

Tetraaqua[1-[(1*H*-1,2,3-benzotriazol-1-yl)methyl]-1*H*-imidazole]sulfato-manganese(II) dihydrate

 Ying Wang^{a*} and Ying-Ying Sun^b

^aDepartment of Geriatrics, The First Affiliated Hospital, Zhengzhou University, Zhengzhou 450000, People's Republic of China, and ^bDepartment of Pharmacy, The Third Affiliated Hospital of Henan University of Traditional Chinese Medicine, Zhengzhou 450008, People's Republic of China
Correspondence e-mail: 13623712409@139.com

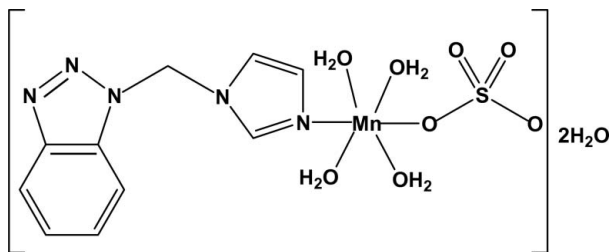
Received 25 May 2011; accepted 8 June 2011

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.038; wR factor = 0.087; data-to-parameter ratio = 17.8.

In the title complex, $[\text{Mn}(\text{SO}_4)(\text{C}_{10}\text{H}_9\text{N}_5)(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$, the Mn^{2+} cation is six-coordinated by one N atom from a 1-[(1*H*-1,2,3-benzotriazol-1-yl)methyl]-1*H*-imidazole ligand and five O atoms from one monodentate sulfate ligand and four water molecules in a distorted octahedral geometry. In the crystal, adjacent molecules are linked through $\text{O}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds into a three-dimensional network.

Related literature

For background to complexes based on flexible organic ligands, see: Ma *et al.* (2011); Meng *et al.* (2009); Sanchez *et al.* (2002).



Experimental

Crystal data

$[\text{Mn}(\text{SO}_4)(\text{C}_{10}\text{H}_9\text{N}_5)(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$
 $M_r = 458.32$
 Triclinic, $P\bar{1}$
 $a = 7.5824$ (15) Å
 $b = 8.5237$ (17) Å
 $c = 15.972$ (3) Å
 $\alpha = 98.33$ (3)°
 $\beta = 91.11$ (3)°

$\gamma = 115.21$ (3)°
 $V = 920.3$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.89$ mm⁻¹
 $T = 293$ K
 $0.20 \times 0.18 \times 0.15$ mm

Data collection

Rigaku Saturn diffractometer
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku/MS, 2006)
 $T_{\min} = 0.842$, $T_{\max} = 0.878$

11432 measured reflections
 4337 independent reflections
 3890 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.087$
 $S = 1.03$
 4337 reflections

244 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.88$ e Å⁻³
 $\Delta\rho_{\min} = -0.42$ e Å⁻³

Table 1

Selected bond lengths (Å).

Mn1—O5	2.1543 (16)	Mn1—N1	2.2043 (17)
Mn1—O8	2.1854 (15)	Mn1—O6	2.2142 (17)
Mn1—O7	2.1860 (16)	Mn1—O1	2.2269 (16)

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
O5—H1W \cdots O10	0.85	1.79	2.634 (2)	173
O5—H2W \cdots O3	0.85	1.92	2.729 (3)	159
O9—H9W \cdots O4	0.85	2.02	2.843 (3)	163
O6—H3W \cdots O9 ⁱ	0.85	1.98	2.824 (2)	170
O8—H8W \cdots O1 ⁱ	0.85	2.04	2.885 (2)	176
O7—H6W \cdots O4 ⁱⁱ	0.85	2.03	2.855 (3)	163
O6—H4W \cdots O4 ⁱⁱ	0.85	1.96	2.805 (2)	173
O7—H5W \cdots O9 ⁱⁱ	0.85	1.99	2.813 (2)	162
O8—H7W \cdots O2 ⁱⁱⁱ	0.85	1.87	2.712 (2)	172
O10—H11W \cdots O2 ⁱⁱⁱ	0.85	2.08	2.842 (3)	150
O10—H12W \cdots N5 ^{iv}	0.85	1.99	2.840 (3)	173
O9—H10W \cdots O1 ^v	0.85	2.24	3.083 (2)	173

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

Data collection: *CrystalClear* (Rigaku/MS, 2006); 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: *XP in SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2495).

