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Di-μ-sulfato-κ^4O:O'-bis[diaqua(1*H*-imidazo[4,5-*f*][1,10]phenanthroline)-manganese(II)] dihydrate

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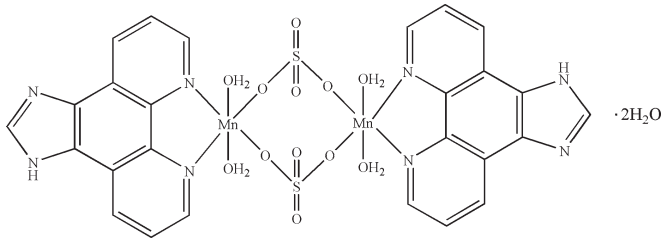
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.082; data-to-parameter ratio = 13.7.

In the title centrosymmetric dinuclear compound, $[Mn_2(SO_4)_2(C_{13}H_8N_4)_2(H_2O)_4]\cdot 2H_2O$, the Mn^{II} atom is octahedrally coordinated by two N atoms from a 1*H*-imidazo-[4,5-*f*][1,10]phenanthroline (ip) ligand, two O atoms belonging to two bridging sulfate anions and two water O atoms. In the crystal structure, the complex molecules and the uncoodinated water molecules are connected by O—H···O, O—H···N and N—H···O hydrogen bonds into a three-dimensional network. A π–π stacking interaction between the pyridyl ring of the ip ligand and the benzene ring of the neighboring ligand [centroid–centroid distance = 3.579 (2) Å] is also observed.

Related literature

For general background to the crystal engineering of functional materials, see: Aoyama (1998); Bassani *et al.* (2000); Kahn (2000); Matsuda *et al.* (2005); Miller (2000); Rowsell *et al.* (2004). For related structures, see: Gong *et al.* (2009); Wang *et al.* (2008); Wu *et al.* (1997); Yang *et al.* (2010); Yu (2009); Zeng *et al.* (2009).



Experimental

Crystal data

$[Mn_2(SO_4)_2(C_{13}H_8N_4)_2(H_2O)_4]\cdot 2H_2O$
M_r = 850.58
Monoclinic, $P2_1/c$
a = 10.467 (7) Å
b = 9.171 (6) Å
c = 17.025 (11) Å
β = 98.758 (12)°
V = 1615.2 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 293 K
1.00 × 0.80 × 0.60 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
T_{min} = 0.432, T_{max} = 1.000
11099 measured reflections
3544 independent reflections
3251 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.082
S = 1.05
3544 reflections
259 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—O1	2.1366 (17)	Mn1—O6	2.1751 (17)
Mn1—O3^{i}	2.1641 (16)	Mn1—N1	2.2718 (19)
Mn1—O5	2.2590 (16)	Mn1—N2	2.2715 (19)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1···O2^{i}	0.85 (1)	1.95 (1)	2.789 (2)	165 (3)
O5—H2···N4^{ii}	0.86 (3)	1.99 (3)	2.824 (2)	164 (3)
O6—H3···O7^{iii}	0.84 (1)	1.80 (1)	2.644 (3)	172 (3)
O6—H4···O2	0.84 (2)	1.97 (1)	2.745 (2)	154 (2)
O7—H5···O2^{iv}	0.85 (1)	1.98 (1)	2.828 (3)	171 (3)
O7—H6···O4	0.84 (1)	2.04 (2)	2.833 (3)	157 (3)
N3—H3*B*···O4^{v}	0.86	2.04	2.890 (2)	167

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

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); 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: HY2338).

