0260 (15)	0.047 (2)	0.065 (2)	−0.0131 (15)	0.0074 (15)	−0.0301 (17)
O7	0.0205 (12)	0.0259 (16)	0.0313 (14)	0.0006 (11)	−0.0070 (11)	0.0080 (12)
O8	0.0227 (13)	0.0288 (16)	0.0226 (12)	−0.0054 (12)	−0.0035 (10)	0.0006 (11)
Mn1	0.0198 (3)	0.0200 (3)	0.0207 (3)	−0.0005 (2)	−0.0016 (2)	0.0007 (2)
Mn2	0.0165 (3)	0.0188 (3)	0.0166 (3)	0.0002 (2)	−0.0029 (2)	0.0014 (2)

Geometric parameters (Å, °)

C1—O3	1.252 (4)	O1—Mn2	2.360 (3)
C1—O4	1.267 (4)	O2—Mn2	2.247 (2)
C1—C2	1.515 (5)	O1W—Mn1	2.185 (3)
C2—C3	1.512 (5)	O1W—HW11	0.850 (10)
C2—H2A	0.9700	O1W—HW12	0.854 (10)
C2—H2B	0.9700	O3—Mn2	2.163 (3)
C3—C4	1.542 (5)	O2W—Mn1	2.211 (3)
C3—C3^{i}	1.549 (7)	O2W—HW22	0.843 (10)
C3—H3	0.9800	O2W—HW21	0.845 (10)
C4—O8	1.257 (4)	O4—Mn1^{iii}	2.140 (2)
C4—O7	1.262 (4)	O3W—Mn2	2.160 (3)
C5—O2	1.251 (4)	O3W—HW31	0.850 (10)
C5—O1	1.258 (4)	O3W—HW32	0.849 (10)
C5—C6	1.510 (5)	O5—Mn1	2.267 (3)
C6—C7	1.521 (5)	O4W—HW41	0.86 (12)
C6—C6^{ii}	1.546 (7)	O4W—HW42	0.85 (13)

C6—H6	0.9800	O6—Mn2^{iv}	2.160 (3)
C7—C8	1.494 (6)	O7—Mn2^{v}	2.217 (3)
C7—H7A	0.9700	O8—Mn1^{v}	2.127 (3)
C7—H7B	0.9700	Mn1—O8^{vi}	2.127 (3)
C8—O6	1.245 (5)	Mn1—O4^{vii}	2.140 (2)
C8—O5	1.271 (5)	Mn2—O6^{viii}	2.160 (3)
O1—Mn1	2.207 (3)	Mn2—O7^{vi}	2.217 (3)
O3—C1—O4	123.3 (3)	C1—O3—Mn2	135.5 (2)
O3—C1—C2	117.5 (3)	Mn1—O2W—HW22	128 (3)
O4—C1—C2	119.2 (3)	Mn1—O2W—HW21	116 (3)
C1—C2—C3	115.7 (3)	HW22—O2W—HW21	106.4 (17)
C1—C2—H2A	108.3	C1—O4—Mn1^{iii}	126.9 (2)
C3—C2—H2A	108.3	Mn2—O3W—HW31	120 (3)
C1—C2—H2B	108.3	Mn2—O3W—HW32	106 (3)
C3—C2—H2B	108.3	HW31—O3W—HW32	104.9 (16)
H2A—C2—H2B	107.4	C8—O5—Mn1	148.3 (3)
C2—C3—C4	112.3 (3)	HW41—O4W—HW42	101 (13)
C2—C3—C3^{i}	112.5 (4)	C8—O6—Mn2^{iv}	101.8 (2)
C4—C3—C3^{i}	108.3 (3)	C4—O7—Mn2^{v}	123.3 (2)
C2—C3—H3	107.8	C4—O8—Mn1^{v}	144.9 (2)
C4—C3—H3	107.8	O8^{vi}—Mn1—O4^{vii}	90.20 (9)
C3^{i}—C3—H3	107.8	O8^{vi}—Mn1—O1W	166.12 (11)
O8—C4—O7	124.7 (3)	O4^{vii}—Mn1—O1W	101.26 (10)
O8—C4—C3	116.5 (3)	O8^{vi}—Mn1—O1	87.51 (10)
O7—C4—C3	118.8 (3)	O4^{vii}—Mn1—O1	85.02 (10)
O2—C5—O1	120.3 (3)	O1W—Mn1—O1	101.15 (11)
O2—C5—C6	120.9 (3)	O8^{vi}—Mn1—O2W	83.53 (12)
O1—C5—C6	118.7 (3)	O4^{vii}—Mn1—O2W	87.77 (11)
C5—C6—C7	110.8 (3)	O1W—Mn1—O2W	89.06 (14)
C5—C6—C6^{ii}	107.9 (4)	O1—Mn1—O2W	168.48 (11)
C7—C6—C6^{ii}	111.8 (4)	O8^{vi}—Mn1—O5	92.08 (10)
C5—C6—H6	108.8	O4^{vii}—Mn1—O5	171.42 (10)
C7—C6—H6	108.8	O1W—Mn1—O5	77.75 (11)
C6^{ii}—C6—H6	108.8	O1—Mn1—O5	86.81 (9)
C8—C7—C6	114.5 (3)	O2W—Mn1—O5	100.70 (11)
C8—C7—H7A	108.6	O3W—Mn2—O6^{viii}	83.43 (13)
C6—C7—H7A	108.6	O3W—Mn2—O3	86.20 (11)
C8—C7—H7B	108.6	O6^{viii}—Mn2—O3	92.23 (12)
C6—C7—H7B	108.6	O3W—Mn2—O7^{vi}	99.22 (11)
H7A—C7—H7B	107.6	O6^{viii}—Mn2—O7^{vi}	87.70 (12)
O6—C8—O5	121.2 (4)	O3—Mn2—O7^{vi}	174.53 (10)
O6—C8—C7	115.8 (3)	O3W—Mn2—O2	133.95 (12)
O5—C8—C7	123.0 (4)	O6^{viii}—Mn2—O2	142.39 (11)