References

- Ma, L.-F., Li, X.-Q., Meng, Q.-L., Wang, L.-Y., Du, M. & Hou, H.-W. (2011). *Cryst. Growth Des.* **11**, 175–184.
 Meng, X., Zhu, X., Qi, Y., Hou, H. & Fan, Y. (2009). *J. Mol. Struct.* **934**, 28–36.
 Rigaku/MS (2006). *CrystalClear*. Rigaku/MS Inc., The Woodlands, Texas, USA, and Rigaku Corporation, Tokyo, Japan.
 Sanchez, V., Storr, A. & Thompson, R. C. (2002). *Can. J. Chem.* **80**, 133–140.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2011). E67, m920 [doi:10.1107/S1600536811022197]

Tetraaqua{1-[(1*H*-1,2,3-benzotriazol-1-yl)methyl]-1*H*-imidazole}sulfatomanganese(II) dihydrate

Y. Wang and Y.-Y. Sun

Comment

A large number of metal-organic frameworks based on flexible organic ligands have been reported since they are good linkers and can influence the structural diversification of the products, including the formation of supramolecular isomers (Ma *et al.*, 2011; Meng *et al.*, 2009; Sanchez *et al.*, 2002). In order to further explore complexes with novel structures, in this work, through the reaction of 1-[(1*H*-1,2,3-benzotriazol-1-yl)methyl]-1*H*-1,3-imidazole (bmi) with manganese sulfate at room temperature, we obtained the title complex, $[\text{Mn}(\text{SO}_4)(\text{C}_{10}\text{H}_9\text{N}_5)(\text{H}_2\text{O})_4](\text{H}_2\text{O})_2$, which is reported here.

As shown in Figure 1, the Mn(II) ion features a distorted octahedral coordination geometry and is surrounded by five oxygen atoms from four water molecules and one monodentate sulfate ligand as well as one nitrogen atom from the bmi ligand. Atoms O1, O5, O6, O7 form the equatorial plane, whereas O8 and N1 atoms are located in the apical positions. The bond angle of O(8)—Mn(1)—N(1) is 176.71 (6)°. Intramolecular O—H···O hydrogen bonds stabilize the molecular configuration and O—H···O, O—H···N hydrogen bonds between adjacent molecules consolidate the crystal packing (Fig. 2).

Experimental

The ligand 1-[(1*H*-1,2,3-benzotriazol-1-yl)methyl]-1*H*-1,3-imidazole (0.1 mmol) in methanol (4 ml) was added dropwise to an aqueous solution (2 ml) of manganese sulfate (0.1 mmol). The resulting solution was allowed to stand at room temperature. After four weeks colorless crystals with good quality were obtained from the filtrate and dried in air.

Refinement

H atoms are positioned geometrically and refined as riding atoms, with C-H = 0.93 (aromatic) and 0.97 (CH₂) Å and O-H = 0.85 Å, and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{O})$.

Figures

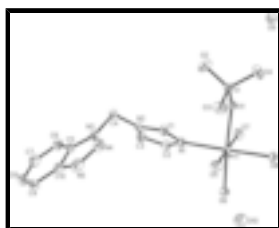


Fig. 1. View of the title complex, showing the labelling of the 30% probability ellipsoids. H atoms are omitted for clarity.

