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catena-Poly[[tetraaquamanganese(II)]-μ-6,6′-dihydroxy-3,3′-diazenediyldibenzoato-κ^2O:O']

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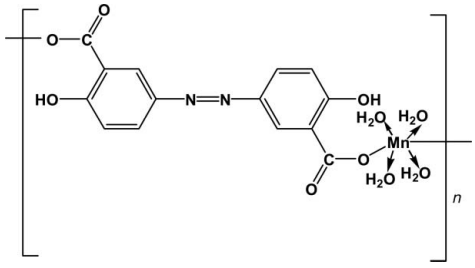
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.102; data-to-parameter ratio = 11.8.

In the title compound, $[Mn(C_{14}H_8N_2O_6)(H_2O)_4]_n$, each 6,6′-dihydroxy-3,3′-diazenediyldibenzoate ligand acts as a carboxylate bridge, leading to the formation of polymeric chains running in the [110] direction. The Mn atom is hexacoordinated in a distorted octahedral geometry by six O atoms from two ligands and four water molecules [Mn—O = 2.1379 (16)–2.2082 (15) Å]. The crystal packing is stabilized by π–π interactions [centroid-to-centroid distances 3.830 (16) and 4.476 (17) Å] and intermolecular O—H···O and O—H···N hydrogen bonds.

Related literature

For related literature, see: Riordan & Blair (1979); Klotz (2005); Tang, Tan & Cao (2007); Tang, Tan, Chen & Cao (2007); Tang, Yang *et al.* (2007).



Experimental

Crystal data

$[Mn(C_{14}H_8N_2O_6)(H_2O)_4]$
M_r = 427.23
Monoclinic, $P2_1/c$
a = 9.486 (2) Å
b = 11.490 (3) Å
c = 16.322 (4) Å
β = 106.076 (3)°
V = 1709.4 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 293 (2) K
0.31 × 0.23 × 0.21 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.80, T_{max} = 0.84
8959 measured reflections
3341 independent reflections
2933 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.102
S = 1.55
3341 reflections
284 parameters
16 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O3*W*	2.1380 (15)	Mn1—O6	2.1654 (14)
Mn1—O1*W*	2.1588 (16)	Mn1—O2^{i}	2.1713 (15)
Mn1—O4*W*	2.1619 (14)	Mn1—O2*W*	2.2083 (15)
O3*W*—Mn1—O1*W*	177.68 (6)	O4*W*—Mn1—O2^{i}	94.95 (6)
O3*W*—Mn1—O4*W*	92.16 (6)	O6—Mn1—O2^{i}	86.75 (6)
O1*W*—Mn1—O4*W*	90.15 (6)	O3*W*—Mn1—O2*W*	88.16 (7)
O3*W*—Mn1—O6	88.88 (6)	O1*W*—Mn1—O2*W*	91.84 (8)
O1*W*—Mn1—O6	88.80 (6)	O4*W*—Mn1—O2*W*	86.06 (6)
O4*W*—Mn1—O6	178.02 (5)	O6—Mn1—O2*W*	92.30 (6)
O3*W*—Mn1—O2^{i}	89.06 (7)	O2^{i}—Mn1—O2*W*	177.08 (7)
O1*W*—Mn1—O2^{i}	90.90 (8)		

Symmetry code: (i) $x+1, y+1, z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4*W*—H4*WB*···O1^{i}	0.85	1.98	2.728 (2)	147
O4*W*—H4*WA*···N2^{ii}	0.85	2.24	3.043 (2)	157
O3—H3*A*···O6	0.84	1.71	2.519 (2)	161
O3*W*—H3*WB*···N1^{iii}	0.85	2.07	2.894 (2)	165
O4—H4*A*···O2	0.87	1.73	2.519 (2)	150
O1*W*—H1*WB*···O5^{ii}	0.85	1.84	2.688 (2)	175
O3*W*—H3*WA*···O1^{ii}	0.85	1.83	2.652 (3)	161
O1*W*—H1*WA*···O4^{iv}	0.85	2.09	2.887 (3)	155
O2*W*—H2*WA*···O5	0.85	1.85	2.678 (2)	165

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXL97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: RT2011).

