

# Poly[tetraqua( $\mu_6$ -9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylato)dimanganese(II)]

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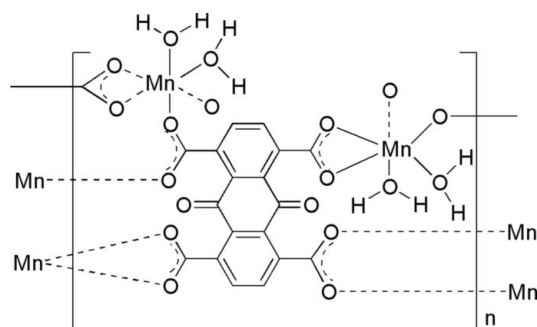
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 Key indicators: single-crystal X-ray study;  $T = 273$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.028;  $wR$  factor = 0.076; data-to-parameter ratio = 9.5.

The title complex,  $[\text{Mn}_2(\text{C}_{18}\text{H}_4\text{O}_{10})(\text{H}_2\text{O})_4]_n$ , was synthesized from manganese(II) chloride tetrahydrate and 9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylic acid ( $\text{H}_4\text{AQTC}$ ) in water. The anthraquinone unit is located about a crystallographic center of inversion. Each asymmetric unit therefore contains one  $\text{Mn}^{\text{II}}$  atom, two water ligands and one half  $\text{AQTC}^{4-}$  anion. The  $\text{Mn}^{\text{II}}$  atom is coordinated in a distorted octahedral geometry by four O atoms from three  $\text{AQTC}^{4-}$  ligands and two water O atoms. Two of the carboxylate groups coordinate one  $\text{Mn}^{\text{II}}$  atom in a chelating mode, whereas the others each coordinate two  $\text{Mn}^{\text{II}}$  atoms. Each  $\text{AQTC}^{4-}$  tetra-anion therefore coordinates six different  $\text{Mn}^{\text{II}}$  ions and, as a result, a three-dimensional coordination polymer is formed.  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, some of them bifurcated, between water ligands and neighboring water or anthraquinone ligands are observed in the crystal structure.

## Related literature

For general background to metal-organic frameworks, see: Li *et al.* (1999, 2012); Cheng *et al.* (2010); Hong *et al.* (2009); Miller & Gatteschi (2011); Liu *et al.* (2010).



## Experimental

### Crystal data

$[\text{Mn}_2(\text{C}_{18}\text{H}_4\text{O}_{10})(\text{H}_2\text{O})_4]$	$V = 917.9$ (2) Å <sup>3</sup>
$M_r = 562.16$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 11.2255$ (16) Å	$\mu = 1.46$ mm <sup>-1</sup>
$b = 8.4153$ (13) Å	$T = 273$ K
$c = 9.7252$ (14) Å	$0.46 \times 0.32 \times 0.26$ mm
$\beta = 92.355$ (2)°	

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	4340 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	1609 independent reflections
$T_{\min} = 0.553$ , $T_{\max} = 0.702$	1499 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.065$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.076$	
$S = 1.08$	
1609 reflections	
170 parameters	
2 restraints	

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O8}-\text{H3}\cdots\text{O2}^{\text{i}}$	0.78 (3)	2.03 (3)	2.775 (2)	160 (3)
$\text{O8}-\text{H4}\cdots\text{O3}^{\text{ii}}$	0.89 (4)	1.86 (4)	2.742 (2)	174 (3)
$\text{O8}-\text{H4}\cdots\text{O6}^{\text{ii}}$	0.89 (4)	2.60 (3)	3.159 (2)	121 (3)
$\text{O9}-\text{H5}\cdots\text{O8}^{\text{iii}}$	0.81 (1)	2.03 (1)	2.832 (3)	168 (4)
$\text{O9}-\text{H6}\cdots\text{O6}^{\text{ii}}$	0.81 (1)	2.38 (2)	3.135 (3)	157 (5)
$\text{O9}-\text{H6}\cdots\text{O7}^{\text{iii}}$	0.81 (1)	2.50 (4)	3.031 (3)	124 (4)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: IM2383).