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supporting information

Acta Cryst. (2010). E**66**, m1115–m1116 [https://doi.org/10.1107/S1600536810031909]

Di-μ-sulfato-κ^4O:O'-bis[diaqua(1*H*-imidazo[4,5-*f*][1,10]phenanthroline)manganese(II)] dihydrate

Ming-Xing Yang, Shen Lin, Li-Juan Chen and Xiao-Hua Chen

S1. Comment

An important aspect of crystal engineering is to understand and attempt to control the manner in which molecules are arranged in crystal lattices through the use of noncovalent interactions such as electrostatic interactions, hydrogen bonding, dispersion and induction forces, and π-π stacking interactions. These materials have attracted much interest due to their strong potential for a variety of applications including gas storage (Matsuda *et al.*, 2005; Rowsell *et al.*, 2004), catalytic properties (Aoyama, 1998; Bassani *et al.*, 2000) and magnetism (Kahn, 2000; Miller, 2000). One approach to forming networks of discrete transition metal complexes is to use a chelating ligand that has additional interactional functionality attached to its backbone, such as additional coordination sites or hydrogen bonding groups, or extended π systems. 1*H*-Imidazo[5,f][1,10]phenanthroline (ip) has been used to form metal complexes with novel supramolecular architectures due to their excellent coordinating ability, large conjugated systems and strong hydrogen bonding donor and acceptor groups (Gong *et al.*, 2009; Wang *et al.*, 2008; Wu *et al.*, 1997; Yang *et al.*, 2010; Yu, 2009; Zeng *et al.*, 2009). In the present paper,we hydrothermally synthesized a new coordination complex constructed from $MnSO_4$ and ip.

The title dimeric complex is generated by an inversion center (Fig. 1). The Mn^{II} atom is six-coordinated by two N atoms from one ip ligand, two O atoms from water molecules and two O atoms from two sulfate anions in a distorted octahedral geometry (Table 1). The equatorial plane is defined by N2, O6, O1 and O5 and the axial coordination sites are occupied by N1 and $O3^{i}$ atoms [symmetry code: (i) -x, 1-y, -z]. The sulfate anion acts as a bidentate bridging ligand connecting two Mn^{II} ions, thus generating a binuclear complex. The hydrogen bonds play a key role in the structural stability (Table 2). The uncoordinated water molecule is a hydrogen bond acceptor from the coordinated water, and a hydrogen bond donor to two O atoms of two sulfate anions in two neighboring complex molecules. So each free water is hydrogen bonded to three different complex molecules. The ip ligand is a hydrogen bond donor through the imidazolyl NH group to a sulfate O atom of an adjacent complex molecule and a hydrogen bond acceptor from the coordinated water molecule (O5) of another adjacent complex molecule through the other imidazolyl N atom, forming a three-dimensional network structure, as illustrated in Fig. 2. There is also a π–π stacking interaction between the pyridyl ring of the ip ligand and the benzene ring of the neighboring ip ligand, with a centroid–centroid distance of 3.579 (2) Å.

S2. Experimental

The ip ligand was synthesized according to literature (Wu *et al.*, 1997). A mixture of $MnSO_4$, ip and H_2O in a molar ratio of 1:1:556 was stirred for an hour, then sealed in an 18 ml Teflon-lined stainless steel reactor and heated for 3 d at 433 K and autogeneous pressure. After allowing the reaction mixture to cool down to room temperature, yellow crystals were collected, washed with water and dried at room temperature.

S3. Refinement

C- and N-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 and N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N). The water H atoms were located in a difference Fourier map and refined isotropically, with restraints of O—H = 0.84 (1) and H···H = 1.44 (1) Å.

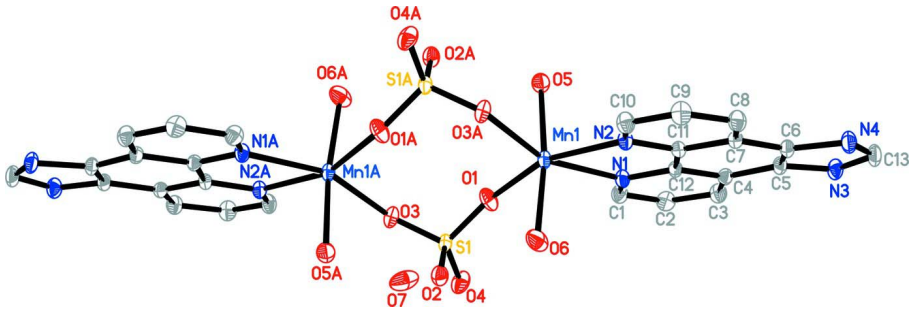

Figure 1

Molecular structure of the title compound. H atoms have been omitted for clarity. [Symmetry code: (A) -x, 1-y, -z.]