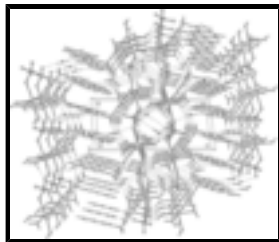


Fig. 2. Packing plot of the title complex, showing the hydrogen bonding (dashed lines)

Tetraaqua{1-[(1*H*-1,2,3-benzotriazol-1-yl)methyl]-1*H*-imidazole}sulfatomanganese(II) dihydrate

Crystal data

[Mn(SO₄)(C₁₀H₉N₅)(H₂O)₄].2H₂O

$M_r = 458.32$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.5824$ (15) Å

$b = 8.5237$ (17) Å

$c = 15.972$ (3) Å

$\alpha = 98.33$ (3)°

$\beta = 91.11$ (3)°

$\gamma = 115.21$ (3)°

$V = 920.3$ (3) Å³

$Z = 2$

$F(000) = 474$

$D_x = 1.654$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2952 reflections

$\theta = 2.6$ – 27.9 °

$\mu = 0.89$ mm⁻¹

$T = 293$ K

Prism, colourless

$0.20 \times 0.18 \times 0.15$ mm

Data collection

Rigaku Saturn
diffractometer

Radiation source: fine-focus sealed tube
graphite

Detector resolution: 28.5714 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*CrystalClear*; Rigaku/MSC, 2006)

$T_{\min} = 0.842$, $T_{\max} = 0.878$

11432 measured reflections

4337 independent reflections

3890 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\max} = 27.9$ °, $\theta_{\min} = 2.6$ °

$h = -9 \rightarrow 9$

$k = -9 \rightarrow 11$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.087$

$S = 1.03$

4337 reflections

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

$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.6298P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

244 parameters

$$\Delta\rho_{\max} = 0.88 \text{ e } \text{\AA}^{-3}$$

0 restraints

$$\Delta\rho_{\min} = -0.42 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	1.09479 (4)	0.68072 (4)	0.368939 (17)	0.02329 (9)
N1	0.9825 (2)	0.8445 (2)	0.31175 (11)	0.0291 (4)
N2	0.7818 (2)	0.9044 (2)	0.23568 (10)	0.0286 (4)
N3	0.6756 (3)	0.8884 (2)	0.09051 (11)	0.0335 (4)
N4	0.6786 (3)	0.7462 (3)	0.04108 (13)	0.0463 (5)
N5	0.7294 (3)	0.7876 (3)	-0.03268 (13)	0.0502 (5)
O1	0.7941 (2)	0.51495 (19)	0.40066 (9)	0.0329 (3)
O2	0.4595 (3)	0.4090 (3)	0.34648 (13)	0.0563 (5)
O3	0.6674 (3)	0.3117 (2)	0.26847 (10)	0.0474 (4)
O4	0.5682 (3)	0.2154 (2)	0.40145 (11)	0.0477 (4)
O5	1.0451 (2)	0.5238 (2)	0.24469 (9)	0.0369 (3)
H1W	1.1290	0.4924	0.2231	0.044*
H2W	0.9310	0.4400	0.2415	0.044*
O6	1.4025 (2)	0.84945 (19)	0.34976 (10)	0.0354 (3)
H3W	1.4870	0.8318	0.3776	0.042*
H4W	1.4499	0.9610	0.3610	0.042*
O7	1.1386 (2)	0.8208 (2)	0.49917 (9)	0.0391 (4)
H5W	1.1708	0.9306	0.5100	0.047*
H6W	1.2073	0.8024	0.5358	0.047*
O8	1.1938 (2)	0.5052 (2)	0.42073 (10)	0.0380 (4)
H7W	1.2767	0.4702	0.4012	0.046*
H8W	1.1915	0.4943	0.4728	0.046*
O9	0.3306 (2)	0.1900 (2)	0.53910 (10)	0.0399 (4)
H9W	0.4033	0.2189	0.4988	0.048*
H10W	0.3046	0.2747	0.5596	0.048*
O10	1.3276 (3)	0.4486 (2)	0.18654 (11)	0.0510 (4)
H11W	1.3663	0.4031	0.2225	0.061*
H12W	1.3172	0.3753	0.1423	0.061*
S1	0.62136 (7)	0.36114 (6)	0.35346 (3)	0.02383 (11)
C1	0.8275 (3)	0.7791 (3)	0.25673 (14)	0.0323 (4)

