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Hexaaquamanganese(II) 4,4′-(1,2-dihydroxyethane-1,2-diyl)dibenzoate monohydrate

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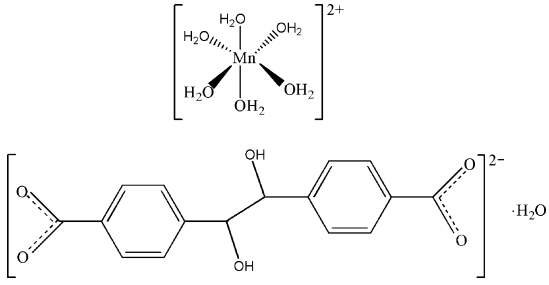
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.057; wR factor = 0.140; data-to-parameter ratio = 13.4.

In the title compound, $[Mn(H_2O)_6](C_{16}H_{12}O_6)\cdot H_2O$, the $[Mn(H_2O)_6]^{2+}$ complex cation lies on a mirror plane, the 4,4′-(1,2-dihydroxyethane-1,2-diyl)dibenzoate anion is located on an inversion center and the solvent water molecule also lies on a mirror plane. Extensive O—H···O hydrogen-bonding interactions between the cations, anions and water molecules stabilize the three-dimensional network.

Related literature

For the intriguing architectures and potential applications of polymeric coordination networks, see: Carlucci *et al.* (2003); Rosi *et al.* (2003).



Experimental

Crystal data

$[Mn(H_2O)_6](C_{16}H_{12}O_6)\cdot H_2O$
M_r = 481.31
Monoclinic, $P2_1/m$
a = 6.0803 (6) Å
b = 20.643 (2) Å
c = 8.6610 (9) Å
β = 104.420 (1)°
V = 1052.84 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.69 mm^{-1}
T = 298 K
0.42 × 0.21 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.760, T_{max} = 0.886
5275 measured reflections
1899 independent reflections
1647 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.140
S = 1.23
1899 reflections
142 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1^{i}	0.82	2.02	2.830 (5)	172
O4—H4*C*···O1^{ii}	0.85	1.86	2.712 (4)	177
O5—H5*C*···O4^{iii}	0.85	1.93	2.777 (6)	175
O5—H5*D*···O8^{iii}	0.85	1.88	2.728 (7)	175
O6—H6*C*···O3^{iv}	0.85	1.99	2.840 (5)	178
O6—H6*D*···O8	0.85	2.19	3.040 (6)	178
O7—H7*C*···O1^{v}	0.85	1.95	2.799 (5)	180
O7—H7*D*···O2^{ii}	0.85	1.82	2.673 (4)	180
O8—H8*C*···O2^{vi}	0.85	1.92	2.767 (5)	172

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

The authors acknowledge Pingdingshan University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2318).

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supporting information

Acta Cryst. (2010). E**66**, m809 [doi:10.1107/S1600536810022300]

Hexaaquamanganese(II) 4,4′-(1,2-dihydroxyethane-1,2-diyl)dibenzoate monohydrate

Cheng-Jun Hao and Yun-Li Cao

S1. Comment

Current interest in polymeric coordination networks is rapidly expanding for their intriguing architectures (Carlucci *et al.*, 2003) and potential applications (Rosi *et al.*, 2003). We have reacted 1,2-bis(4-carboxyphenyl)-1,2-ethanediol with $MnCl_2$ under hydrothermal conditions to obtain the title compound and its structure is reported here.

As illustrated in Fig. 1, the title compound contains one $[Mn(H_2O)_6]^{2+}$ complex cation lying on a mirror plan, one 1,2-dihydroxyethane-1,2-bis(4-benzenecarboxylate) anion located on an inversion center and one solvent water molecule lying on a mirror plan. The carboxylate group lies in the plane of the benzene ring as indicated by the O1—C1—C2—C3 and O2—C1—C2—C7 torsion angles of -3.0 (6) and -1.2 (6)°. The benzene ring is nearly planar with maximum deviations from the mean plane being -0.003 (6) Å for C6. The cation, anion and solvent water molecule interact via O—H···O hydrogen bonds, consolidating the three-dimensional network (Fig. 2, Table 1).