C5—O1—Mn1	119.0 (2)	O3—Mn2—O2	87.30 (10)
C5—O1—Mn2	89.0 (2)	O7^{vi}—Mn2—O2	89.42 (10)
Mn1—O1—Mn2	121.45 (11)	O3W—Mn2—O1	78.19 (11)
C5—O2—Mn2	94.4 (2)	O6^{viii}—Mn2—O1	161.24 (11)
Mn1—O1W—HW11	110 (3)	O3—Mn2—O1	90.28 (10)
Mn1—O1W—HW12	114 (4)	O7^{vi}—Mn2—O1	91.54 (10)
HW11—O1W—HW12	104.7 (16)	O2—Mn2—O1	56.30 (9)

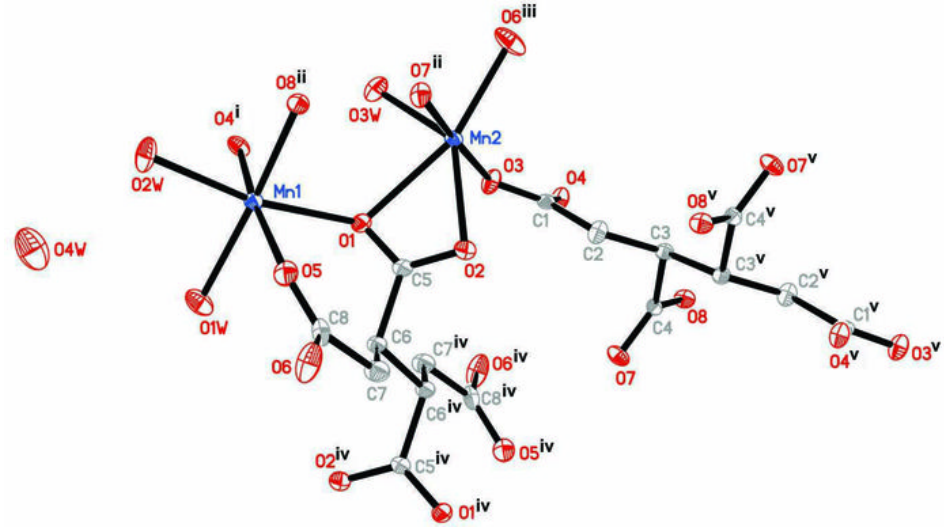
Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+2; (ii) −*x*+2, −*y*+1, −*z*+2; (iii) −*x*+5/2, *y*+1/2, −*z*+3/2; (iv) −*x*+3/2, *y*−1/2, −*z*+3/2; (v) *x*+1/2, −*y*+3/2, *z*+1/2; (vi) *x*−1/2, −*y*+3/2, *z*−1/2; (vii) −*x*+5/2, *y*−1/2, −*z*+3/2; (viii) −*x*+3/2, *y*+1/2, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2W—HW22···O6^{ix}	0.843 (10)	2.46 (5)	2.998 (4)	122 (4)
O2W—HW22···O4W	0.843 (10)	2.39 (4)	2.985 (10)	128 (4)
O3W—HW31···O4^{vii}	0.850 (10)	2.075 (19)	2.874 (4)	156 (4)
O4W—HW41···O1^{vii}	0.86 (12)	2.43 (14)	3.091 (12)	133 (16)
O4W—HW42···O6^{iv}	0.85 (13)	2.58 (14)	3.124 (11)	123 (14)
O1W—HW11···O7^{ii}	0.850 (10)	2.098 (11)	2.944 (4)	173 (4)
O1W—HW12···O3^{vii}	0.854 (10)	2.39 (4)	2.935 (4)	123 (3)
O2W—HW21···O2^{iv}	0.845 (10)	1.919 (18)	2.731 (4)	161 (4)
O3W—HW32···O2W^{x}	0.849 (10)	2.333 (17)	3.155 (5)	163 (5)

Symmetry codes: (ix) *x*+1/2, −*y*+1/2, *z*−1/2; (vii) −*x*+5/2, *y*−1/2, −*z*+3/2; (iv) −*x*+3/2, *y*−1/2, −*z*+3/2; (ii) −*x*+2, −*y*+1, −*z*+2; (x) −*x*+2, −*y*+1, −*z*+1.

Fig. 1


O6iii
O7ii
O8ii
O4i
O3W
Mn2
O2W
Mn1
O3
O4
O7v
O8v
C4v
C1
C2
C3
C3v
C2v
O4W
O1
O5
C5
O2
O1W
C8
C6
C7iv
O6iv
O6
C7
C8iv
C6iv
C4
O8
C1v
O4v
O3v
O7
O2iv
C5iv
O5iv
O1iv