Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aqua{6,6′-dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}(formato-κO)-manganese(III) dihydrate

See Mun Lee, Kong Mun Lo and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

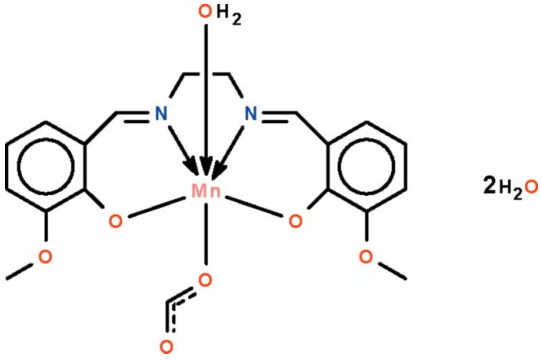
Received 9 May 2011; accepted 10 May 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.067; wR factor = 0.192; data-to-parameter ratio = 16.4.

The Mn^{III} atom in the title complex, $[Mn(C_{18}H_{18}N_2O_4)(CHO_2)(H_2O)]\cdot 2H_2O$, is O,N,N',O'-chelated by the deprotonated Schiff base; the four chelating atoms form an approximate square, with the O atoms of the water molecule and the formate ion in axial positions above and below the square plane. Two metal-bearing molecules are linked by an O—$H_{water}\cdots$O hydrogen bond about a center of inversion, generating a hydrogen-bonded dinuclear species; adjacent dinuclear units are linked through the lattice water molecules, forming a three-dimensional network.

Related literature

For related Mn^{III} compounds with the same Schiff base, see: Bermejo *et al.* (2007); Li *et al.* (2009); Zhang *et al.* (1999, 2000).



Experimental

Crystal data

$[Mn(C_{18}H_{18}N_2O_4)(CHO_2)(H_2O)]\cdot 2H_2O$
M_r = 480.35
Monoclinic, $P2_1/c$
a = 11.5670 (2) Å
b = 19.9312 (3) Å
c = 8.7701 (1) Å
β = 96.859 (1)°
V = 2007.42 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 100 K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.932, T_{max} = 0.932
18245 measured reflections
4600 independent reflections
3660 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.192
S = 1.12
4600 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O3^{i}	0.84	2.01	2.730 (4)	143
O1w—H12···O2^{i}	0.84	2.09	2.813 (4)	145
O2w—H21···O6	0.84	2.04	2.793 (5)	148
O2w—H22···O3w	0.84	1.96	2.762 (7)	161
O3w—H31···O2w^{ii}	0.84	1.94	2.782 (7)	179

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank the University of Malaya (grant No. RG020/09AFR) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5546).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bermejo, M. R., Fernandez, M. I., Gomez-Forneas, E., Gonzalez-Noya, A., Maneiro, M., Pedrido, R. & Rodriguez, M. J. (2007). *Eur. J. Inorg. Chem.* pp. 3789–3797.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, Z.-X., Li, X., Zhang, L.-F. & Yu, M.-M. (2009). *Acta Cryst.* E**65**, m153.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Zhang, C.-G., Tian, G.-H., Ma, Z.-F. & Yan, D.-Y. (2000). *Transition Met. Chem.* **25**, 270–273.
Zhang, C.-G., Wu, D., Zhao, C.-X., Sun, J. & Kong, X.-F. (1999). *Transition Met. Chem.* **24**, 718–721.

supporting information

Acta Cryst. (2011). E**67**, m746 [doi:10.1107/S1600536811017648]

Aqua{6,6′-dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}(formato-κO)manganese(III) dihydrate

See Mun Lee, Kong Mun Lo and Seik Weng Ng

S1. Comment

The 6,6′-dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenol Schiff base functions as a tetradentate dianionic ligand in a small number of manganese(III) derivatives (Bermejo *et al.*, 2007; Li *et al.* 2009; Zhang *et al.*, 1999, 2000). The counterion that balances the positive charge on the metal is involved in coordination. In the present study, the acetate portion of the manganese(III) acetate reactant undergoes carbon-carbon cleave to form a formate ion. The Mn^{III} atom in $Mn(H_2O)(CHO_2)(C_{18}H_{18}N_2O_4)\cdot 2H_2O$ (Scheme I) is *O*,*N*,*N*′,*O*′-chelated by the deprotonated Schiff base; the four atoms involved in chelating form a square, above and below which are the O atoms of the water molecule and the formate ion (Fig. 1). Two molecules are linked by an $O–H_{water}\cdots O$ hydrogen bond dinuclear species; adjacent dinuclear units are linked through the lattice water molecules, forming a three-dimensional network (Table 1).