S2. Experimental

A mixture of $MnCl_2$ (0.1 mmol, 0.013 g), 1,2-bis(4-carboxyphenyl)-1,2-ethanediol (0.1 mmol, 0.03 g) and 10 ml of H_2O was sealed in a 20 ml Telflon-lined stainless steel vessel and heated at 303 K for 2 d. Colorless crystals were obtained when the solution was cooled to room temperature slowly.

S3. Refinement

H atoms bound to C atoms were placed at calculated positions and were treated as riding on the parent atoms, with C—H = 0.93 (aromatic) and 0.98 (CH) Å and with U_{iso}(H) = 1.2U_{eq}(C). H atoms of hydroxyl group and water molecules were located in a difference Fourier map and refined as riding, with O—H = 0.85 Å and U_{iso}(H) = 1.2(1.5 for hydroxyl)U_{eq}(O).

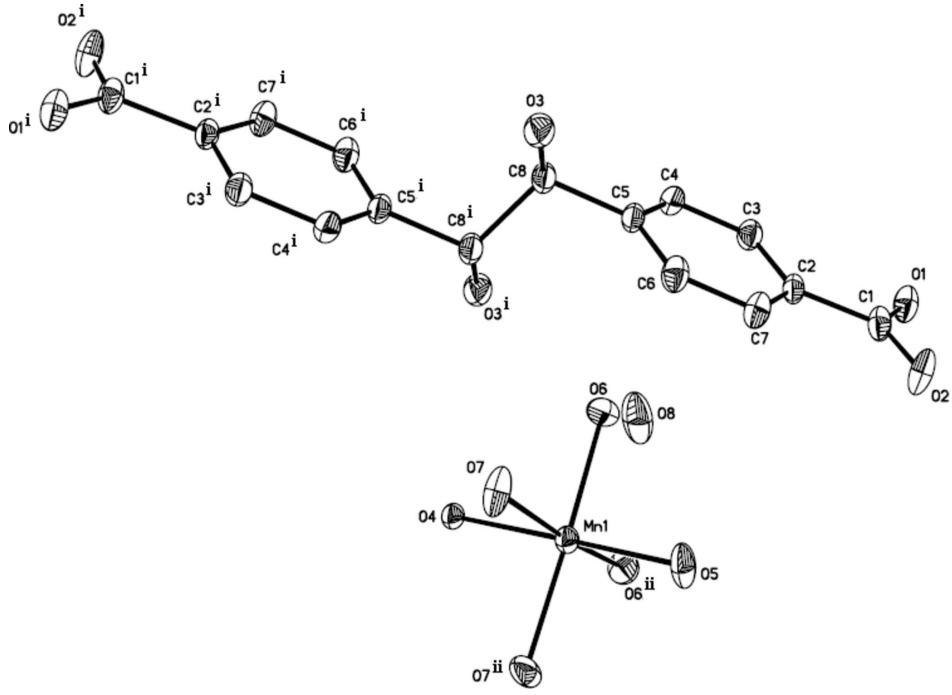

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are shown at the 30% probability level. H atoms and water molecule are omitted for clarity. [Symmetry codes: (i) 1-x, 1-y, 1-z; (ii) x, 3/2-y, z.]