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References

Bruker (2000). *SMART*, *SAINT*, *SHELXTL* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Klotz, U. (2005). *Dig. Liver Dis.* **37**, 381–388.
Riordan, J. E. & Blair, H. S. (1979). *Polymer*, **20**, 196–202.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tang, Y.-Z., Tan, Y.-H. & Cao, Y.-W. (2007). *Acta Cryst.* E**63**, m1175–m1176.
Tang, Y. Z., Tan, Y. H., Chen, S. H. & Cao, Y. W. (2007). *Z. Anorg. Allg. Chem.* **633**, 332–335.
Tang, Y. Z., Yang, S. P., Tan, Y. H., Chen, S. H., Cao, Y. W. & Wang, P. (2007). *Chin. J. Inorg. Chem.* **23**, 70–74.

supplementary materials

Acta Cryst. (2007). E**63**, m2948-m2949 [**doi:10.1107/S1600536807055717**]

catena-Poly[[tetraaquamanganese(II)]-μ-6,6'-dihydroxy-3,3'-diazenediyldibenzoato-κ^2O:O']

Y.-H. Tan, Z.-Q. Huang, S.-H. Chen, X.-B. Xie and L.-B. Xia

Comment

Olsalazine − 3,3-azo-bis(6-hydroxybenzoic acid) - has been widely used to prevent and treat the inflammatory bowel diseases, such as ulcerative colitis (Klotz, 2005). Recently, we have successfully synthesized a serial of Zn (Tang, Tan, Chen & Cao, 2007), Cd and Co (Tang, Yang *et al.*, 2007) complexes with olsalazine as building block. Also, we have reported a Mn complex of olsalazine crystallized in chiral group P4(3)2(1)2 (Tang, Tan & Cao, 2007), however in the condition of UV light- illumination with wavenumber 365 nm, to our surprise, we found the colour of the crystals turn from orange to deep red after two weeks. The further investigation by X-ray single-crystal structure analysis revealed that the space group change from P4(3)2(1)2 to P2(1)/c. Here we reported the new crystal structure of the title compound, (I)− a new Manganese complex of olsalazine.

In (I) (Fig. 1), the Mn atom is hexacoordinated (Fig. 1) by two O atoms from two *L* ligands (H_2L = 3,3-azo-bis(6-hydroxybenzoic acid)) and four water molecules in a distorted octahedral geometry (Table 1). Two ligands are *cis* to each other in an octahedral environment. Each ligand *L* acts as a carboxylate bridge, that leads to formation of polymeric chain running in the direction [110]. Two neighbouring polymeric chains are paired by π···π interactions between the aromatic rings - the distances $Cg1\cdots Cg1^{i}$ and $Cg2\cdots Cg2^{i}$ are 3.830 (16) and 4.476 (17) Å, respectively [*Cg*1 and *Cg*2 are centroids of C3/C8/C10/C6/C12/C9 and C1/C2/C7/C13/C11/C5 rings, respectively; symmetry code: (i) *1 − x*,*-y*,*- -z*; (ii) *-x*,*-1 − y*,*- -z*]. The crystal packing is further stabilized by the intermolecular O—H···O and O—H···N hydrogen bonds (Table 2).

Experimental

$MnCl_2$ was acquired from Aldrich, and 3,3-azo-bis(6-hydroxybenzoic acid) was synthesized according to the literature (Riordan & Blair, 1979). To a solution of 3,3-azo-bis(6-hydroxybenzoic acid) (301 mg, 1 mmol) in water (60 ml) and sodium hydroxide (1 *M*, 2 ml), $MnCl_2$ (349 mg, 1 mmol) was added. The mixture was stirred at 373 K for 12 h and then filtered. Single-crystals were grown from the filtrate after six weeks (Tang *et al.*, 2007), then moved to a box with UV light (365 nm)- illumination in room temperature. The orange crystals turned to deep red crystals about two weeks later. We collected and separated them carefully, then dried in a desiccator. The yield reaches 92 percent based on the orange crystals. Compound (I) is stable in air and insoluble in water.