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## supporting information

*Acta Cryst.* (2012). E68, m957 [https://doi.org/10.1107/S1600536812027158]

## Poly[tetraaqua( $\mu_6$ -9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylato)dimanganese(II)]

Rui Xu and Jian-Lan Liu

### S1. Comment

Porous solid materials, such as MOFs (metal-organic frameworks) have been widely studied for their potential applications in gas absorption, separation, catalysis and magnetic materials. Explorations of advanced porous materials for these applications are an intense subject of scientific research (Li *et al.*, 1999; Li *et al.*, 2012; Cheng *et al.*, 2010; Hong *et al.*, 2009; Miller & Gatteschi, 2011; Liu *et al.*, 2010.) Herein we report the crystal structure of the title compound.

The molecular structure of (I) is illustrated in Fig. 1., a summary of the observed hydrogen bonds and the corresponding angles are given in Table 1.

Each asymmetric unit therefore contains one manganese(II) atom, two water ligands and one half AQTC<sup>4-</sup> ligand. The coordination sphere around manganese is distorted octahedral due to the coordination of four O atoms from three AQTC<sup>4-</sup> ligands and two O atoms from two water molecules. Two of the carboxylate groups coordinate one manganese in a chelating mode whereas the others each coordinate two manganese center. Each AQTC<sup>4-</sup> therefore coordinates six different manganese ions and as a result a three-dimensional coordination polymer is formed.

### S2. Experimental

A mixture of 9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylic acid (H<sub>4</sub>AQTC; 0.025 mmol, 9.8 mg) was added to distilled water (4 ml) and ultra-sounded for 10 min. The pH value of the mixture was then adjusted to 7.0 with sodium hydroxide (0.5 mol L<sup>-1</sup>), prior to the addition of manganese(II) chloride tetrahydrate (0.05 mmol, 9.9 mg). The reactants were placed in a Teflon-lined stainless steel vessel, heated for 3 days, and then cooled to ambient temperature over 12 h. The solution was exposed to air for three days leading to the precipitation of brown crystals (yield 10%).

### S3. Refinement

All non-hydrogen atoms were refined anisotropically. H atoms of the H<sub>2</sub>O ligands were determined in difference Fourier maps and refined isotropically with distance restraints for O9—H5 and O9—H6 of 0.82 Å. H atoms of AQTC<sup>4-</sup> ligands calculated in idealized positions with C—H = 0.93 Å and refined as riding atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