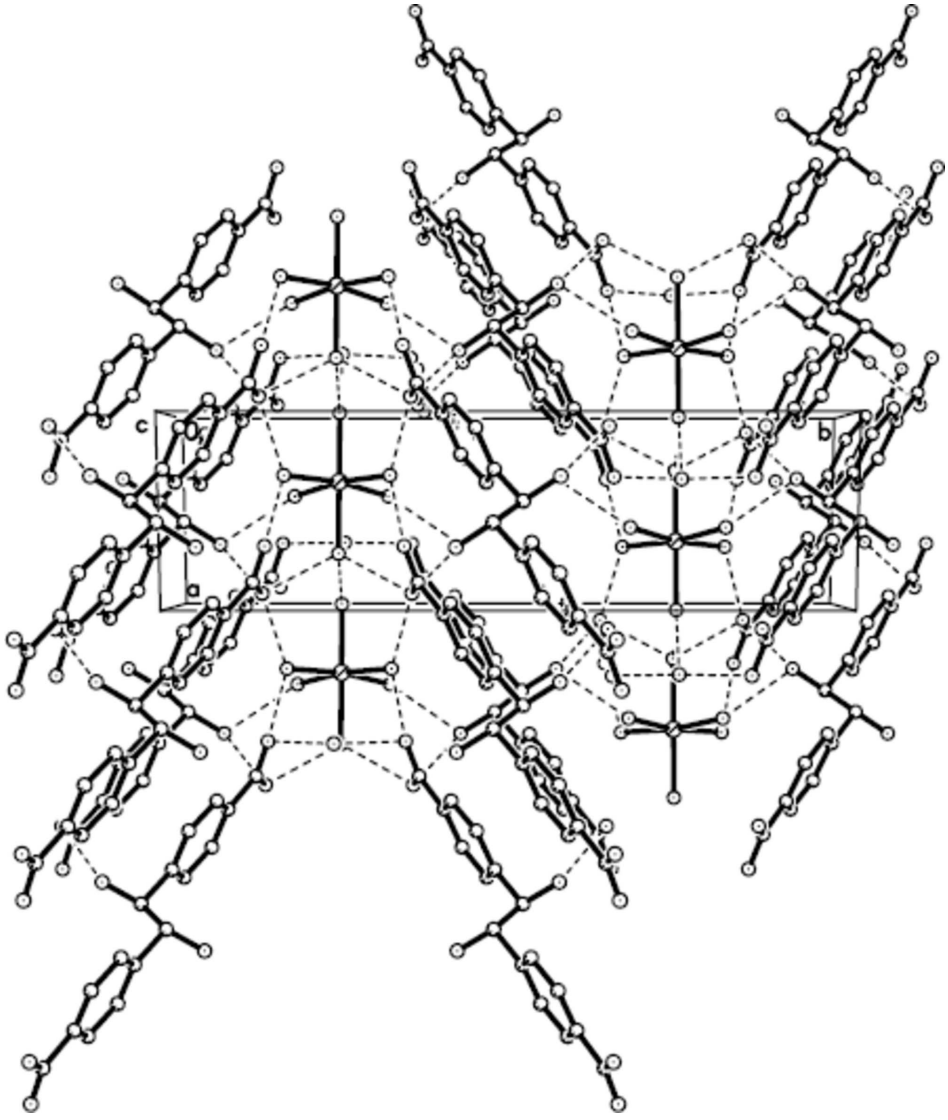

Figure 2

View of the three-dimensional network constructed by O—H···O hydrogen bonds (dashed lines). H atoms are omitted for clarity.

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Crystal data

$[Mn(H_2O)_6](C_{16}H_{12}O_6)\cdot H_2O$
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Hall symbol: -P 2yb
$a = 6.0803$ (6) Å
$b = 20.643$ (2) Å
$c = 8.6610$ (9) Å
$\beta = 104.420$ (1)°
$V = 1052.84$ (19) Å^3
$Z = 2$
$F(000) = 502$
$D_x = 1.518$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2215 reflections
$\theta = 2.5$–24.0°
$\mu = 0.69$ mm^{-1}
$T = 298$ K
Block, colorless
0.42 × 0.21 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.760, T_{max} = 0.886
5275 measured reflections
1899 independent reflections
1647 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°, θ_{min} = 2.0°
$h = -7 \rightarrow 6$
$k = -24 \rightarrow 22$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.140
S = 1.23
1899 reflections
142 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0292P)^2 + 3.0592P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.65486 (15)	0.7500	0.46088 (10)	0.0289 (3)
O1	1.0818 (5)	0.64065 (16)	1.2067 (4)	0.0444 (8)
O2	1.3265 (5)	0.64967 (19)	1.0567 (4)	0.0567 (10)
O3	0.6710 (6)	0.42818 (15)	0.5229 (4)	0.0472 (9)
H3	0.7538	0.4103	0.6004	0.071*
O4	0.2836 (6)	0.7500	0.3483 (5)	0.0296 (9)
H4C	0.2168	0.7166	0.3015	0.036*
O5	1.0130 (7)	0.7500	0.5635 (5)	0.0533 (14)
H5C	1.0885	0.7500	0.4931	0.064*
H5D	1.1062	0.7500	0.6548	0.064*
O6	0.5811 (6)	0.67978 (16)	0.6304 (4)	0.0477 (8)
H6C	0.5029	0.6476	0.5861	0.057*
H6D	0.5095	0.6985	0.6904	0.057*
O7	0.6863 (5)	0.67266 (18)	0.2996 (4)	0.0548 (10)
H7C	0.8061	0.6629	0.2710	0.066*
H7D	0.5724	0.6653	0.2220	0.066*
O8	0.3346 (10)	0.7500	0.8464 (6)	0.090 (2)
H8C	0.3323	0.7167	0.9035	0.109*
C1	1.1422 (7)	0.6306 (2)	1.0792 (5)	0.0377 (11)
C2	0.9858 (7)	0.5932 (2)	0.9471 (5)	0.0321 (10)
C3	0.7845 (7)	0.5675 (2)	0.9661 (5)	0.0364 (10)
H3A	0.7415	0.5747	1.0605	0.044*
C4	0.6454 (7)	0.5311 (2)	0.8455 (5)	0.0371 (10)
H4	0.5098	0.5144	0.8597	0.045*
C5	0.7062 (7)	0.5195 (2)	0.7053 (5)	0.0335 (10)