Refinement

The hydroxy and C-bound H atoms were placed in calculated postions (C—H = 0.93 Å, O—H = 0.82 Å) and included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C,*O*). The water H atoms were located in a difference Fourier map and isotropically refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å.

Figures

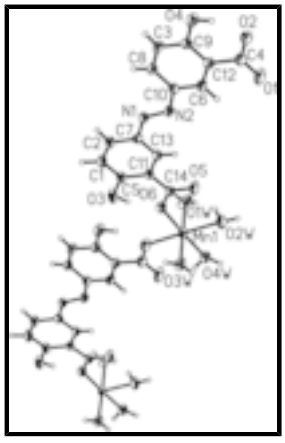


Fig. 1. The structure of a portion of the polymeric chain in (I), showing displacement ellipsoids drawn at the 30% probability level and the atomic labelling. Unlabelled atoms are related to labelled atoms by the symmetry code ($x-1, y-1, z$).

catena-Poly[[tetraaquamanganese(II)]-μ-6,6'-dihydroxy-3,3'- diazenediyldibenzoato-$\kappa^2O:O'$]

Crystal data

$[Mn(C_{14}H_8N_2O_6)(H_2O_1)_4]$	F_{000} = 876
M_r = 427.23	D_x = 1.660 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 935 reflections
a = 9.486 (2) Å	θ = 2.2–26º
b = 11.490 (3) Å	μ = 0.83 mm^{-1}
c = 16.322 (4) Å	T = 293 (2) K
β = 106.076 (3)º	Block, red
V = 1709.4 (7) Å^3	0.31 × 0.23 × 0.21 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3341 independent reflections
Radiation source: fine-focus sealed tube	2933 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
T = 293(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −11→11
T_{min} = 0.80, T_{max} = 0.84	k = −13→14
8959 measured reflections	l = −20→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.0368P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.55$	$(\Delta/\sigma)_{max} = 0.001$
3341 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
284 parameters	$\Delta\rho_{min} = -0.37$ e Å^{-3}
16 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}
Mn1	0.71229 (3)	0.36073 (2)	0.210538 (18)	0.03035 (13)
O4W	0.84712 (17)	0.45769 (13)	0.31718 (7)	0.0454 (4)
O6	0.57181 (16)	0.26262 (12)	0.10622 (9)	0.0378 (3)
N2	0.09166 (19)	−0.14057 (13)	0.00328 (11)	0.0331 (4)
O5	0.4699 (2)	0.13827 (14)	0.17648 (10)	0.0518 (5)
O4	−0.30717 (19)	−0.50644 (14)	−0.04431 (10)	0.0503 (4)
N1	0.12243 (19)	−0.10512 (15)	−0.06254 (10)	0.0311 (4)
C14	0.4863 (2)	0.17786 (17)	0.10958 (12)	0.0322 (4)
O3	0.5107 (2)	0.25868 (15)	−0.05407 (10)	0.0563 (5)
O3W	0.88504 (19)	0.23991 (14)	0.21347 (7)	0.0525 (4)
O2W	0.6512 (2)	0.25207 (16)	0.30695 (10)	0.0540 (4)
C13	0.3039 (2)	0.03679 (17)	0.02394 (13)	0.0299 (4)
C12	−0.1180 (2)	−0.39112 (18)	0.04972 (13)	0.0333 (4)
C11	0.4008 (2)	0.12786 (16)	0.02602 (13)	0.0292 (4)
C10	−0.0114 (2)	−0.23392 (16)	−0.01245 (12)	0.0310 (4)
C9	−0.2083 (2)	−0.41852 (17)	−0.03162 (13)	0.0345 (4)
C8	−0.1046 (2)	−0.26171 (19)	−0.09284 (13)	0.0372 (5)
O1W	0.5321 (2)	0.47858 (14)	0.20352 (11)	0.0637 (5)
C7	0.2227 (2)	−0.01053 (16)	−0.05305 (12)	0.0309 (4)
C6	−0.0207 (2)	−0.29866 (18)	0.05741 (12)	0.0362 (5)

