Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[diaqua(μ_2-5,5-dioxodibenzo[*b*,*d*]thiophene-3,7-dicarboxylato)(μ_2-ethylene glycol)manganese(II)] dimethylacetamide solvate]

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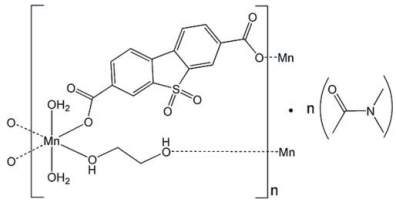
Received 22 October 2010; accepted 5 November 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.083; data-to-parameter ratio = 17.1.

In the title complex, $\{[Mn(C_{14}H_6O_6S)(C_2H_6O_2)(H_2O)_2]\cdot C_4H_9NO\}_n$, the Mn^{II} ion is six-coordinated in a *trans*-octahedral geometry by two carboxylate O atoms from two 5,5-dioxodibenzo[*b*,*d*]thiophene-3,7-dicarboxylate (*L*) ligands in a monodentate mode, two O atoms from two ethylene glycol (EG) molecules and two aqua O atoms. The metal ions are linked by the EG and *L* ligands, forming two-dimensional coordination networks, which are associated into the three-dimensional structure through O—H···O hydrogen bonds.

Related literature

For the use of H_2L ligands in the construction of coordination polymers, including metal-organic frameworks with functionalized pores, see: Neofotistou *et al.* (2010). Kanaizuka *et al.* (2010). Yan *et al.* (2009). For the ligand synthesis, see: Neofotistou *et al.* (2009).



Experimental

Crystal data

$[Mn(C_{14}H_6O_6S)(C_2H_6O_2)(H_2O)_2]\cdot C_4H_9NO$
M_r = 542.41
Monoclinic, $P2_1/c$
a = 7.0564 (3) Å
b = 11.8142 (4) Å
c = 28.0008 (10) Å
β = 100.544 (1)°
V = 2294.89 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 296 K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.811, T_{max} = 0.931
30673 measured reflections
5716 independent reflections
5221 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.083
S = 1.07
5716 reflections
335 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—O9	2.1191 (12)	Mn1—O10	2.1897 (12)
Mn1—O3^{i}	2.1437 (10)	Mn1—O8^{ii}	2.2138 (12)
Mn1—O1	2.1710 (10)	Mn1—O7	2.2253 (11)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7···O4^{iii}	0.84 (2)	1.83 (2)	2.6623 (16)	175 (2)
O8—H8···O2^{iv}	0.82 (2)	1.88 (2)	2.6865 (16)	169 (2)
O9—H9*C*···O11	0.83 (2)	1.89 (2)	2.7086 (17)	171 (2)
O9—H9*B*···O2	0.83 (2)	1.84 (2)	2.6135 (16)	156 (2)
O10—H10*C*···O11^{iv}	0.83 (3)	1.96 (3)	2.7877 (19)	172 (2)
O10—H10*B*···O4^{i}	0.82 (3)	1.98 (3)	2.7663 (16)	161 (3)

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

Data collection: *APEX2* (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*.

We are thankful for financial support from the NSFC (20771038) and the Shanghai Leading Academic Discipline Project (B409).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FK2028).

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Yan, L., Yue, Q., Jia, Q.-X., Lemercier, G. & Gao, E.-Q. (2009). *Cryst. Growth Des.* **9**, 2984–2987.

supporting information

Acta Cryst. (2010). E**66**, m1554 [https://doi.org/10.1107/S1600536810045411]

Poly[[diaqua(μ_2-5,5-dioxodibenzo[*b*,*d*]thiophene-3,7-dicarboxylato)(μ_2-ethylene glycol)manganese(II)] dimethylacetamide solvate]