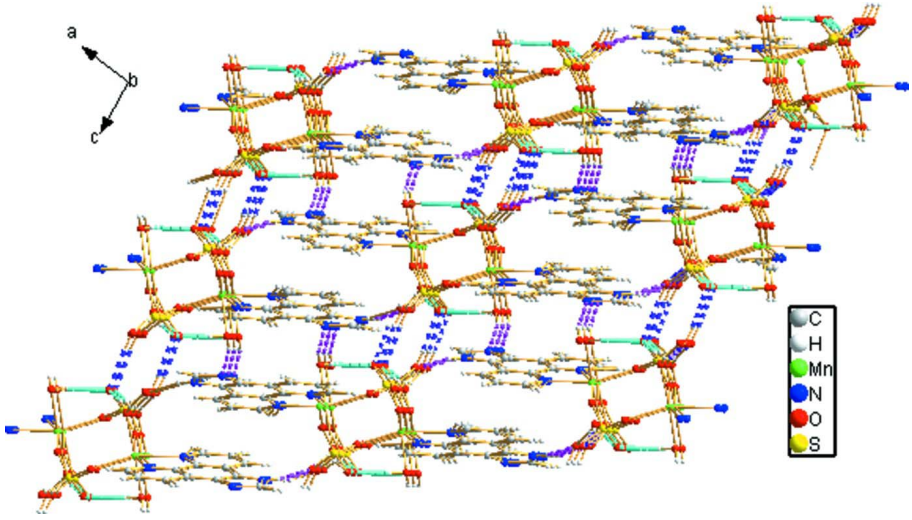

Figure 2

The three-dimensional hydrogen bonding network in the title compound.

Di-μ-sulfato-κ^4O:O'- bis[diaqua(1*H*-imidazo-[4,5-*f*][1,10]phenanthroline)manganese(II)] dihydrate

Crystal data

$[Mn_2(SO_4)_2(C_{13}H_8N_4)_2(H_2O)_4]\cdot 2H_2O$
M_r = 850.58
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.467 (7) Å
b = 9.171 (6) Å
c = 17.025 (11) Å
β = 98.758 (12)°
V = 1615.2 (18) Å^3
Z = 2
$F(000)$ = 868
D_x = 1.749 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4851 reflections
θ = 3.3–27.4°
μ = 1.00 mm^{-1}
T = 293 K
Prism, yellow
1.00 × 0.80 × 0.60 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 14.6306 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
T_{min} = 0.432, T_{max} = 1.000

11099 measured reflections
3544 independent reflections
3251 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.4°, θ_{min} = 2.5°
h = −13→13
k = −11→11
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.082
S = 1.05
3544 reflections
259 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 0.5623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Mn1	0.18299 (2)	0.67998 (3)	0.039544 (16)	0.02452 (10)
S1	0.03061 (4)	0.40185 (4)	0.11921 (2)	0.02399 (11)
O1	0.13383 (12)	0.47205 (14)	0.08303 (9)	0.0374 (3)
O2	−0.06301 (12)	0.51435 (14)	0.13804 (8)	0.0316 (3)
O3	−0.03679 (12)	0.29274 (14)	0.06387 (8)	0.0311 (3)
O4	0.08663 (14)	0.32790 (15)	0.19348 (9)	0.0400 (3)
O5	0.29524 (13)	0.55706 (16)	−0.04252 (8)	0.0339 (3)
H1	0.2295 (19)	0.519 (3)	−0.0712 (14)	0.074 (9)*
H2	0.329 (3)	0.626 (3)	−0.0665 (16)	0.096 (12)*
O6	0.05988 (16)	0.77338 (17)	0.11855 (10)	0.0484 (4)
H3	0.065 (2)	0.8546 (15)	0.1421 (14)	0.059 (8)*
H4	0.012 (2)	0.7107 (19)	0.1349 (14)	0.056 (8)*
O7	0.0949 (3)	0.01928 (19)	0.20000 (11)	0.0714 (6)
H5	0.090 (3)	0.008 (3)	0.2492 (7)	0.076 (10)*
H6	0.088 (3)	0.1066 (16)	0.1844 (15)	0.084 (10)*
N1	0.37913 (14)	0.68351 (15)	0.11788 (9)	0.0257 (3)
N2	0.25995 (13)	0.91094 (15)	0.03511 (9)	0.0252 (3)
N3	0.74601 (14)	1.01809 (18)	0.20156 (9)	0.0321 (3)
H3B	0.8055	0.9678	0.2297	0.039*
N4	0.64434 (15)	1.21029 (17)	0.13915 (10)	0.0338 (4)
C1	0.43732 (18)	0.56818 (19)	0.15534 (11)	0.0303 (4)
H1A	0.3930	0.4800	0.1522	0.036*
C2	0.56195 (18)	0.5734 (2)	0.19914 (12)	0.0333 (4)
H2B	0.5993	0.4901	0.2240	0.040*