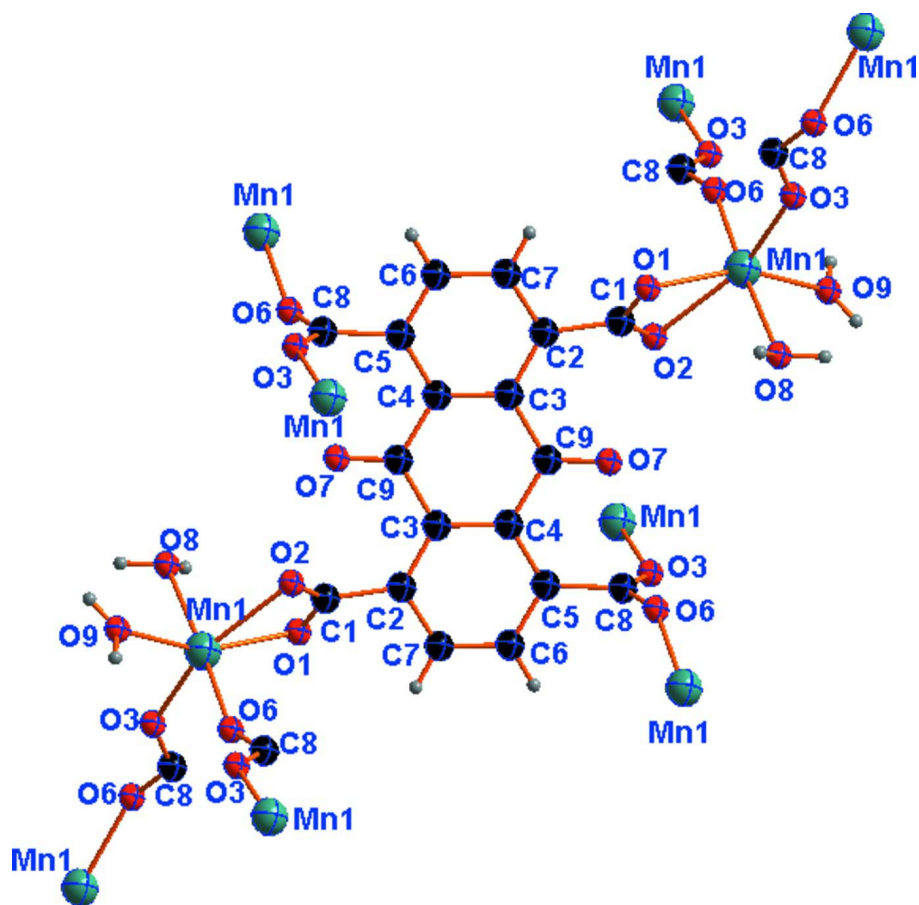


Figure 1

One repeating unit of the coordination polymer, showing displacement ellipsoids at the 30% probability level. [Symmetry codes: (#1)  $x + 1, -y, -z + 1$ ; (#2)  $x + 1, y + 1/2, -z + 1/2$ ; (#3)  $x + 1, -y + 1, -z + 1$ ; (#4)  $x + 1, y - 1/2, -z + 1/2$ .]

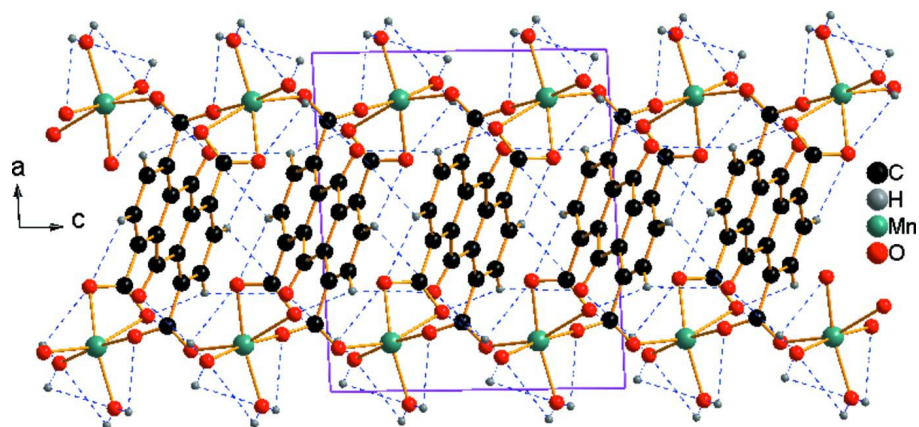


Figure 2

A view of the crystal structure of the title compound.

Poly[tetraaqua( $\mu_6$ -9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylato)dimanganese(II)]

## Crystal data

[Mn<sub>2</sub>(C<sub>18</sub>H<sub>4</sub>O<sub>10</sub>)(H<sub>2</sub>O)<sub>4</sub>] $M_r = 562.16$ Monoclinic,  $P2_1/c$ 

Hall symbol: -P 2ybc

 $a = 11.2255 (16) \text{ \AA}$  $b = 8.4153 (13) \text{ \AA}$  $c = 9.7252 (14) \text{ \AA}$  $\beta = 92.355 (2)^\circ$  $V = 917.9 (2) \text{ \AA}^3$  $Z = 2$  $F(000) = 564$  $D_x = 2.034 \text{ Mg m}^{-3}$ Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$ 

Cell parameters from 5133 reflections

 $\theta = 2.2\text{--}27.6^\circ$  $\mu = 1.46 \text{ mm}^{-1}$  $T = 273 \text{ K}$ 

Block, brown

 $0.46 \times 0.32 \times 0.26 \text{ mm}$ 

## Data collection

Bruker SMART APEX CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\phi$  and  $\omega$  scansAbsorption correction: multi-scan  
(SADABS; Bruker, 2000) $T_{\min} = 0.553$ ,  $T_{\max} = 0.702$ 

4340 measured reflections

1609 independent reflections

1499 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.065$  $\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 3.0^\circ$  $h = -12 \rightarrow 13$  $k = -10 \rightarrow 7$  $l = -11 \rightarrow 11$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.028$  $wR(F^2) = 0.076$  $S = 1.08$ 