Xiu-Chun Yi, Li Yan and En-Qing Gao

S1. Comment

In this paper, we report the coordination and hydrogen-bond structure of the title complex (I) derived from *S*,*S*-dioxodibenzothiophen-3,7-dicarboxylic acid (H_2L). These sulfone-functionalized dicarboxylic ligands have recently been used to construct coordination polymers, including metal-organic frameworks with functionalized pores (Kanaizuka *et al.* (2010); Neofotistou *et al.* (2010); Neofotistou *et al.* (2009); Yan *et al.* (2009)). The asymmetric unit of I contains a Mn(II) ion, an *L* ligand, two aqua ligands, an ethylene glycol (EG) ligand, and an *N*,*N*-dimethylacetamide (DMA) solvent molecule (Fig. 1). Each Mn atom resides in a *trans*-octahedral coordination geometry completed by two carboxylate O atoms (O1 and O3) from two *L* ligands, two O atoms (O7 and O8) from two EG molecules, and two O atoms (O9 and O10) from two water molecules. The Mn—O distances lie in the range of 2.1191 (12)–2.2253 (11) Å (Table 1). The *L* ligand binds two Mn atoms through two monodentate carboxylate groups, and the EG ligand also binds two Mn atoms through its two hydroxyl groups. Consequently, the metal ions are linked into a two-dimensional layer (Fig. 2). The carboxylate, hydroxyl, and aqua groups from the coordination sphere and the carbonyl group from the DMA molecule provide plenty of sites for hydrogen bonding (Table 2). Each uncoordinated carboxylate oxygen atom (O2 or O4) serves as a bifurcate acceptor to form an intralayer hydrogen bond with a coordinated aqua molecule and an interlayer one with a EG hydroxyl group from the neighboring layer. The oxygen atom (O11) of the DMA solvent is also bifurcately hydrogen-bonded, to two independent aqua ligands from different coordination layers. The above hydrogen bonds collaborate to assemble the two-dimensional coordination layers into a three-dimensional structure.

S2. Experimental

The ligand was synthesized from dimethyl ester of 4,4′-biphenyldicarboxylic acid and H_2SO_4, 20%SO_3 (oleum) according to the procedure for similar compounds (Neofotistou *et al.*, 2009). The ligand (0.006 g, 0.03 mmol) and $MnCl_2.6H_2O$ (0.006 g, 0.03 mmol) were dissolved under stirring in a mixture of ethylene glycol (1.0 ml) and DMA (2.0 ml). The resulting solution was left to stand at room temperature for 20 days to afford colorless block crystals of the title compound.

S3. Refinement

All hydrogen atoms attached to carbon atoms were placed at calculated positions and refined with the riding model using AFIX 43 and AFIX 23 instructions for aromatic C—H and secondary CH_2. The hydrogen atoms from EG and water were initially located from difference Fourier maps and refined isotropically with restraints on O—H distance (0.85 Å) and H—O—H angles.