C3	0.62820 (17)	0.7031 (2)	0.20480 (12)	0.0314 (4)
H3C	0.7105	0.7093	0.2343	0.038*
C4	0.56986 (15)	0.82664 (18)	0.16534 (10)	0.0239 (3)
C5	0.62700 (15)	0.96855 (19)	0.16508 (10)	0.0257 (4)
C6	0.56533 (16)	1.08776 (18)	0.12661 (10)	0.0253 (3)
C7	0.43740 (15)	1.07578 (18)	0.08161 (10)	0.0236 (3)
C8	0.36759 (18)	1.19078 (18)	0.04063 (12)	0.0302 (4)
H8A	0.4032	1.2838	0.0414	0.036*
C9	0.24595 (18)	1.1648 (2)	−0.00075 (12)	0.0337 (4)
H9A	0.1977	1.2403	−0.0269	0.040*
C10	0.19618 (16)	1.0231 (2)	−0.00289 (11)	0.0306 (4)
H10A	0.1150	1.0060	−0.0321	0.037*
C11	0.37862 (15)	0.93635 (17)	0.07832 (10)	0.0220 (3)
C12	0.44406 (15)	0.81270 (17)	0.12160 (10)	0.0222 (3)
C13	0.75016 (19)	1.1614 (2)	0.18408 (12)	0.0370 (4)
H13A	0.8209	1.2205	0.2020	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.02168 (14)	0.02247 (15)	0.02823 (17)	−0.00592 (9)	−0.00001 (11)	−0.00163 (10)
S1	0.0223 (2)	0.0203 (2)	0.0272 (2)	−0.00508 (14)	−0.00289 (16)	0.00196 (15)
O1	0.0317 (7)	0.0248 (6)	0.0578 (9)	−0.0043 (5)	0.0138 (6)	0.0050 (6)
O2	0.0289 (6)	0.0270 (6)	0.0384 (7)	−0.0024 (5)	0.0037 (5)	−0.0046 (5)
O3	0.0290 (6)	0.0253 (6)	0.0354 (8)	−0.0023 (5)	−0.0067 (5)	−0.0044 (5)
O4	0.0475 (8)	0.0336 (7)	0.0330 (8)	−0.0034 (6)	−0.0129 (6)	0.0068 (6)
O5	0.0305 (7)	0.0349 (7)	0.0361 (8)	−0.0022 (5)	0.0040 (6)	−0.0011 (6)
O6	0.0599 (9)	0.0302 (8)	0.0626 (10)	−0.0153 (7)	0.0334 (8)	−0.0142 (7)
O7	0.1428 (19)	0.0306 (9)	0.0456 (11)	−0.0169 (10)	0.0295 (12)	−0.0072 (7)
N1	0.0253 (7)	0.0215 (7)	0.0292 (8)	−0.0046 (5)	0.0008 (6)	0.0003 (5)
N2	0.0209 (6)	0.0247 (7)	0.0287 (8)	−0.0030 (5)	0.0000 (6)	0.0014 (6)
N3	0.0235 (7)	0.0369 (9)	0.0323 (9)	−0.0062 (6)	−0.0073 (6)	0.0023 (7)
N4	0.0326 (8)	0.0295 (8)	0.0376 (9)	−0.0113 (6)	−0.0004 (7)	0.0004 (7)
C1	0.0348 (9)	0.0221 (8)	0.0330 (10)	−0.0035 (7)	0.0026 (8)	0.0010 (7)
C2	0.0363 (9)	0.0266 (9)	0.0352 (11)	0.0049 (7)	0.0002 (8)	0.0060 (7)
C3	0.0244 (8)	0.0342 (10)	0.0335 (10)	0.0018 (7)	−0.0023 (7)	0.0032 (8)
C4	0.0217 (7)	0.0251 (8)	0.0240 (9)	−0.0023 (6)	0.0006 (6)	−0.0010 (6)
C5	0.0200 (7)	0.0293 (9)	0.0263 (9)	−0.0046 (6)	−0.0011 (6)	−0.0012 (7)
C6	0.0253 (8)	0.0234 (8)	0.0266 (9)	−0.0068 (6)	0.0022 (7)	−0.0018 (6)
C7	0.0241 (8)	0.0224 (8)	0.0241 (8)	−0.0032 (6)	0.0032 (7)	−0.0012 (6)
C8	0.0327 (9)	0.0207 (8)	0.0364 (11)	−0.0025 (6)	0.0029 (8)	0.0005 (7)
C9	0.0319 (9)	0.0278 (9)	0.0393 (11)	0.0050 (7)	−0.0019 (8)	0.0064 (8)
C10	0.0218 (8)	0.0316 (9)	0.0362 (10)	0.0006 (7)	−0.0023 (7)	0.0042 (8)
C11	0.0196 (7)	0.0220 (8)	0.0240 (9)	−0.0025 (6)	0.0024 (6)	−0.0007 (6)
C12	0.0214 (7)	0.0216 (8)	0.0232 (9)	−0.0030 (6)	0.0019 (6)	−0.0008 (6)
C13	0.0318 (9)	0.0387 (11)	0.0380 (11)	−0.0177 (8)	−0.0029 (8)	−0.0020 (8)