C5	0.4158 (2)	0.17191 (19)	−0.05163 (13)	0.0369 (5)
C3	−0.2000 (3)	−0.35306 (19)	−0.10170 (15)	0.0411 (5)
C2	0.2400 (3)	0.0341 (2)	−0.12885 (14)	0.0412 (5)
C1	0.3339 (3)	0.1242 (2)	−0.12874 (14)	0.0470 (6)
C4	−0.1291 (3)	−0.45639 (19)	0.12689 (14)	0.0422 (5)
O2	−0.22138 (18)	−0.53993 (13)	0.11428 (10)	0.0474 (4)
O1	−0.0512 (2)	−0.42829 (17)	0.19838 (10)	0.0677 (6)
H13A	0.301 (2)	0.0110 (17)	0.0730 (14)	0.030 (5)*
H8A	−0.111 (3)	−0.2182 (17)	−0.1412 (15)	0.036 (6)*
H1A	0.336 (3)	0.165 (2)	−0.1854 (17)	0.047 (6)*
H2A	0.178 (4)	0.012 (3)	−0.178 (2)	0.079 (10)*
H5A	−0.261 (3)	−0.3663 (18)	−0.1493 (18)	0.042 (7)*
H6A	0.0455 (7)	−0.2856 (8)	0.11412 (19)	0.062 (8)*
H2WB	0.6323	0.2541	0.3549	0.055 (8)*
H4WB	0.9093	0.4932	0.2975	0.074 (10)*
H3A	0.5395 (5)	0.2747 (2)	−0.00175 (8)	0.058 (8)*
H4WA	0.8832	0.4458	0.3703	0.085 (11)*
H3WB	0.8753	0.2116	0.1641	0.098 (12)*
H1WB	0.5363	0.5277	0.2431	0.075 (10)*
H3WA	0.9322	0.1924	0.2511	0.097 (12)*
H4A	−0.2990 (4)	−0.5379 (3)	0.00539 (10)	0.061 (8)*
H1WA	0.4804	0.5058	0.1563	0.086 (11)*
H2WA	0.5834	0.2157	0.2710	0.114 (14)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0338 (2)	0.03079 (19)	0.02409 (19)	−0.00292 (12)	0.00414 (13)	−0.00169 (11)
O4W	0.0477 (9)	0.0535 (9)	0.0323 (8)	−0.0134 (8)	0.0067 (7)	−0.0077 (7)
O6	0.0439 (8)	0.0385 (8)	0.0290 (7)	−0.0167 (7)	0.0068 (6)	−0.0067 (6)
N2	0.0363 (10)	0.0348 (9)	0.0263 (9)	−0.0097 (7)	0.0055 (7)	0.0003 (7)
O5	0.0692 (12)	0.0565 (10)	0.0254 (8)	−0.0264 (8)	0.0061 (8)	0.0029 (7)
O4	0.0569 (10)	0.0485 (9)	0.0370 (9)	−0.0288 (8)	−0.0014 (7)	0.0031 (7)
N1	0.0334 (9)	0.0325 (8)	0.0268 (8)	−0.0077 (7)	0.0071 (7)	−0.0021 (7)
C14	0.0342 (11)	0.0320 (10)	0.0296 (10)	−0.0048 (8)	0.0077 (8)	−0.0014 (8)
O3	0.0746 (12)	0.0654 (10)	0.0304 (8)	−0.0439 (9)	0.0168 (8)	−0.0058 (7)
O3W	0.0617 (11)	0.0620 (10)	0.0317 (8)	0.0259 (9)	0.0098 (7)	−0.0018 (8)
O2W	0.0654 (11)	0.0650 (10)	0.0335 (9)	−0.0240 (9)	0.0169 (8)	−0.0025 (8)
C13	0.0340 (11)	0.0304 (10)	0.0257 (10)	−0.0044 (8)	0.0090 (8)	−0.0002 (8)
C12	0.0350 (11)	0.0325 (10)	0.0298 (11)	−0.0088 (8)	0.0047 (8)	0.0017 (8)
C11	0.0301 (10)	0.0316 (10)	0.0255 (10)	−0.0039 (8)	0.0069 (8)	−0.0021 (8)
C10	0.0328 (10)	0.0314 (9)	0.0286 (10)	−0.0076 (8)	0.0078 (8)	−0.0003 (8)
C9	0.0342 (11)	0.0334 (10)	0.0335 (11)	−0.0099 (9)	0.0052 (9)	−0.0013 (8)
C8	0.0374 (11)	0.0445 (12)	0.0273 (10)	−0.0089 (9)	0.0051 (9)	0.0056 (9)
O1W	0.0627 (12)	0.0665 (11)	0.0470 (10)	0.0277 (10)	−0.0096 (9)	−0.0223 (9)
C7	0.0291 (10)	0.0322 (10)	0.0305 (10)	−0.0072 (8)	0.0068 (8)	−0.0027 (8)
C6	0.0403 (11)	0.0402 (11)	0.0240 (10)	−0.0123 (9)	0.0020 (8)	0.0015 (8)
C5	0.0421 (12)	0.0397 (11)	0.0304 (11)	−0.0144 (9)	0.0123 (9)	−0.0021 (9)