S2. Experimental

N,N′-Ethylenebis(4-methoxysalicylindeneaminate) was prepared by reacting 0.2 ml (3.1 mmol) of ethylenediamine with 0.9 g (6 mmol) of 2-hydroxy-4-methoxybenzaldehyde in 50 ml of ethanol. An aqueous solution of 0.18 g (1 mmol) of manganese(II) nitrate was added to a hot methanol solution (100 ml) containing 0. 32 g (1 mmol) of the ligand and 0.28 g (2 mmol) of sodium acetate trihydrate. The immediate brown solution was refluxed for an hour, after which it was filtered. Slow evaporation of the filtrate gave brown crystals. Under the reaction conditions, the acetate ion used in the synthesis was converted to the formate ion in the product; the carbon-carbon bond cleavage was accompanied by oxidation of the Mn^{II} to Mn^{III}.

S3. Refinement

Carbon- and oxygen-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.98, O—H 0.84 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2–1.5 times U_{eq}(C). The water H atoms were placed on the basis of hydrogen bonding interactions. The O3w atom forms one only hydrogen bond; the O atom appears to be a little disordered but the disorder could not be modeled. The H31 atom is 1.99 Å from another H atom.

The final differerence Fourier map had a peak in the vicinity of Mn1.

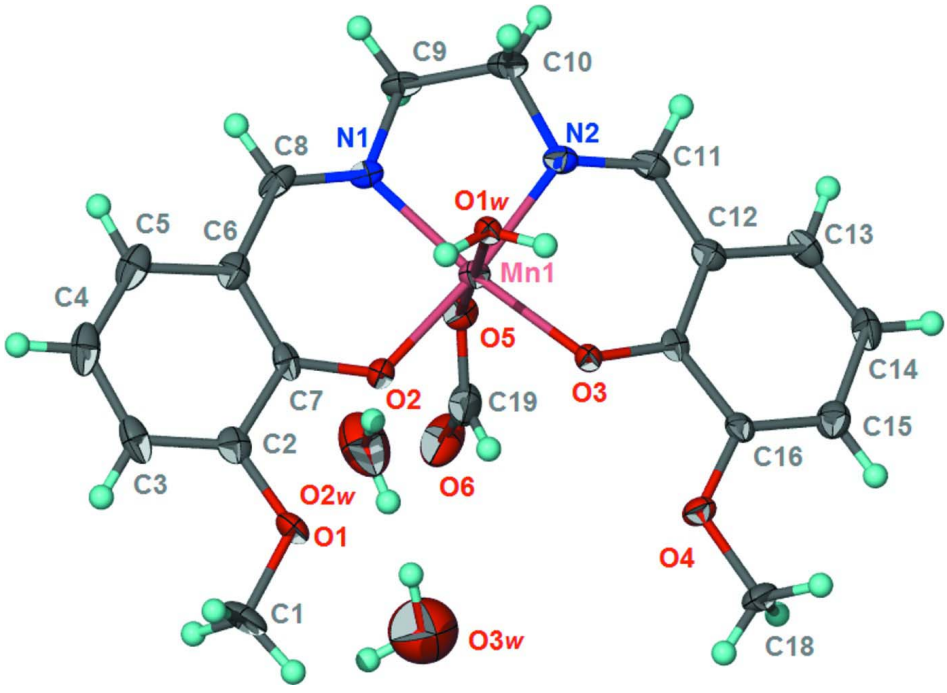


Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $Mn(H_2O)(CHO_2)(C_{18}H_{18}N_2O_4)\cdot 2H_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Aqua{6,6′-dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}(formato-κO)manganese(III) dihydrate