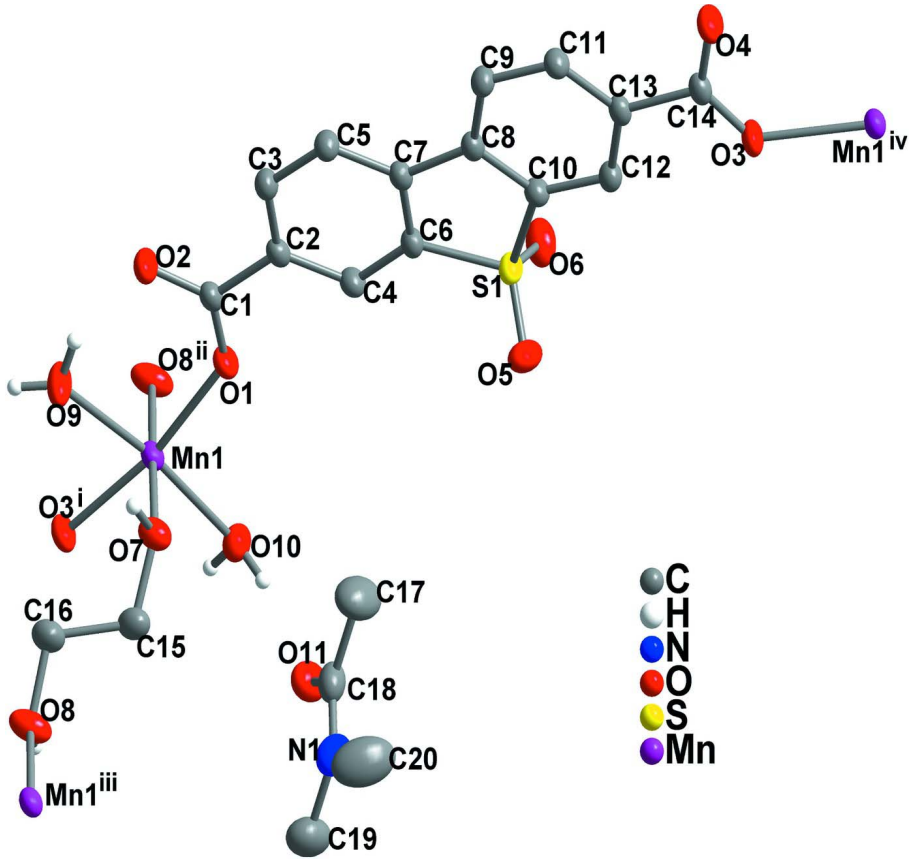

Figure 1

Coordination enviroment in the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and the H atoms attached to C are omitted for clarity. [Symmetry code: (i)-1/2 + *x*, 1/2 - *y*, 1/2 + *z* (ii) 1 + *x*, *y*, *z* (iii) -1 + *x*, *y*, *z* (iv)1/2 + *x*, 1/2 - *y*, -1/2 + *z*]

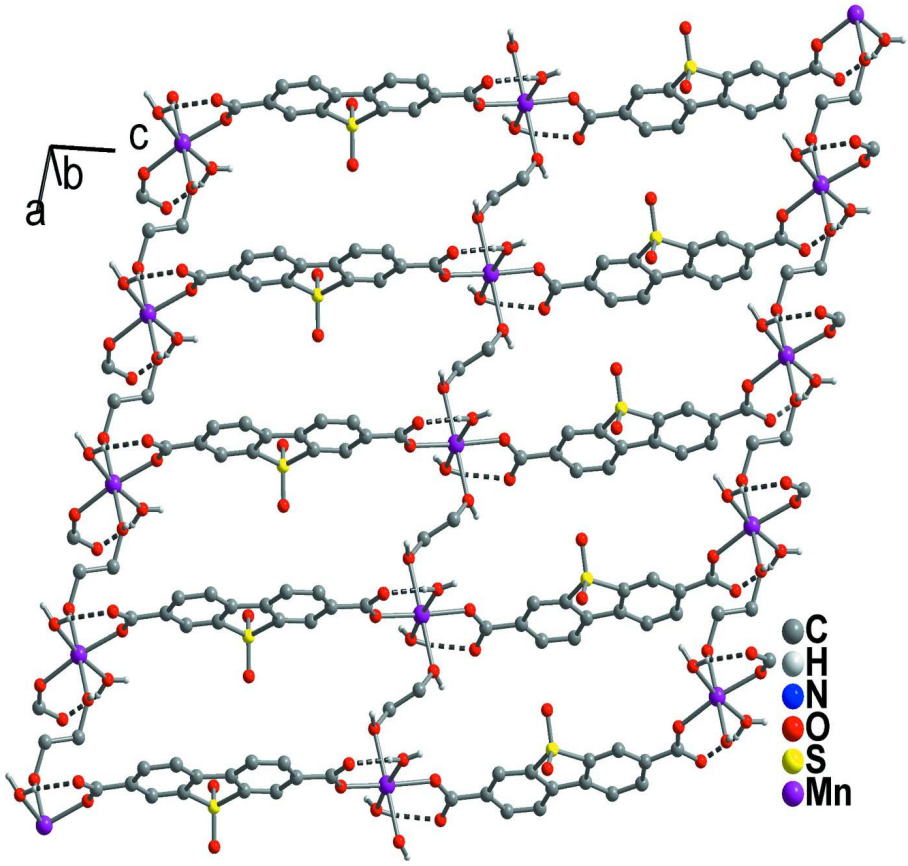

Figure 2

Two-dimensional layer connected through *L* and EG. The intralayer hydrogen bonds are shown as dot lines. The H atoms attached to C are omitted for clarity.