C3	0.0440 (13)	0.0483 (13)	0.0245 (10)	−0.0154 (10)	−0.0014 (10)	−0.0002 (9)
C2	0.0463 (13)	0.0512 (13)	0.0243 (10)	−0.0171 (11)	0.0069 (9)	−0.0051 (9)
C1	0.0579 (15)	0.0576 (14)	0.0259 (11)	−0.0252 (12)	0.0126 (10)	−0.0005 (10)
C4	0.0463 (13)	0.0428 (12)	0.0334 (11)	−0.0167 (10)	0.0044 (10)	0.0040 (9)
O2	0.0531 (10)	0.0464 (9)	0.0375 (8)	−0.0238 (8)	0.0039 (7)	0.0087 (7)
O1	0.0855 (14)	0.0753 (12)	0.0312 (9)	−0.0476 (11)	−0.0025 (9)	0.0096 (8)

Geometric parameters (Å, °)

Mn1—O3W	2.1380 (15)	C13—C7	1.390 (3)
Mn1—O1W	2.1588 (16)	C13—H13A	0.86 (2)
Mn1—O4W	2.1619 (14)	C12—C6	1.390 (3)
Mn1—O6	2.1654 (14)	C12—C9	1.402 (3)
Mn1—O2^{i}	2.1713 (15)	C12—C4	1.495 (3)
Mn1—O2W	2.2083 (15)	C11—C5	1.408 (3)
O4W—H4WB	0.8501	C10—C6	1.384 (3)
O4W—H4WA	0.8500	C10—C8	1.401 (3)
O6—C14	1.278 (2)	C9—C3	1.389 (3)
N2—N1	1.256 (2)	C8—C3	1.367 (3)
N2—C10	1.426 (2)	C8—H8A	0.92 (2)
O5—C14	1.232 (3)	O1W—H1WB	0.8501
O4—C9	1.355 (2)	O1W—H1WA	0.8500
O4—H4A	0.872 (3)	C7—C2	1.391 (3)
N1—C7	1.424 (2)	C6—H6A	0.975 (4)
C14—C11	1.495 (3)	C5—C1	1.395 (3)
O3—C5	1.351 (2)	C3—H5A	0.84 (3)
O3—H3A	0.8418 (19)	C2—C1	1.365 (3)
O3W—H3WB	0.8502	C2—H2A	0.90 (3)
O3W—H3WA	0.8502	C1—H1A	1.04 (3)
O2W—H2WB	0.8501	C4—O1	1.239 (3)
O2W—H2WA	0.8500	C4—O2	1.277 (2)
C13—C11	1.387 (3)	O2—Mn1^{ii}	2.1713 (15)
O3W—Mn1—O1W	177.68 (6)	C13—C11—C5	118.74 (18)
O3W—Mn1—O4W	92.16 (6)	C13—C11—C14	120.05 (17)
O1W—Mn1—O4W	90.15 (6)	C5—C11—C14	121.21 (17)
O3W—Mn1—O6	88.88 (6)	C6—C10—C8	118.78 (17)
O1W—Mn1—O6	88.80 (6)	C6—C10—N2	116.91 (17)
O4W—Mn1—O6	178.02 (5)	C8—C10—N2	124.29 (17)
O3W—Mn1—O2^{i}	89.06 (7)	O4—C9—C3	118.19 (18)
O1W—Mn1—O2^{i}	90.90 (8)	O4—C9—C12	121.86 (18)
O4W—Mn1—O2^{i}	94.95 (6)	C3—C9—C12	119.94 (18)
O6—Mn1—O2^{i}	86.75 (6)	C3—C8—C10	120.11 (19)
O3W—Mn1—O2W	88.16 (7)	C3—C8—H8A	116.1 (14)
O1W—Mn1—O2W	91.84 (8)	C10—C8—H8A	123.6 (14)
O4W—Mn1—O2W	86.06 (6)	Mn1—O1W—H1WB	120.4
O6—Mn1—O2W	92.30 (6)	Mn1—O1W—H1WA	121.9
O2^{i}—Mn1—O2W	177.08 (7)	H1WB—O1W—H1WA	109.7

