

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

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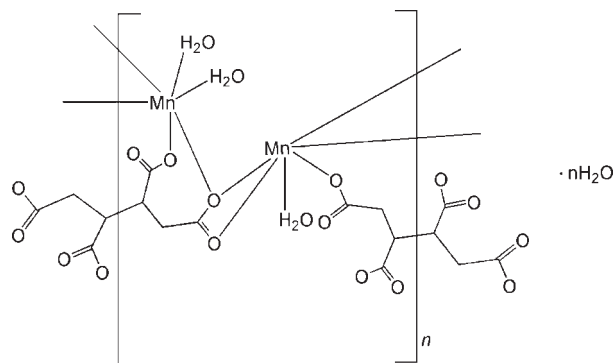
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.041; wR factor = 0.106; data-to-parameter ratio = 13.4.

The asymmetric unit of the title Mn^{II} coordination polymer, $\{[\text{Mn}_2(\text{C}_8\text{H}_6\text{O}_8)(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}\}_n$, 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 $\text{O}-\text{H}\cdots\text{O}$ 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

 $[\text{Mn}_2(\text{C}_8\text{H}_6\text{O}_8)(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$
 $M_r = 824.14$

 Monoclinic, $P2_1/n$
 $a = 8.1962$ (4) Å

 $b = 12.3291$ (7) Å

 $c = 12.9758$ (6) Å

 $\beta = 97.760$ (5)°

 $V = 1299.22$ (11) Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 2.01$ mm⁻¹
 $T = 293$ K

 $0.33 \times 0.21 \times 0.17$ mm

Data collection

Bruker APEX CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{\text{min}} = 0.764$, $T_{\text{max}} = 0.852$

7085 measured reflections

3031 independent reflections

 1990 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

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

 $\Delta\rho_{\text{max}} = 0.63$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.83$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O}2\text{W}-\text{HW}22\cdots\text{O}6^{\text{i}}$	0.843 (10)	2.46 (5)	2.998 (4)	122 (4)
$\text{O}2\text{W}-\text{HW}22\cdots\text{O}4\text{W}$	0.843 (10)	2.39 (4)	2.985 (10)	128 (4)
$\text{O}3\text{W}-\text{HW}31\cdots\text{O}4^{\text{ii}}$	0.850 (10)	2.075 (19)	2.874 (4)	156 (4)
$\text{O}4\text{W}-\text{HW}41\cdots\text{O}1^{\text{ii}}$	0.86 (12)	2.43 (14)	3.091 (12)	133 (16)
$\text{O}4\text{W}-\text{HW}42\cdots\text{O}6^{\text{iii}}$	0.85 (13)	2.58 (14)	3.124 (11)	123 (14)
$\text{O}1\text{W}-\text{HW}11\cdots\text{O}7^{\text{iv}}$	0.850 (10)	2.098 (11)	2.944 (4)	173 (4)
$\text{O}1\text{W}-\text{HW}12\cdots\text{O}3^{\text{ii}}$	0.854 (10)	2.39 (4)	2.935 (4)	123 (3)
$\text{O}2\text{W}-\text{HW}21\cdots\text{O}2^{\text{iii}}$	0.845 (10)	1.919 (18)	2.731 (4)	161 (4)
$\text{O}3\text{W}-\text{HW}32\cdots\text{O}2\text{W}^{\text{v}}$	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.

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

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supporting information

Acta Cryst. (2009). E65, m1425 [https://doi.org/10.1107/S1600536809042998]

Poly[[triqua(butane-1,2,3,4-tetracarboxylato)dimanganese(II)] monohydrate]**Ling Wu****S1. 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-tetracarboxylic 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 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**).

S2. Experimental

A mixture of $Mn(NO_3)_2 \cdot 6H_2O$ (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).

S3. Refinement

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

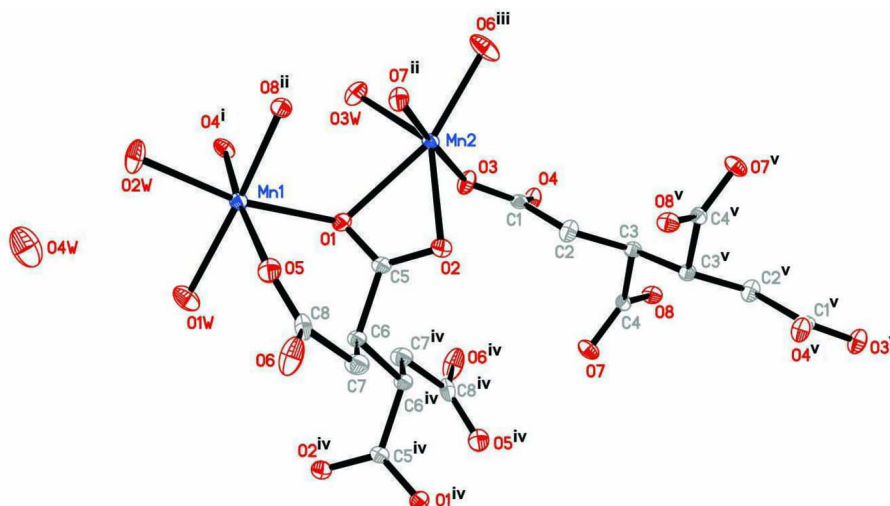


Figure 1

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

[Mn₂(C₈H₆O₈)(H₂O)₃]-H₂O

M_r = 824.14

Monoclinic, *P*2₁/*n*

Hall symbol: -*P* 2yn

a = 8.1962 (4) Å

b = 12.3291 (7) Å

c = 12.9758 (6) Å

β = 97.760 (5)°

V = 1299.22 (11) Å³

Z = 2

F(000) = 832

D_x = 2.107 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 3031 reflections

θ = 3.0–29.1°

μ = 2.01 mm⁻¹

T = 293 K

Block, colorless

0.33 × 0.21 × 0.17 mm

Data collection

Bruker APEX CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

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* > 2σ(*I*)

R_{int} = 0.040

θ_{max} = 29.1°, θ_{min} = 3.0°

h = -11→7

k = -12→15

l = -17→17

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.041

wR(*F*²) = 0.106

S = 0.88

3031 reflections

227 parameters

12 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0651P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.63 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.83 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (Å²)

	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 (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2W—HW22 \cdots O6 ^{ix}	0.84 (1)	2.46 (5)	2.998 (4)	122 (4)
O2W—HW22 \cdots O4W	0.84 (1)	2.39 (4)	2.985 (10)	128 (4)
O3W—HW31 \cdots O4 ^{vii}	0.85 (1)	2.08 (2)	2.874 (4)	156 (4)
O4W—HW41 \cdots O1 ^{vii}	0.86 (12)	2.43 (14)	3.091 (12)	133 (16)
O4W—HW42 \cdots O6 ^{iv}	0.85 (13)	2.58 (14)	3.124 (11)	123 (14)
O1W—HW11 \cdots O7 ⁱⁱ	0.85 (1)	2.10 (1)	2.944 (4)	173 (4)
O1W—HW12 \cdots O3 ^{vii}	0.85 (1)	2.39 (4)	2.935 (4)	123 (3)
O2W—HW21 \cdots O2 ^{iv}	0.85 (1)	1.92 (2)	2.731 (4)	161 (4)
O3W—HW32 \cdots O2W ^x	0.85 (1)	2.33 (2)	3.155 (5)	163 (5)

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