Poly[[diaqua(μ_2-5,5-dioxodibenzo[*b*,*d*]thiophene- 3,7-dicarboxylato)(μ_2-ethylene glycol)manganese(II)] dimethylacetamide solvate]

Crystal data

$[Mn(C_{14}H_6O_6S)(C_2H_6O_2)(H_2O)_2]\cdot C_4H_9NO$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.0564\ (3)$ Å
$b = 11.8142\ (4)$ Å
$c = 28.0008\ (10)$ Å
$\beta = 100.544\ (1)°$
$V = 2294.89\ (15)$ Å^3
$Z = 4$
$F(000) = 1124$
$D_x = 1.570$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9208 reflections
$\theta = 2.3–26°$
$\mu = 0.73$ mm^{-1}
$T = 296$ K
Columnar, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.811$, $T_{max} = 0.931$
30673 measured reflections
5716 independent reflections

5221 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 28.4°$, $\theta_{min} = 1.5°$
$h = -9 \rightarrow 7$
$k = -15 \rightarrow 14$
$l = -37 \rightarrow 36$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.083$
$S = 1.07$
5716 reflections
335 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: geom and difmap
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 1.0021P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0011 (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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.22688 (3)	0.673463 (17)	0.267191 (7)	0.02227 (7)
C1	0.43784 (19)	0.86846 (12)	0.33374 (5)	0.0236 (3)
C2	0.53981 (19)	0.90349 (12)	0.38359 (5)	0.0225 (3)
C3	0.5765 (2)	1.01741 (12)	0.39461 (5)	0.0249 (3)
H3A	0.5433	1.0713	0.3703	0.030*
C4	0.5922 (2)	0.82195 (11)	0.41959 (5)	0.0247 (3)
H4A	0.5704	0.7454	0.4130	0.030*
C5	0.6613 (2)	1.05261 (12)	0.44092 (5)	0.0247 (3)
H5A	0.6842	1.1290	0.4476	0.030*
C6	0.67736 (19)	0.85829 (12)	0.46533 (5)	0.0229 (3)
C7	0.71153 (19)	0.97220 (11)	0.47712 (5)	0.0216 (2)
C8	0.79778 (19)	0.98999 (11)	0.52870 (5)	0.0213 (2)
C9	0.8502 (2)	1.09104 (11)	0.55269 (5)	0.0244 (3)
H9A	0.8314	1.1596	0.5362	0.029*
C10	0.8262 (2)	0.88924 (11)	0.55495 (5)	0.0229 (3)
C11	0.9316 (2)	1.08823 (12)	0.60187 (5)	0.0242 (3)
H11A	0.9687	1.1557	0.6180	0.029*
C12	0.90422 (19)	0.88466 (12)	0.60378 (5)	0.0235 (3)
H12A	0.9199	0.8161	0.6203	0.028*
C13	0.95877 (18)	0.98663 (11)	0.62747 (5)	0.0215 (3)