1609 reflections

170 parameters

2 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sitesH atoms treated by a mixture of independent  
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0357P)^2 + 0.3487P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 0.35 \text{ e \AA}^{-3}$  $\Delta\rho_{\min} = -0.41 \text{ e \AA}^{-3}$ 

## 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.32095 (18)	0.3515 (2)	0.3203 (2)	0.0199 (4)
C2	0.44180 (17)	0.2999 (2)	0.37593 (19)	0.0182 (4)
C3	0.47029 (17)	0.1544 (2)	0.43842 (19)	0.0174 (4)

C4	0.58569 (16)	0.1290 (2)	0.49497 (19)	0.0168 (4)
C5	0.67291 (17)	0.2464 (2)	0.4857 (2)	0.0176 (4)
C6	0.64515 (18)	0.3863 (2)	0.4181 (2)	0.0214 (4)
H1	0.7036	0.4632	0.4081	0.026*
C7	0.53093 (18)	0.4128 (2)	0.3654 (2)	0.0214 (4)
H2	0.5133	0.5087	0.3217	0.026*
C8	0.79987 (17)	0.2271 (2)	0.5408 (2)	0.0187 (4)
C9	0.38273 (18)	0.0223 (2)	0.4344 (2)	0.0173 (4)
Mn1	0.14215 (3)	0.50978 (3)	0.21336 (3)	0.02054 (15)
O1	0.31881 (13)	0.4118 (2)	0.20209 (15)	0.0305 (4)
O2	0.23044 (12)	0.35278 (18)	0.39148 (15)	0.0261 (4)
O3	0.87242 (12)	0.15778 (18)	0.46563 (15)	0.0245 (3)
O6	0.82943 (13)	0.28802 (18)	0.65405 (15)	0.0274 (4)
O7	0.28972 (13)	0.03344 (17)	0.36714 (16)	0.0244 (4)
O8	0.09489 (15)	0.2961 (2)	0.08600 (17)	0.0267 (4)
O9	-0.04028 (17)	0.5190 (3)	0.2639 (2)	0.0489 (6)
H3	0.143 (3)	0.273 (4)	0.034 (3)	0.053 (10)*
H4	0.024 (3)	0.306 (4)	0.042 (4)	0.068 (10)*
H5	-0.064 (3)	0.590 (3)	0.312 (3)	0.079 (13)*
H6	-0.091 (3)	0.457 (5)	0.239 (5)	0.114 (17)*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0197 (10)	0.0151 (10)	0.0247 (11)	-0.0006 (8)	-0.0031 (8)	0.0011 (8)
C2	0.0176 (10)	0.0206 (10)	0.0166 (10)	0.0002 (8)	0.0007 (7)	0.0003 (8)
C3	0.0157 (9)	0.0201 (10)	0.0163 (10)	0.0020 (8)	0.0004 (7)	-0.0001 (8)
C4	0.0171 (9)	0.0186 (10)	0.0147 (10)	0.0016 (8)	-0.0007 (7)	-0.0010 (7)
C5	0.0172 (10)	0.0191 (10)	0.0163 (10)	0.0015 (8)	-0.0002 (7)	-0.0031 (8)
C6	0.0183 (10)	0.0225 (11)	0.0233 (11)	-0.0042 (8)	0.0000 (8)	0.0011 (8)
C7	0.0223 (10)	0.0191 (10)	0.0225 (10)	0.0012 (8)	-0.0008 (8)	0.0042 (8)
C8	0.0177 (10)	0.0154 (10)	0.0228 (11)	-0.0029 (8)	-0.0027 (8)	0.0029 (8)
C9	0.0158 (10)	0.0183 (10)	0.0178 (10)	0.0016 (8)	0.0002 (8)	-0.0015 (8)
Mn1	0.0173 (2)	0.0225 (2)	0.0215 (2)	0.00180 (12)	-0.00320 (14)	-0.00052 (12)
O1	0.0221 (8)	0.0426 (10)	0.0265 (8)	0.0031 (7)	-0.0023 (6)	0.0113 (7)
O2	0.0205 (8)	0.0280 (8)	0.0299 (8)	0.0030 (6)	0.0035 (6)	0.0038 (6)
O3	0.0166 (7)	0.0319 (8)	0.0247 (8)	0.0000 (6)	-0.0016 (6)	-0.0063 (6)
O6	0.0260 (8)	0.0289 (8)	0.0266 (8)	-0.0003 (7)	-0.0069 (6)	-0.0097 (7)
O7	0.0183 (8)	0.0225 (7)	0.0315 (9)	0.0000 (6)	-0.0105 (6)	0.0041 (6)
O8	0.0185 (8)	0.0339 (9)	0.0276 (9)	0.0005 (7)	-0.0007 (7)	-0.0065 (7)
O9	0.0217 (9)	0.0638 (14)	0.0617 (14)	-0.0095 (9)	0.0059 (9)	-0.0353 (11)