Mn1—O4W—H4WB	105.1	C13—C7—C2	119.17 (18)
Mn1—O4W—H4WA	136.0	C13—C7—N1	125.68 (17)
H4WB—O4W—H4WA	109.7	C2—C7—N1	115.13 (17)
C14—O6—Mn1	128.50 (12)	C10—C6—C12	121.88 (18)
N1—N2—C10	113.58 (15)	C10—C6—H6A	121.9 (3)
C9—O4—H4A	106.7 (2)	C12—C6—H6A	116.1 (3)
N2—N1—C7	117.43 (15)	O3—C5—C1	118.21 (18)
O5—C14—O6	123.82 (18)	O3—C5—C11	121.75 (18)
O5—C14—C11	119.81 (17)	C1—C5—C11	120.03 (18)
O6—C14—C11	116.36 (16)	C8—C3—C9	121.0 (2)
C5—O3—H3A	99.4 (4)	C8—C3—H5A	120.1 (16)
Mn1—O3W—H3WB	110.2	C9—C3—H5A	118.6 (16)
Mn1—O3W—H3WA	132.8	C1—C2—C7	121.1 (2)
H3WB—O3W—H3WA	109.6	C1—C2—H2A	119 (2)
Mn1—O2W—H2WB	143.5	C7—C2—H2A	119 (2)
Mn1—O2W—H2WA	94.8	C2—C1—C5	120.0 (2)
H2WB—O2W—H2WA	109.7	C2—C1—H1A	120.7 (14)
C11—C13—C7	121.00 (18)	C5—C1—H1A	118.9 (14)
C11—C13—H13A	115.6 (14)	O1—C4—O2	123.5 (2)
C7—C13—H13A	123.4 (14)	O1—C4—C12	120.01 (19)
C6—C12—C9	118.27 (18)	O2—C4—C12	116.53 (18)
C6—C12—C4	120.50 (18)	C4—O2—Mn1^{ii}	126.99 (14)
C9—C12—C4	121.20 (18)		