C14	1.05227 (19)	0.98394 (12)	0.68052 (5)	0.0224 (3)
O1	0.39522 (15)	0.76549 (9)	0.32753 (4)	0.0290 (2)
O2	0.39864 (18)	0.94438 (10)	0.30224 (4)	0.0366 (3)
O3	1.05942 (16)	0.88879 (9)	0.70073 (4)	0.0316 (2)
O4	1.11941 (17)	1.07339 (9)	0.70058 (4)	0.0339 (2)
O5	0.5980 (2)	0.71159 (11)	0.53019 (4)	0.0437 (3)
O6	0.92266 (19)	0.70701 (10)	0.51083 (4)	0.0411 (3)
S1	0.75616 (5)	0.77206 (3)	0.516692 (12)	0.02602 (9)
C15	−0.2116 (2)	0.65002 (14)	0.28938 (6)	0.0334 (3)
H15A	−0.2780	0.6571	0.3167	0.040*
H15B	−0.1888	0.5702	0.2847	0.040*
C16	−0.3383 (2)	0.69648 (15)	0.24442 (6)	0.0334 (3)
H16A	−0.3629	0.7761	0.2490	0.040*
H16B	−0.2730	0.6894	0.2169	0.040*
O7	−0.03049 (15)	0.70750 (10)	0.30054 (4)	0.0312 (2)
H7	−0.052 (3)	0.777 (2)	0.3005 (8)	0.048 (6)*
O8	−0.51664 (16)	0.63629 (11)	0.23467 (5)	0.0381 (3)
H8	−0.495 (3)	0.5748 (15)	0.2233 (8)	0.052 (6)*
O9	0.1821 (2)	0.83273 (10)	0.23213 (5)	0.0471 (3)
H9C	0.135 (3)	0.854 (2)	0.2043 (6)	0.056 (7)*
H9B	0.246 (3)	0.8828 (18)	0.2484 (7)	0.057 (7)*
O10	0.24423 (19)	0.49977 (10)	0.29494 (5)	0.0352 (3)
H10C	0.182 (3)	0.474 (2)	0.3150 (9)	0.057 (7)*
H10B	0.210 (4)	0.463 (2)	0.2701 (10)	0.072 (9)*
C17	−0.0751 (4)	1.0498 (2)	0.08416 (8)	0.0639 (6)
H17A	−0.1888	1.0591	0.0981	0.096*
H17B	−0.1115	1.0281	0.0507	0.096*
H17C	−0.0053	1.1199	0.0863	0.096*
C18	0.0504 (3)	0.95932 (15)	0.11144 (6)	0.0391 (4)
C19	0.3395 (3)	0.8464 (2)	0.12584 (8)	0.0578 (5)
H19A	0.2600	0.7865	0.1344	0.087*
H19B	0.4142	0.8782	0.1548	0.087*
H19C	0.4244	0.8168	0.1057	0.087*
C20	0.2899 (5)	0.9857 (2)	0.05873 (11)	0.0830 (9)
H20A	0.2025	1.0437	0.0443	0.125*
H20B	0.3005	0.9288	0.0349	0.125*
H20C	0.4144	1.0184	0.0703	0.125*
O11	−0.0072 (2)	0.90934 (12)	0.14522 (4)	0.0461 (3)
N1	0.2175 (2)	0.93427 (13)	0.09933 (6)	0.0440 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.02329 (11)	0.02213 (11)	0.01900 (11)	−0.00047 (7)	−0.00245 (8)	−0.00162 (7)
C1	0.0221 (6)	0.0278 (7)	0.0191 (6)	−0.0016 (5)	−0.0007 (5)	−0.0006 (5)
C2	0.0211 (6)	0.0267 (6)	0.0184 (6)	−0.0021 (5)	0.0002 (5)	−0.0018 (5)
C3	0.0283 (7)	0.0253 (7)	0.0193 (6)	−0.0009 (5)	−0.0004 (5)	0.0015 (5)
C4	0.0268 (7)	0.0227 (6)	0.0228 (6)	−0.0024 (5)	−0.0006 (5)	−0.0026 (5)