Crystal data

$[Mn(C_{18}H_{18}N_2O_4)(CHO_2)(H_2O)]\cdot 2H_2O$
$M_r = 480.35$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.5670$ (2) Å
$b = 19.9312$ (3) Å
$c = 8.7701$ (1) Å
$\beta = 96.859$ (1)°
$V = 2007.42$ (5) Å^3
$Z = 4$
$F(000) = 1000$
$D_x = 1.589$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5455 reflections
$\theta = 2.6$–$28.0°$
$\mu = 0.72$ mm^{-1}
$T = 100$ K
Prism, brown
0.10 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.932$, $T_{max} = 0.932$
18245 measured reflections
4600 independent reflections
3660 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.1°$
$h = -15\rightarrow 15$
$k = -25\rightarrow 25$
$l = -11\rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.192$
$S = 1.12$
4600 reflections
280 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
$w = 1/[\sigma^2(F_o^2) + (0.0885P)^2 + 6.8815P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.67$ e Å^{-3}
$\Delta\rho_{min} = -0.96$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.40763 (5)	0.60235 (3)	0.45697 (6)	0.01376 (19)
O1	0.6169 (2)	0.53984 (14)	0.8928 (3)	0.0177 (6)
O2	0.5069 (2)	0.58740 (13)	0.6460 (3)	0.0144 (5)
O3	0.3207 (2)	0.52060 (13)	0.4678 (3)	0.0125 (5)
O4	0.2108 (2)	0.42353 (13)	0.5778 (3)	0.0158 (6)
O5	0.2946 (2)	0.65306 (13)	0.5659 (3)	0.0162 (6)
O6	0.2078 (3)	0.65735 (18)	0.7803 (4)	0.0348 (8)
O1W	0.5237 (2)	0.55239 (13)	0.3407 (3)	0.0126 (5)
H11	0.5894	0.5451	0.3896	0.019*
H12	0.4944	0.5155	0.3105	0.019*
O2W	0.1084 (3)	0.7667 (2)	0.9154 (4)	0.0449 (10)
H21	0.1510	0.7465	0.8592	0.067*
H22	0.0809	0.7383	0.9721	0.067*
O3W	−0.0064 (5)	0.6998 (3)	1.1285 (6)	0.0685 (14)
H31	0.0274	0.7096	1.2158	0.103*
H32	−0.0035	0.6581	1.1146	0.103*
N1	0.4905 (3)	0.68849 (16)	0.4208 (4)	0.0136 (6)
N2	0.3178 (3)	0.62522 (16)	0.2534 (4)	0.0143 (6)
C1	0.6694 (4)	0.5152 (2)	1.0374 (5)	0.0246 (9)
H1A	0.6264	0.4758	1.0668	0.037*
H1B	0.6676	0.5502	1.1155	0.037*
H1C	0.7504	0.5026	1.0294	0.037*
C2	0.6672 (3)	0.5951 (2)	0.8350 (4)	0.0161 (8)
C3	0.7689 (3)	0.6259 (2)	0.8983 (5)	0.0202 (8)
H3	0.8092	0.6095	0.9916	0.024*
C4	0.8127 (4)	0.6813 (2)	0.8249 (5)	0.0233 (9)
H4	0.8836	0.7017	0.8672	0.028*
C5	0.7536 (3)	0.7061 (2)	0.6929 (5)	0.0209 (9)
H5	0.7838	0.7438	0.6445	0.025*
C6	0.6482 (3)	0.67655 (19)	0.6269 (4)	0.0155 (7)
C7	0.6036 (3)	0.61946 (19)	0.6976 (4)	0.0138 (7)
C8	0.5872 (3)	0.70852 (19)	0.4923 (5)	0.0170 (8)
H8	0.6216	0.7474	0.4542	0.020*
C9	0.4287 (4)	0.72776 (19)	0.2943 (5)	0.0184 (8)