*Geometric parameters (Å, °)*

C1—O2	1.253 (3)	C8—O3	1.260 (2)
C1—O1	1.256 (2)	C9—O7	1.212 (2)
C1—C2	1.504 (3)	C9—C4 <sup>i</sup>	1.483 (3)
C2—C7	1.386 (3)	Mn1—O9	2.1270 (19)

C2—C3	1.398 (3)	Mn1—O3 <sup>ii</sup>	2.1412 (15)
C3—C4	1.403 (3)	Mn1—O6 <sup>iii</sup>	2.1508 (15)
C3—C9	1.483 (3)	Mn1—O1	2.1547 (15)
C4—C5	1.396 (3)	Mn1—O8	2.2350 (16)
C4—C9 <sup>i</sup>	1.483 (3)	Mn1—O2	2.3637 (15)
C5—C6	1.378 (3)	O3—Mn1 <sup>iv</sup>	2.1412 (15)
C5—C8	1.511 (3)	O6—Mn1 <sup>iii</sup>	2.1508 (15)
C6—C7	1.379 (3)	O8—H3	0.78 (3)
C6—H1	0.9300	O8—H4	0.89 (4)
C7—H2	0.9300	O9—H5	0.812 (10)
C8—O6	1.247 (2)	O9—H6	0.809 (10)
O2—C1—O1	121.11 (18)	C4 <sup>i</sup> —C9—C3	119.05 (17)
O2—C1—C2	122.96 (18)	O9—Mn1—O3 <sup>ii</sup>	97.16 (8)
O1—C1—C2	115.40 (17)	O9—Mn1—O6 <sup>iii</sup>	87.31 (7)
C7—C2—C3	118.63 (18)	O3 <sup>ii</sup> —Mn1—O6 <sup>iii</sup>	91.81 (6)
C7—C2—C1	114.76 (17)	O9—Mn1—O1	157.30 (8)
C3—C2—C1	126.59 (18)	O3 <sup>ii</sup> —Mn1—O1	102.77 (5)
C2—C3—C4	119.69 (18)	O6 <sup>iii</sup> —Mn1—O1	102.67 (6)
C2—C3—C9	120.34 (17)	O9—Mn1—O8	87.05 (7)
C4—C3—C9	119.75 (18)	O3 <sup>ii</sup> —Mn1—O8	90.52 (6)
C5—C4—C3	120.36 (18)	O6 <sup>iii</sup> —Mn1—O8	174.13 (6)
C5—C4—C9 <sup>i</sup>	118.84 (17)	O1—Mn1—O8	82.05 (6)
C3—C4—C9 <sup>i</sup>	120.80 (17)	O9—Mn1—O2	103.28 (8)
C6—C5—C4	119.34 (17)	O3 <sup>ii</sup> —Mn1—O2	159.49 (5)
C6—C5—C8	116.90 (17)	O6 <sup>iii</sup> —Mn1—O2	87.45 (6)
C4—C5—C8	123.71 (17)	O1—Mn1—O2	57.61 (5)
C5—C6—C7	120.24 (19)	O8—Mn1—O2	92.25 (6)
C5—C6—H1	119.9	C1—O1—Mn1	95.23 (12)
C7—C6—H1	119.9	C1—O2—Mn1	85.71 (12)
C6—C7—C2	121.64 (19)	C8—O3—Mn1 <sup>iv</sup>	135.36 (13)
C6—C7—H2	119.2	C8—O6—Mn1 <sup>iii</sup>	151.88 (14)
C2—C7—H2	119.2	Mn1—O8—H3	114 (2)
O6—C8—O3	123.22 (18)	Mn1—O8—H4	112 (2)
O6—C8—C5	118.82 (17)	H3—O8—H4	110 (3)
O3—C8—C5	117.82 (17)	Mn1—O9—H5	120 (3)
O7—C9—C4 <sup>i</sup>	120.01 (18)	Mn1—O9—H6	126 (4)
O7—C9—C3	120.77 (18)	H5—O9—H6	114 (5)
O2—C1—C2—C7	−122.6 (2)	C4—C5—C8—O3	84.0 (2)
O1—C1—C2—C7	49.1 (3)	C2—C3—C9—O7	6.4 (3)
O2—C1—C2—C3	55.6 (3)	C4—C3—C9—O7	−168.17 (19)
O1—C1—C2—C3	−132.7 (2)	C2—C3—C9—C4 <sup>i</sup>	−178.27 (17)
C7—C2—C3—C4	3.3 (3)	C4—C3—C9—C4 <sup>i</sup>	7.1 (3)
C1—C2—C3—C4	−174.94 (18)	O2—C1—O1—Mn1	6.2 (2)
C7—C2—C3—C9	−171.33 (17)	C2—C1—O1—Mn1	−165.70 (15)
C1—C2—C3—C9	10.5 (3)	O9—Mn1—O1—C1	−39.0 (2)
C2—C3—C4—C5	−1.8 (3)	O3 <sup>ii</sup> —Mn1—O1—C1	170.17 (12)