C5	0.0302 (7)	0.0217 (6)	0.0207 (6)	−0.0010 (5)	0.0009 (5)	−0.0008 (5)
C6	0.0244 (6)	0.0235 (6)	0.0190 (6)	0.0005 (5)	−0.0006 (5)	0.0014 (5)
C7	0.0212 (6)	0.0247 (6)	0.0177 (6)	−0.0004 (5)	0.0005 (5)	−0.0012 (5)
C8	0.0216 (6)	0.0236 (6)	0.0178 (6)	0.0000 (5)	0.0013 (5)	−0.0002 (5)
C9	0.0301 (7)	0.0212 (6)	0.0204 (6)	0.0001 (5)	0.0010 (5)	0.0014 (5)
C10	0.0255 (6)	0.0211 (6)	0.0206 (6)	−0.0014 (5)	0.0006 (5)	−0.0020 (5)
C11	0.0276 (6)	0.0225 (6)	0.0209 (6)	−0.0011 (5)	0.0004 (5)	−0.0026 (5)
C12	0.0257 (6)	0.0231 (6)	0.0203 (6)	0.0011 (5)	0.0003 (5)	0.0020 (5)
C13	0.0203 (6)	0.0255 (6)	0.0176 (6)	0.0015 (5)	0.0002 (5)	−0.0005 (5)
C14	0.0213 (6)	0.0256 (6)	0.0187 (6)	0.0031 (5)	−0.0004 (5)	−0.0007 (5)
O1	0.0348 (5)	0.0260 (5)	0.0221 (5)	−0.0033 (4)	−0.0054 (4)	−0.0028 (4)
O2	0.0494 (7)	0.0311 (6)	0.0234 (5)	−0.0091 (5)	−0.0092 (5)	0.0045 (4)
O3	0.0397 (6)	0.0270 (5)	0.0222 (5)	−0.0004 (4)	−0.0094 (4)	0.0035 (4)
O4	0.0472 (6)	0.0264 (5)	0.0234 (5)	−0.0010 (5)	−0.0062 (4)	−0.0033 (4)
O5	0.0572 (8)	0.0372 (6)	0.0347 (6)	−0.0207 (6)	0.0036 (5)	0.0026 (5)
O6	0.0543 (7)	0.0313 (6)	0.0340 (6)	0.0154 (5)	−0.0022 (5)	−0.0037 (5)
S1	0.03603 (19)	0.01997 (16)	0.01953 (16)	−0.00206 (13)	−0.00157 (13)	−0.00020 (11)
C15	0.0273 (7)	0.0319 (7)	0.0406 (8)	−0.0013 (6)	0.0048 (6)	0.0038 (6)
C16	0.0256 (7)	0.0369 (8)	0.0372 (8)	−0.0023 (6)	0.0044 (6)	−0.0012 (6)
O7	0.0269 (5)	0.0278 (5)	0.0375 (6)	0.0006 (4)	0.0022 (4)	−0.0058 (4)
O8	0.0257 (5)	0.0373 (6)	0.0516 (7)	−0.0023 (5)	0.0076 (5)	−0.0186 (5)
O9	0.0779 (10)	0.0270 (6)	0.0266 (6)	−0.0056 (6)	−0.0164 (6)	0.0035 (5)
O10	0.0474 (7)	0.0284 (6)	0.0280 (6)	−0.0012 (5)	0.0018 (5)	0.0029 (5)
C17	0.0792 (16)	0.0631 (14)	0.0481 (12)	0.0237 (12)	0.0083 (11)	0.0178 (10)
C18	0.0535 (10)	0.0349 (8)	0.0253 (7)	0.0019 (7)	−0.0021 (7)	−0.0032 (6)
C19	0.0607 (13)	0.0621 (13)	0.0526 (12)	0.0184 (11)	0.0155 (10)	0.0050 (10)
C20	0.103 (2)	0.0651 (16)	0.095 (2)	0.0174 (15)	0.0574 (18)	0.0312 (15)
O11	0.0525 (8)	0.0550 (8)	0.0298 (6)	0.0113 (6)	0.0049 (5)	0.0074 (5)
N1	0.0569 (10)	0.0382 (8)	0.0377 (8)	0.0020 (7)	0.0109 (7)	−0.0011 (6)