supplementary materials

H1A	0.7579	0.6599	0.2350	0.039*
C2	1.0396 (3)	1.0233 (3)	0.32650 (14)	0.0349 (5)
H2A	1.1463	1.1055	0.3629	0.042*
C3	0.9168 (4)	1.0606 (3)	0.27995 (15)	0.0392 (5)
H3A	0.9230	1.1714	0.2783	0.047*
C4	0.6192 (3)	0.8766 (3)	0.17646 (13)	0.0364 (5)
H4A	0.5134	0.7615	0.1773	0.044*
H4B	0.5714	0.9640	0.1945	0.044*
C5	0.7249 (3)	1.0253 (3)	0.04678 (12)	0.0309 (4)
C6	0.7348 (3)	1.1929 (3)	0.06646 (15)	0.0409 (5)
H6A	0.7078	1.2356	0.1192	0.049*
C7	0.7875 (4)	1.2921 (4)	0.00210 (19)	0.0544 (7)
H7A	0.7978	1.4061	0.0120	0.065*
C8	0.8259 (4)	1.2264 (5)	-0.07757 (19)	0.0605 (8)
H8A	0.8619	1.2985	-0.1187	0.073*
C9	0.8125 (4)	1.0620 (5)	-0.09655 (16)	0.0546 (7)
H9A	0.8369	1.0195	-0.1499	0.065*
C10	0.7603 (3)	0.9581 (3)	-0.03262 (13)	0.0391 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.02459 (15)	0.02428 (16)	0.02242 (15)	0.01142 (12)	0.00181 (11)	0.00560 (11)
N1	0.0309 (9)	0.0280 (9)	0.0306 (9)	0.0139 (7)	-0.0007 (7)	0.0086 (7)
N2	0.0300 (9)	0.0348 (9)	0.0258 (8)	0.0169 (7)	0.0011 (7)	0.0107 (7)
N3	0.0370 (10)	0.0413 (10)	0.0267 (9)	0.0203 (8)	0.0001 (7)	0.0085 (8)
N4	0.0532 (13)	0.0501 (12)	0.0432 (11)	0.0313 (11)	-0.0020 (10)	0.0033 (10)
N5	0.0543 (13)	0.0665 (15)	0.0378 (11)	0.0376 (12)	-0.0010 (10)	-0.0032 (10)
O1	0.0280 (7)	0.0301 (8)	0.0295 (7)	0.0027 (6)	0.0038 (6)	0.0030 (6)
O2	0.0394 (10)	0.0640 (12)	0.0746 (13)	0.0333 (9)	0.0045 (9)	0.0049 (10)
O3	0.0467 (10)	0.0523 (10)	0.0286 (8)	0.0102 (8)	0.0061 (7)	-0.0020 (7)
O4	0.0593 (11)	0.0292 (8)	0.0443 (9)	0.0072 (8)	-0.0041 (8)	0.0141 (7)
O5	0.0410 (9)	0.0341 (8)	0.0321 (8)	0.0144 (7)	0.0066 (6)	0.0007 (6)
O6	0.0276 (7)	0.0313 (8)	0.0443 (9)	0.0088 (6)	0.0024 (6)	0.0096 (7)
O7	0.0515 (10)	0.0356 (8)	0.0262 (7)	0.0178 (7)	-0.0043 (7)	-0.0021 (6)
O8	0.0497 (9)	0.0482 (9)	0.0346 (8)	0.0354 (8)	0.0111 (7)	0.0171 (7)
O9	0.0427 (9)	0.0342 (8)	0.0448 (9)	0.0181 (7)	0.0105 (7)	0.0071 (7)
O10	0.0652 (12)	0.0600 (11)	0.0368 (9)	0.0376 (10)	0.0053 (8)	0.0019 (8)
S1	0.0226 (2)	0.0225 (2)	0.0259 (2)	0.00928 (18)	0.00274 (17)	0.00440 (18)
C1	0.0345 (11)	0.0261 (10)	0.0348 (11)	0.0112 (8)	-0.0036 (9)	0.0076 (8)
C2	0.0382 (11)	0.0275 (10)	0.0353 (11)	0.0121 (9)	-0.0060 (9)	0.0024 (9)
C3	0.0492 (14)	0.0281 (11)	0.0437 (13)	0.0201 (10)	-0.0024 (10)	0.0071 (9)
C4	0.0312 (11)	0.0560 (14)	0.0296 (10)	0.0226 (10)	0.0040 (8)	0.0180 (10)
C5	0.0262 (10)	0.0422 (12)	0.0241 (9)	0.0139 (9)	-0.0011 (7)	0.0083 (8)
C6	0.0378 (12)	0.0407 (13)	0.0371 (12)	0.0119 (10)	-0.0067 (10)	0.0021 (10)
C7	0.0431 (14)	0.0435 (14)	0.0670 (18)	0.0068 (11)	-0.0070 (13)	0.0209 (13)
C8	0.0390 (14)	0.085 (2)	0.0531 (16)	0.0126 (14)	0.0050 (12)	0.0427 (16)
C9	0.0408 (14)	0.094 (2)	0.0303 (12)	0.0269 (14)	0.0104 (10)	0.0222 (13)