C9—C3—C4—C5	172.81 (17)	O6 <sup>iii</sup> —Mn1—O1—C1	75.34 (13)
C2—C3—C4—C9 <sup>i</sup>	178.11 (17)	O8—Mn1—O1—C1	-101.11 (13)
C9—C3—C4—C9 <sup>i</sup>	-7.3 (3)	O2—Mn1—O1—C1	-3.32 (11)
C3—C4—C5—C6	-1.2 (3)	O1—C1—O2—Mn1	-5.63 (19)
C9 <sup>i</sup> —C4—C5—C6	178.86 (18)	C2—C1—O2—Mn1	165.63 (18)
C3—C4—C5—C8	-178.52 (18)	O9—Mn1—O2—C1	169.94 (12)
C9 <sup>i</sup> —C4—C5—C8	1.6 (3)	O3 <sup>ii</sup> —Mn1—O2—C1	-15.1 (2)
C4—C5—C6—C7	2.8 (3)	O6 <sup>iii</sup> —Mn1—O2—C1	-103.43 (12)
C8—C5—C6—C7	-179.76 (18)	O1—Mn1—O2—C1	3.32 (11)
C5—C6—C7—C2	-1.3 (3)	O8—Mn1—O2—C1	82.44 (12)
C3—C2—C7—C6	-1.8 (3)	O6—C8—O3—Mn1 <sup>iv</sup>	168.36 (14)
C1—C2—C7—C6	176.64 (19)	C5—C8—O3—Mn1 <sup>iv</sup>	-15.9 (3)
C6—C5—C8—O6	82.5 (2)	O3—C8—O6—Mn1 <sup>iii</sup>	112.0 (3)
C4—C5—C8—O6	-100.1 (2)	C5—C8—O6—Mn1 <sup>iii</sup>	-63.7 (4)
C6—C5—C8—O3	-93.4 (2)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O8—H3 $\cdots$ O2 <sup>v</sup>	0.78 (3)	2.03 (3)	2.775 (2)	160 (3)
O8—H4 $\cdots$ O3 <sup>vi</sup>	0.89 (4)	1.86 (4)	2.742 (2)	174 (3)
O8—H4 $\cdots$ O6 <sup>vi</sup>	0.89 (4)	2.60 (3)	3.159 (2)	121 (3)
O9—H5 $\cdots$ O8 <sup>vii</sup>	0.81 (1)	2.03 (1)	2.832 (3)	168 (4)
O9—H6 $\cdots$ O6 <sup>vi</sup>	0.81 (1)	2.38 (2)	3.135 (3)	157 (5)
O9—H6 $\cdots$ O7 <sup>vii</sup>	0.81 (1)	2.50 (4)	3.031 (3)	124 (4)

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