Geometric parameters (Å, º)

Mn1—O9	2.1191 (12)	C14—O3	1.2553 (17)
Mn1—O3^{i}	2.1437 (10)	O3—Mn1^{iii}	2.1437 (10)
Mn1—O1	2.1710 (10)	O5—S1	1.4329 (13)
Mn1—O10	2.1897 (12)	O6—S1	1.4382 (13)
Mn1—O8^{ii}	2.2138 (12)	C15—O7	1.4303 (18)
Mn1—O7	2.2253 (11)	C15—C16	1.508 (2)
C1—O2	1.2529 (17)	C15—H15A	0.9700
C1—O1	1.2576 (18)	C15—H15B	0.9700
C1—C2	1.5066 (18)	C16—O8	1.4275 (19)
C2—C3	1.3943 (19)	C16—H16A	0.9700
C2—C4	1.3945 (19)	C16—H16B	0.9700
C3—C5	1.3889 (19)	O7—H7	0.84 (2)
C3—H3A	0.9300	O8—Mn1^{iv}	2.2138 (11)
C4—C6	1.3799 (18)	O8—H8	0.818 (16)
C4—H4A	0.9300	O9—H9C	0.827 (15)
C5—C7	1.3871 (18)	O9—H9B	0.827 (15)

C5—H5A	0.9300	O10—H10C	0.83 (3)
C6—C7	1.3961 (19)	O10—H10B	0.82 (3)
C6—S1	1.7671 (14)	C17—C18	1.504 (3)
C7—C8	1.4762 (17)	C17—H17A	0.9600
C8—C9	1.3864 (18)	C17—H17B	0.9600
C8—C10	1.3941 (18)	C17—H17C	0.9600
C9—C11	1.3919 (18)	C18—O11	1.245 (2)
C9—H9A	0.9300	C18—N1	1.318 (2)
C10—C12	1.3784 (18)	C19—N1	1.461 (3)
C10—S1	1.7648 (13)	C19—H19A	0.9600
C11—C13	1.3932 (19)	C19—H19B	0.9600
C11—H11A	0.9300	C19—H19C	0.9600
C12—C13	1.3950 (19)	C20—N1	1.462 (3)
C12—H12A	0.9300	C20—H20A	0.9600
C13—C14	1.5114 (17)	C20—H20B	0.9600
C14—O4	1.2488 (17)	C20—H20C	0.9600

O9—Mn1—O3^{i}	83.73 (4)	C1—O1—Mn1	132.45 (9)
O9—Mn1—O1	85.98 (4)	C14—O3—Mn1^{iii}	131.98 (9)
O3^{i}—Mn1—O1	169.61 (4)	O5—S1—O6	117.10 (8)
O9—Mn1—O10	172.07 (5)	O5—S1—C10	112.10 (7)
O3^{i}—Mn1—O10	88.43 (4)	O6—S1—C10	110.15 (7)
O1—Mn1—O10	101.89 (4)	O5—S1—C6	110.96 (7)
O9—Mn1—O8^{ii}	92.82 (6)	O6—S1—C6	110.93 (7)
O3^{i}—Mn1—O8^{ii}	86.40 (4)	C10—S1—C6	93.06 (6)
O1—Mn1—O8^{ii}	92.72 (4)	O7—C15—C16	112.28 (13)
O10—Mn1—O8^{ii}	87.89 (5)	O7—C15—H15A	109.1
O9—Mn1—O7	88.29 (6)	C16—C15—H15A	109.1
O3^{i}—Mn1—O7	93.65 (4)	O7—C15—H15B	109.1
O1—Mn1—O7	87.44 (4)	C16—C15—H15B	109.1
O10—Mn1—O7	91.00 (5)	H15A—C15—H15B	107.9
O8^{ii}—Mn1—O7	178.89 (5)	O8—C16—C15	110.22 (14)
O2—C1—O1	125.37 (12)	O8—C16—H16A	109.6
O2—C1—C2	117.52 (12)	C15—C16—H16A	109.6
O1—C1—C2	117.09 (12)	O8—C16—H16B	109.6
C3—C2—C4	119.54 (12)	C15—C16—H16B	109.6
C3—C2—C1	120.53 (12)	H16A—C16—H16B	108.1
C4—C2—C1	119.90 (12)	C15—O7—Mn1	125.99 (10)
C5—C3—C2	121.77 (13)	C15—O7—H7	108.4 (15)
C5—C3—H3A	119.1	Mn1—O7—H7	109.7 (16)
C2—C3—H3A	119.1	C16—O8—Mn1^{iv}	125.51 (10)
C6—C4—C2	117.96 (12)	C16—O8—H8	107.4 (16)
C6—C4—H4A	121.0	Mn1^{iv}—O8—H8	123.9 (16)
C2—C4—H4A	121.0	Mn1—O9—H9C	134.6 (16)
C7—C5—C3	119.08 (13)	Mn1—O9—H9B	111.1 (16)
C7—C5—H5A	120.5	H9C—O9—H9B	113 (2)
C3—C5—H5A	120.5	Mn1—O10—H10C	125.2 (17)
C4—C6—C7	123.13 (12)	Mn1—O10—H10B	102 (2)