Geometric parameters (Å, º)

Mn1—O1	2.1366 (17)	N3—H3B	0.8600
Mn1—O3^{i}	2.1641 (16)	N4—C13	1.325 (3)
Mn1—O5	2.2590 (16)	N4—C6	1.392 (2)
Mn1—O6	2.1751 (17)	C1—C2	1.401 (3)
Mn1—N1	2.2718 (19)	C1—H1A	0.9300
Mn1—N2	2.2715 (19)	C2—C3	1.373 (3)
S1—O1	1.4711 (14)	C2—H2B	0.9300
S1—O4	1.4753 (16)	C3—C4	1.408 (2)
S1—O3	1.4779 (14)	C3—H3C	0.9300
S1—O2	1.4910 (14)	C4—C12	1.416 (2)
O3—Mn1^{i}	2.1641 (16)	C4—C5	1.433 (2)
O5—H1	0.85 (1)	C5—C6	1.383 (2)
O5—H2	0.86 (3)	C6—C7	1.442 (2)
O6—H3	0.84 (1)	C7—C8	1.406 (2)
O6—H4	0.84 (2)	C7—C11	1.416 (2)
O7—H5	0.85 (1)	C8—C9	1.379 (3)
O7—H6	0.84 (1)	C8—H8A	0.9300
N1—C1	1.333 (2)	C9—C10	1.398 (3)
N1—C12	1.363 (2)	C9—H9A	0.9300
N2—C10	1.338 (2)	C10—H10A	0.9300
N2—C11	1.364 (2)	C11—C12	1.464 (2)
N3—C13	1.350 (3)	C13—H13A	0.9300
N3—C5	1.381 (2)		