H9A	0.4841	0.7575	0.2491	0.022*
H9B	0.3683	0.7560	0.3333	0.022*
C10	0.3726 (4)	0.6793 (2)	0.1728 (5)	0.0189 (8)
H10A	0.3133	0.7029	0.1015	0.023*
H10B	0.4322	0.6605	0.1127	0.023*
C11	0.2202 (3)	0.59919 (19)	0.1976 (4)	0.0162 (7)
H11A	0.1824	0.6176	0.1049	0.019*
C12	0.1639 (3)	0.54401 (19)	0.2656 (4)	0.0143 (7)
C13	0.0536 (3)	0.5237 (2)	0.1934 (5)	0.0186 (8)
H13	0.0186	0.5475	0.1060	0.022*
C14	−0.0036 (3)	0.4701 (2)	0.2477 (5)	0.0201 (8)
H14	−0.0770	0.4566	0.1967	0.024*
C15	0.0461 (3)	0.4352 (2)	0.3783 (5)	0.0186 (8)
H15	0.0056	0.3986	0.4167	0.022*
C16	0.1531 (3)	0.45387 (18)	0.4506 (4)	0.0132 (7)
C17	0.2160 (3)	0.50826 (18)	0.3954 (4)	0.0116 (7)
C18	0.1525 (4)	0.3688 (2)	0.6400 (5)	0.0195 (8)
H18A	0.2013	0.3508	0.7297	0.029*
H18B	0.1376	0.3335	0.5622	0.029*
H18C	0.0783	0.3843	0.6709	0.029*
C19	0.2604 (4)	0.6283 (2)	0.6891 (5)	0.0232 (9)
H19	0.2783	0.5825	0.7102	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0155 (3)	0.0130 (3)	0.0126 (3)	−0.0006 (2)	0.0011 (2)	0.0015 (2)
O1	0.0182 (14)	0.0221 (14)	0.0117 (13)	−0.0003 (11)	−0.0031 (10)	0.0014 (11)
O2	0.0141 (13)	0.0138 (13)	0.0151 (13)	−0.0037 (10)	0.0006 (10)	0.0000 (10)
O3	0.0129 (12)	0.0119 (12)	0.0119 (12)	−0.0012 (10)	−0.0022 (10)	0.0012 (9)
O4	0.0173 (14)	0.0134 (13)	0.0163 (13)	−0.0013 (10)	0.0007 (10)	0.0039 (10)
O5	0.0158 (13)	0.0145 (13)	0.0187 (14)	0.0010 (10)	0.0040 (11)	−0.0008 (10)
O6	0.038 (2)	0.0346 (19)	0.0353 (19)	−0.0131 (15)	0.0206 (16)	−0.0151 (15)
O1W	0.0116 (12)	0.0134 (12)	0.0122 (12)	−0.0006 (9)	−0.0002 (10)	0.0005 (10)
O2W	0.042 (2)	0.054 (2)	0.039 (2)	0.0025 (18)	0.0034 (17)	−0.0162 (18)
O3W	0.069 (3)	0.066 (3)	0.069 (3)	−0.004 (3)	0.003 (3)	0.004 (3)
N1	0.0152 (15)	0.0119 (15)	0.0142 (15)	0.0004 (12)	0.0036 (12)	0.0025 (12)
N2	0.0170 (16)	0.0128 (15)	0.0134 (15)	0.0022 (12)	0.0023 (12)	0.0032 (12)
C1	0.027 (2)	0.036 (2)	0.0102 (18)	0.0038 (18)	−0.0022 (16)	0.0031 (16)
C2	0.0155 (18)	0.0182 (19)	0.0147 (18)	0.0015 (14)	0.0023 (14)	−0.0046 (14)
C3	0.0149 (19)	0.027 (2)	0.0182 (19)	0.0027 (16)	−0.0017 (15)	−0.0113 (16)
C4	0.0142 (19)	0.026 (2)	0.031 (2)	−0.0031 (16)	0.0043 (16)	−0.0138 (18)
C5	0.0153 (19)	0.0170 (19)	0.032 (2)	−0.0030 (15)	0.0089 (16)	−0.0082 (16)
C6	0.0132 (18)	0.0145 (18)	0.0191 (19)	0.0002 (14)	0.0033 (14)	−0.0051 (14)
C7	0.0120 (17)	0.0161 (18)	0.0136 (17)	0.0016 (13)	0.0026 (14)	−0.0066 (14)
C8	0.0199 (19)	0.0106 (17)	0.022 (2)	−0.0009 (14)	0.0104 (16)	−0.0005 (14)
C9	0.023 (2)	0.0146 (18)	0.0177 (19)	0.0004 (15)	0.0034 (16)	0.0062 (15)
C10	0.020 (2)	0.020 (2)	0.0164 (19)	−0.0007 (15)	0.0041 (15)	0.0060 (15)