C4—C6—S1	126.50 (11)	H10C—O10—H10B	106 (2)
C7—C6—S1	110.38 (10)	C18—C17—H17A	109.5
C5—C7—C6	118.52 (12)	C18—C17—H17B	109.5
C5—C7—C8	128.45 (12)	H17A—C17—H17B	109.5
C6—C7—C8	113.03 (12)	C18—C17—H17C	109.5
C9—C8—C10	118.68 (12)	H17A—C17—H17C	109.5
C9—C8—C7	128.49 (12)	H17B—C17—H17C	109.5
C10—C8—C7	112.83 (12)	O11—C18—N1	121.38 (16)
C8—C9—C11	118.95 (12)	O11—C18—C17	118.61 (18)
C8—C9—H9A	120.5	N1—C18—C17	120.01 (18)
C11—C9—H9A	120.5	N1—C19—H19A	109.5
C12—C10—C8	123.32 (12)	N1—C19—H19B	109.5
C12—C10—S1	126.02 (11)	H19A—C19—H19B	109.5
C8—C10—S1	110.64 (10)	N1—C19—H19C	109.5
C9—C11—C13	121.50 (12)	H19A—C19—H19C	109.5
C9—C11—H11A	119.2	H19B—C19—H19C	109.5
C13—C11—H11A	119.2	N1—C20—H20A	109.5
C10—C12—C13	117.59 (12)	N1—C20—H20B	109.5
C10—C12—H12A	121.2	H20A—C20—H20B	109.5
C13—C12—H12A	121.2	N1—C20—H20C	109.5
C11—C13—C12	119.96 (12)	H20A—C20—H20C	109.5
C11—C13—C14	121.20 (12)	H20B—C20—H20C	109.5
C12—C13—C14	118.82 (12)	C18—N1—C19	120.01 (16)
O4—C14—O3	125.06 (12)	C18—N1—C20	124.28 (18)
O4—C14—C13	119.06 (12)	C19—N1—C20	115.66 (19)
O3—C14—C13	115.87 (12)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7···O4^{v}	0.84 (2)	1.83 (2)	2.6623 (16)	175 (2)
O8—H8···O2^{vi}	0.82 (2)	1.88 (2)	2.6865 (16)	169 (2)
O9—H9*C*···O11	0.83 (2)	1.89 (2)	2.7086 (17)	171 (2)
O9—H9*B*···O2	0.83 (2)	1.84 (2)	2.6135 (16)	156 (2)
O10—H10*C*···O11^{vi}	0.83 (3)	1.96 (3)	2.7877 (19)	172 (2)
O10—H10*B*···O4^{i}	0.82 (3)	1.98 (3)	2.7663 (16)	161 (3)

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