C6	0.9078 (8)	0.5454 (2)	0.6850 (5)	0.0398 (11)
H6	0.9505	0.5381	0.5906	0.048*
C7	1.0457 (7)	0.5820 (2)	0.8053 (5)	0.0387 (11)
H7	1.1802	0.5993	0.7905	0.046*
C8	0.5518 (8)	0.4795 (2)	0.5750 (5)	0.0365 (10)
H8	0.4286	0.4613	0.6160	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0245 (5)	0.0337 (5)	0.0272 (5)	0.000	0.0039 (4)	0.000
O1	0.0364 (17)	0.051 (2)	0.0399 (18)	0.0007 (15)	−0.0016 (14)	−0.0157 (15)
O2	0.0333 (19)	0.078 (3)	0.052 (2)	−0.0144 (18)	−0.0013 (15)	−0.0261 (19)
O3	0.053 (2)	0.0349 (18)	0.0454 (19)	0.0047 (15)	−0.0045 (15)	−0.0064 (15)
O4	0.026 (2)	0.029 (2)	0.031 (2)	0.000	0.0003 (16)	0.000
O5	0.025 (2)	0.100 (4)	0.032 (2)	0.000	0.0016 (19)	0.000
O6	0.058 (2)	0.0403 (19)	0.0434 (19)	−0.0019 (16)	0.0097 (16)	0.0080 (15)
O7	0.0285 (17)	0.078 (3)	0.053 (2)	0.0039 (17)	0.0007 (15)	−0.0328 (19)
O8	0.065 (4)	0.169 (7)	0.037 (3)	0.000	0.012 (3)	0.000
C1	0.030 (2)	0.037 (3)	0.038 (3)	0.009 (2)	−0.0053 (19)	−0.011 (2)
C2	0.028 (2)	0.029 (2)	0.032 (2)	0.0044 (18)	−0.0058 (18)	−0.0058 (18)
C3	0.037 (2)	0.037 (2)	0.032 (2)	−0.001 (2)	0.0018 (18)	−0.0065 (19)
C4	0.033 (2)	0.036 (2)	0.038 (2)	−0.0057 (19)	−0.0007 (19)	−0.003 (2)
C5	0.030 (2)	0.028 (2)	0.035 (2)	0.0017 (18)	−0.0063 (18)	−0.0048 (18)
C6	0.038 (3)	0.044 (3)	0.034 (2)	0.002 (2)	0.0021 (19)	−0.012 (2)
C7	0.027 (2)	0.045 (3)	0.041 (3)	−0.001 (2)	0.0030 (19)	−0.012 (2)
C8	0.037 (2)	0.033 (2)	0.032 (2)	0.001 (2)	−0.0043 (19)	−0.0060 (19)

Geometric parameters (Å, º)