C11	0.0169 (18)	0.0170 (18)	0.0143 (18)	0.0051 (14)	0.0003 (14)	0.0032 (14)
C12	0.0151 (18)	0.0158 (18)	0.0119 (17)	0.0023 (14)	0.0008 (14)	−0.0010 (14)
C13	0.0157 (19)	0.023 (2)	0.0164 (18)	0.0043 (15)	−0.0025 (15)	−0.0015 (15)
C14	0.0141 (18)	0.026 (2)	0.020 (2)	−0.0025 (16)	−0.0020 (15)	−0.0052 (16)
C15	0.0154 (19)	0.021 (2)	0.0200 (19)	−0.0018 (15)	0.0029 (15)	−0.0021 (15)
C16	0.0151 (18)	0.0140 (17)	0.0103 (16)	−0.0005 (14)	0.0010 (13)	−0.0016 (13)
C17	0.0128 (17)	0.0111 (16)	0.0113 (16)	0.0013 (13)	0.0027 (13)	−0.0026 (13)
C18	0.025 (2)	0.0148 (18)	0.0192 (19)	−0.0049 (15)	0.0041 (16)	0.0028 (15)
C19	0.021 (2)	0.027 (2)	0.022 (2)	−0.0087 (17)	0.0062 (17)	−0.0055 (17)

Geometric parameters (Å, º)

Mn1—O3	1.923 (3)	C3—C4	1.403 (6)
Mn1—O2	1.924 (3)	C3—H3	0.9500
Mn1—O5	1.985 (3)	C4—C5	1.364 (6)
Mn1—N2	2.008 (3)	C4—H4	0.9500
Mn1—N1	2.010 (3)	C5—C6	1.414 (5)
Mn1—O1W	2.040 (3)	C5—H5	0.9500
O1—C2	1.371 (5)	C6—C7	1.422 (5)
O1—C1	1.427 (5)	C6—C8	1.449 (6)
O2—C7	1.321 (4)	C8—H8	0.9500
O3—C17	1.322 (4)	C9—C10	1.525 (6)
O4—C16	1.370 (4)	C9—H9A	0.9900
O4—C18	1.426 (5)	C9—H9B	0.9900
O5—C19	1.293 (5)	C10—H10A	0.9900
O6—C19	1.208 (5)	C10—H10B	0.9900
O1W—H11	0.8400	C11—C12	1.443 (5)
O1W—H12	0.8400	C11—H11A	0.9500
O2W—H21	0.8400	C12—C13	1.414 (5)
O2W—H22	0.8399	C12—C17	1.415 (5)
O3W—H31	0.8401	C13—C14	1.371 (6)
O3W—H32	0.8399	C13—H13	0.9500
N1—C8	1.279 (5)	C14—C15	1.403 (6)
N1—C9	1.471 (5)	C14—H14	0.9500
N2—C11	1.285 (5)	C15—C16	1.373 (5)
N2—C10	1.473 (5)	C15—H15	0.9500
C1—H1A	0.9800	C16—C17	1.423 (5)
C1—H1B	0.9800	C18—H18A	0.9800
C1—H1C	0.9800	C18—H18B	0.9800
C2—C3	1.383 (5)	C18—H18C	0.9800
C2—C7	1.421 (5)	C19—H19	0.9500
O3—Mn1—O2	95.04 (11)	C5—C6—C8	117.6 (4)
O3—Mn1—O5	91.70 (11)	C7—C6—C8	122.7 (3)
O2—Mn1—O5	91.35 (11)	O2—C7—C2	117.2 (3)
O3—Mn1—N2	91.04 (12)	O2—C7—C6	125.1 (3)
O2—Mn1—N2	173.53 (12)	C2—C7—C6	117.7 (3)
O5—Mn1—N2	90.68 (12)	N1—C8—C6	125.1 (3)