O1—Mn1—O3^{i}	101.97 (6)	N1—C1—C2	123.22 (16)
O1—Mn1—O6	86.60 (7)	N1—C1—H1A	118.4
O3^{i}—Mn1—O6	92.60 (8)	C2—C1—H1A	118.4
O1—Mn1—O5	86.81 (6)	C3—C2—C1	119.08 (17)
O3^{i}—Mn1—O5	85.67 (7)	C3—C2—H2B	120.5
O6—Mn1—O5	172.68 (5)	C1—C2—H2B	120.5
O1—Mn1—N2	161.64 (6)	C2—C3—C4	119.07 (17)
O3^{i}—Mn1—N2	94.33 (5)	C2—C3—H3C	120.5
O6—Mn1—N2	84.25 (6)	C4—C3—H3C	120.5
O5—Mn1—N2	102.96 (6)	C3—C4—C12	118.63 (15)
O1—Mn1—N1	93.04 (6)	C3—C4—C5	125.55 (16)
O3^{i}—Mn1—N1	160.02 (5)	C12—C4—C5	115.82 (15)
O6—Mn1—N1	101.47 (8)	N3—C5—C6	106.07 (15)
O5—Mn1—N1	82.04 (7)	N3—C5—C4	130.22 (16)
N2—Mn1—N1	73.31 (5)	C6—C5—C4	123.70 (15)
O1—S1—O4	109.79 (9)	C5—C6—N4	110.00 (16)
O1—S1—O3	109.82 (9)	C5—C6—C7	121.34 (15)
O4—S1—O3	108.90 (9)	N4—C6—C7	128.66 (16)
O1—S1—O2	109.62 (9)	C8—C7—C11	117.88 (16)
O4—S1—O2	108.80 (9)	C8—C7—C6	125.22 (15)
O3—S1—O2	109.88 (8)	C11—C7—C6	116.90 (15)
S1—O1—Mn1	140.06 (8)	C9—C8—C7	119.55 (16)

S1—O3—Mn1^{i}	130.55 (8)	C9—C8—H8A	120.2
Mn1—O5—H1	96 (2)	C7—C8—H8A	120.2
Mn1—O5—H2	102 (2)	C8—C9—C10	119.05 (16)
H1—O5—H2	112.2 (16)	C8—C9—H9A	120.5
Mn1—O6—H3	129.9 (16)	C10—C9—H9A	120.5
Mn1—O6—H4	112.2 (16)	N2—C10—C9	123.04 (17)
H3—O6—H4	116.3 (16)	N2—C10—H10A	118.5
H5—O7—H6	114.1 (16)	C9—C10—H10A	118.5
C1—N1—C12	118.64 (15)	N2—C11—C7	122.01 (15)
C1—N1—Mn1	125.14 (11)	N2—C11—C12	117.19 (14)
C12—N1—Mn1	116.06 (11)	C7—C11—C12	120.81 (15)
C10—N2—C11	118.41 (15)	N1—C12—C4	121.34 (15)
C10—N2—Mn1	125.42 (12)	N1—C12—C11	117.28 (15)
C11—N2—Mn1	116.10 (11)	C4—C12—C11	121.39 (14)
C13—N3—C5	106.16 (15)	N4—C13—N3	113.86 (16)
C13—N3—H3B	126.9	N4—C13—H13A	123.1
C5—N3—H3B	126.9	N3—C13—H13A	123.1
C13—N4—C6	103.91 (16)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1···O2^{i}	0.85 (1)	1.95 (1)	2.789 (2)	165 (3)
O5—H2···N4^{ii}	0.86 (3)	1.99 (3)	2.824 (2)	164 (3)
O6—H3···O7^{iii}	0.84 (1)	1.80 (1)	2.644 (3)	172 (3)
O6—H4···O2	0.84 (2)	1.97 (1)	2.745 (2)	154 (2)
O7—H5···O2^{iv}	0.85 (1)	1.98 (1)	2.828 (3)	171 (3)
O7—H6···O4	0.84 (1)	2.04 (2)	2.833 (3)	157 (3)
N3—H3*B*···O4^{v}	0.86	2.04	2.890 (2)	167

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