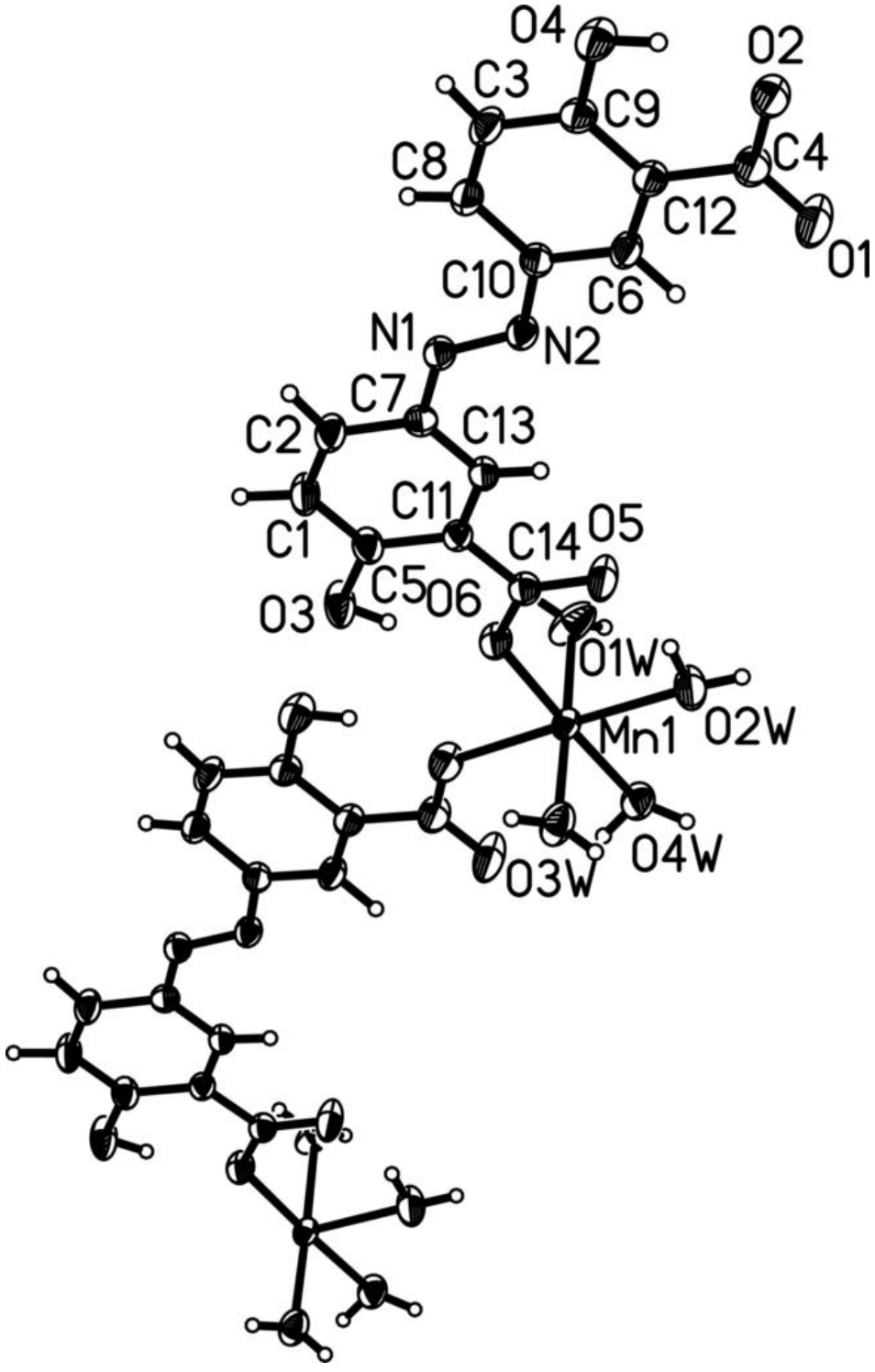
Symmetry codes: (i) *x*+1, *y*+1, *z*; (ii) *x*−1, *y*−1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4W—H4WB···O1^{i}	0.85	1.98	2.728 (2)	147
O4W—H4WA···N2^{iii}	0.85	2.24	3.043 (2)	157
O3—H3A···O6	0.84	1.71	2.519 (2)	161
O3W—H3WB···N1^{iv}	0.85	2.07	2.894 (2)	165
O4—H4A···O2	0.87	1.73	2.519 (2)	150
O1W—H1WB···O5^{iii}	0.85	1.84	2.688 (2)	175
O3W—H3WA···O1^{iii}	0.85	1.83	2.652 (3)	161
O1W—H1WA···O4^{v}	0.85	2.09	2.887 (3)	155
O2W—H2WA···O5	0.85	1.85	2.678 (2)	165

Symmetry codes: (i) *x*+1, *y*+1, *z*; (iii) −*x*+1, *y*+1/2, −*z*+1/2; (iv) −*x*+1, −*y*, −*z*; (v) −*x*, −*y*, −*z*.

Fig. 1


O4
O2
C3
C9
C8
C4
C12
O1
C10
C6
N1
N2
C7
C2
C13
C11
C1
C14
O5
C5
O6
O3
O1W
Mn1
O2W
O3W
O4W