O3—Mn1—N1	173.52 (12)	N1—C8—H8	117.5
O2—Mn1—N1	91.25 (12)	C6—C8—H8	117.5
O5—Mn1—N1	89.71 (12)	N1—C9—C10	108.5 (3)
N2—Mn1—N1	82.62 (13)	N1—C9—H9A	110.0
O3—Mn1—O1W	89.43 (11)	C10—C9—H9A	110.0
O2—Mn1—O1W	89.70 (11)	N1—C9—H9B	110.0
O5—Mn1—O1W	178.39 (11)	C10—C9—H9B	110.0
N2—Mn1—O1W	88.15 (12)	H9A—C9—H9B	108.4
N1—Mn1—O1W	89.05 (12)	N2—C10—C9	107.4 (3)
C2—O1—C1	116.8 (3)	N2—C10—H10A	110.2
C7—O2—Mn1	127.9 (2)	C9—C10—H10A	110.2
C17—O3—Mn1	126.0 (2)	N2—C10—H10B	110.2
C16—O4—C18	116.2 (3)	C9—C10—H10B	110.2
C19—O5—Mn1	119.6 (3)	H10A—C10—H10B	108.5
Mn1—O1W—H11	116.0	N2—C11—C12	124.8 (3)
Mn1—O1W—H12	108.7	N2—C11—H11A	117.6
H11—O1W—H12	108.4	C12—C11—H11A	117.6
H21—O2W—H22	108.4	C13—C12—C17	119.4 (3)
H31—O3W—H32	110.0	C13—C12—C11	117.5 (3)
C8—N1—C9	121.4 (3)	C17—C12—C11	123.1 (3)
C8—N1—Mn1	126.5 (3)	C14—C13—C12	121.0 (4)
C9—N1—Mn1	112.1 (2)	C14—C13—H13	119.5
C11—N2—C10	121.4 (3)	C12—C13—H13	119.5
C11—N2—Mn1	125.8 (3)	C13—C14—C15	120.1 (4)
C10—N2—Mn1	112.7 (2)	C13—C14—H14	119.9
O1—C1—H1A	109.5	C15—C14—H14	119.9
O1—C1—H1B	109.5	C16—C15—C14	120.1 (4)
H1A—C1—H1B	109.5	C16—C15—H15	119.9
O1—C1—H1C	109.5	C14—C15—H15	119.9
H1A—C1—H1C	109.5	O4—C16—C15	125.6 (3)
H1B—C1—H1C	109.5	O4—C16—C17	113.2 (3)
O1—C2—C3	125.9 (4)	C15—C16—C17	121.2 (4)
O1—C2—C7	112.8 (3)	O3—C17—C12	124.8 (3)
C3—C2—C7	121.2 (4)	O3—C17—C16	117.1 (3)
C2—C3—C4	120.1 (4)	C12—C17—C16	118.1 (3)
C2—C3—H3	119.9	O4—C18—H18A	109.5
C4—C3—H3	119.9	O4—C18—H18B	109.5
C5—C4—C3	120.2 (4)	H18A—C18—H18B	109.5
C5—C4—H4	119.9	O4—C18—H18C	109.5
C3—C4—H4	119.9	H18A—C18—H18C	109.5
C4—C5—C6	121.1 (4)	H18B—C18—H18C	109.5
C4—C5—H5	119.5	O6—C19—O5	126.8 (5)
C6—C5—H5	119.5	O6—C19—H19	116.6
C5—C6—C7	119.6 (4)	O5—C19—H19	116.6

O3—Mn1—O2—C7	166.9 (3)	C3—C2—C7—O2	−179.4 (3)
O5—Mn1—O2—C7	−101.3 (3)	O1—C2—C7—C6	−179.7 (3)
N1—Mn1—O2—C7	−11.5 (3)	C3—C2—C7—C6	0.1 (5)