Mn1—O5	2.137 (4)	O7—H7D	0.8500
Mn1—O7	2.161 (3)	O8—H8C	0.8500
Mn1—O7^{i}	2.161 (3)	C1—C2	1.506 (6)
Mn1—O6^{i}	2.187 (3)	C2—C3	1.381 (6)
Mn1—O6	2.187 (3)	C2—C7	1.384 (6)
Mn1—O4	2.225 (4)	C3—C4	1.390 (6)
O1—C1	1.265 (5)	C3—H3A	0.9300
O2—C1	1.248 (6)	C4—C5	1.375 (6)
O3—C8	1.419 (5)	C4—H4	0.9300
O3—H3	0.8200	C5—C6	1.387 (6)
O4—H4C	0.8500	C5—C8	1.520 (6)
O5—H5C	0.8500	C6—C7	1.388 (6)
O5—H5D	0.8500	C6—H6	0.9300
O6—H6C	0.8500	C7—H7	0.9300
O6—H6D	0.8500	C8—C8^{ii}	1.548 (8)
O7—H7C	0.8500	C8—H8	0.9800
O5—Mn1—O7	91.37 (12)	O2—C1—C2	117.7 (4)

O5—Mn1—O7^{i}	91.37 (12)	O1—C1—C2	118.8 (4)
O7—Mn1—O7^{i}	95.3 (2)	C3—C2—C7	118.6 (4)
O5—Mn1—O6^{i}	94.52 (13)	C3—C2—C1	121.1 (4)
O7—Mn1—O6^{i}	171.61 (14)	C7—C2—C1	120.2 (4)
O7^{i}—Mn1—O6^{i}	90.57 (14)	C2—C3—C4	120.6 (4)
O5—Mn1—O6	94.52 (13)	C2—C3—H3A	119.7
O7—Mn1—O6	90.57 (14)	C4—C3—H3A	119.7
O7^{i}—Mn1—O6	171.61 (14)	C5—C4—C3	120.7 (4)
O6^{i}—Mn1—O6	83.01 (19)	C5—C4—H4	119.6
O5—Mn1—O4	178.63 (17)	C3—C4—H4	119.6
O7—Mn1—O4	87.71 (11)	C4—C5—C6	119.0 (4)
O7^{i}—Mn1—O4	87.71 (11)	C4—C5—C8	119.9 (4)
O6^{i}—Mn1—O4	86.50 (12)	C6—C5—C8	121.1 (4)
O6—Mn1—O4	86.50 (12)	C5—C6—C7	120.1 (4)
C8—O3—H3	109.5	C5—C6—H6	119.9
Mn1—O4—H4C	121.4	C7—C6—H6	119.9
Mn1—O5—H5C	112.2	C2—C7—C6	120.9 (4)
Mn1—O5—H5D	139.5	C2—C7—H7	119.5
H5C—O5—H5D	108.3	C6—C7—H7	119.5
Mn1—O6—H6C	113.5	O3—C8—C5	111.9 (3)
Mn1—O6—H6D	109.4	O3—C8—C8^{ii}	105.9 (4)
H6C—O6—H6D	108.4	C5—C8—C8^{ii}	111.9 (4)
Mn1—O7—H7C	125.7	O3—C8—H8	109.0
Mn1—O7—H7D	117.3	C5—C8—H8	109.0
H7C—O7—H7D	108.4	C8^{ii}—C8—H8	109.0
O2—C1—O1	123.5 (4)		

O2—C1—C2—C3	176.5 (4)	C4—C5—C6—C7	0.3 (7)
O1—C1—C2—C3	−3.0 (6)	C8—C5—C6—C7	179.7 (4)
O2—C1—C2—C7	−1.2 (6)	C3—C2—C7—C6	−0.5 (7)
O1—C1—C2—C7	179.3 (4)	C1—C2—C7—C6	177.3 (4)
C7—C2—C3—C4	0.1 (7)	C5—C6—C7—C2	0.3 (7)
C1—C2—C3—C4	−177.6 (4)	C4—C5—C8—O3	−128.0 (4)
C2—C3—C4—C5	0.5 (7)	C6—C5—C8—O3	52.5 (6)
C3—C4—C5—C6	−0.7 (7)	C4—C5—C8—C8^{ii}	113.3 (6)
C3—C4—C5—C8	179.9 (4)	C6—C5—C8—C8^{ii}	−66.1 (6)

Symmetry codes: (i) x, $-y+3/2$, z; (ii) $-x+1$, $-y+1$, $-z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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