O1W—Mn1—O2—C7	77.5 (3)	C5—C6—C7—O2	−179.5 (3)
O2—Mn1—O3—C17	159.0 (3)	C8—C6—C7—O2	3.6 (6)
O5—Mn1—O3—C17	67.5 (3)	C5—C6—C7—C2	1.1 (5)
N2—Mn1—O3—C17	−23.2 (3)	C8—C6—C7—C2	−175.8 (3)
O1W—Mn1—O3—C17	−111.4 (3)	C9—N1—C8—C6	173.9 (3)
O3—Mn1—O5—C19	46.9 (3)	Mn1—N1—C8—C6	−8.3 (6)
O2—Mn1—O5—C19	−48.1 (3)	C5—C6—C8—N1	−179.1 (4)
N2—Mn1—O5—C19	138.0 (3)	C7—C6—C8—N1	−2.1 (6)
N1—Mn1—O5—C19	−139.4 (3)	C8—N1—C9—C10	143.4 (4)
O2—Mn1—N1—C8	12.7 (3)	Mn1—N1—C9—C10	−34.8 (4)
O5—Mn1—N1—C8	104.1 (3)	C11—N2—C10—C9	142.6 (4)
N2—Mn1—N1—C8	−165.2 (3)	Mn1—N2—C10—C9	−34.4 (4)
O1W—Mn1—N1—C8	−76.9 (3)	N1—C9—C10—N2	44.2 (4)
O2—Mn1—N1—C9	−169.2 (3)	C10—N2—C11—C12	176.8 (3)
O5—Mn1—N1—C9	−77.9 (3)	Mn1—N2—C11—C12	−6.5 (6)
N2—Mn1—N1—C9	12.8 (2)	N2—C11—C12—C13	176.8 (4)
O1W—Mn1—N1—C9	101.1 (2)	N2—C11—C12—C17	−6.0 (6)
O3—Mn1—N2—C11	17.3 (3)	C17—C12—C13—C14	0.3 (6)
O5—Mn1—N2—C11	−74.5 (3)	C11—C12—C13—C14	177.6 (4)
N1—Mn1—N2—C11	−164.1 (3)	C12—C13—C14—C15	1.1 (6)
O1W—Mn1—N2—C11	106.6 (3)	C13—C14—C15—C16	−1.1 (6)
O3—Mn1—N2—C10	−165.8 (3)	C18—O4—C16—C15	−1.1 (5)
O5—Mn1—N2—C10	102.5 (3)	C18—O4—C16—C17	179.6 (3)
N1—Mn1—N2—C10	12.9 (3)	C14—C15—C16—O4	−179.4 (4)
O1W—Mn1—N2—C10	−76.4 (3)	C14—C15—C16—C17	−0.3 (6)
C1—O1—C2—C3	5.3 (5)	Mn1—O3—C17—C12	19.2 (5)
C1—O1—C2—C7	−175.0 (3)	Mn1—O3—C17—C16	−162.5 (2)
O1—C2—C3—C4	178.3 (4)	C13—C12—C17—O3	176.7 (3)
C7—C2—C3—C4	−1.5 (6)	C11—C12—C17—O3	−0.4 (6)
C2—C3—C4—C5	1.6 (6)	C13—C12—C17—C16	−1.6 (5)
C3—C4—C5—C6	−0.4 (6)	C11—C12—C17—C16	−178.8 (3)
C4—C5—C6—C7	−1.0 (6)	O4—C16—C17—O3	2.4 (5)
C4—C5—C6—C8	176.1 (4)	C15—C16—C17—O3	−176.8 (3)
Mn1—O2—C7—C2	−174.6 (2)	O4—C16—C17—C12	−179.1 (3)
Mn1—O2—C7—C6	6.0 (5)	C15—C16—C17—C12	1.7 (5)
O1—C2—C7—O2	0.9 (5)	Mn1—O5—C19—O6	167.1 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···O3^{i}	0.84	2.01	2.730 (4)	143
O1w—H12···O2^{i}	0.84	2.09	2.813 (4)	145
O2w—H21···O6	0.84	2.04	2.793 (5)	148
O2w—H22···O3w	0.84	1.96	2.762 (7)	161
O3w—H31···O2w^{ii}	0.84	1.94	2.782 (7)	179

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