C10 0.0309 (11) 0.0607 (15) 0.0266 (10) 0.0216 (10) 0.0025 (8) 0.0047 (10)

Geometric parameters (Å, °)

Mn1—O5	2.1543 (16)	O7—H5W	0.8500
Mn1—O8	2.1854 (15)	O7—H6W	0.8499
Mn1—O7	2.1860 (16)	O8—H7W	0.8500
Mn1—N1	2.2043 (17)	O8—H8W	0.8500
Mn1—O6	2.2142 (17)	O9—H9W	0.8500
Mn1—O1	2.2269 (16)	O9—H10W	0.8501
N1—C1	1.313 (3)	O10—H11W	0.8499
N1—C2	1.377 (3)	O10—H12W	0.8500
N2—C1	1.338 (3)	C1—H1A	0.9300
N2—C3	1.363 (3)	C2—C3	1.347 (3)
N2—C4	1.453 (3)	C2—H2A	0.9300
N3—N4	1.357 (3)	C3—H3A	0.9300
N3—C5	1.365 (3)	C4—H4A	0.9700
N3—C4	1.450 (3)	C4—H4B	0.9700
N4—N5	1.297 (3)	C5—C6	1.387 (3)
N5—C10	1.369 (3)	C5—C10	1.394 (3)
O1—S1	1.4885 (16)	C6—C7	1.382 (4)
O2—S1	1.4560 (17)	C6—H6A	0.9300
O3—S1	1.4561 (16)	C7—C8	1.402 (4)
O4—S1	1.4677 (17)	C7—H7A	0.9300
O5—H1W	0.8501	C8—C9	1.349 (4)
O5—H2W	0.8500	C8—H8A	0.9300
O6—H3W	0.8500	C9—C10	1.401 (3)
O6—H4W	0.8500	C9—H9A	0.9300
O5—Mn1—O8	89.65 (6)	H11W—O10—H12W	98.3
O5—Mn1—O7	175.48 (6)	O2—S1—O3	108.94 (12)
O8—Mn1—O7	86.58 (6)	O2—S1—O4	109.81 (12)
O5—Mn1—N1	87.70 (7)	O3—S1—O4	110.79 (11)
O8—Mn1—N1	176.71 (6)	O2—S1—O1	108.90 (11)
O7—Mn1—N1	95.98 (7)	O3—S1—O1	110.12 (10)
O5—Mn1—O6	92.32 (7)	O4—S1—O1	108.25 (10)
O8—Mn1—O6	88.81 (6)	N1—C1—N2	111.90 (19)
O7—Mn1—O6	90.10 (7)	N1—C1—H1A	124.1
N1—Mn1—O6	93.25 (7)	N2—C1—H1A	124.1
O5—Mn1—O1	92.08 (7)	C3—C2—N1	109.40 (19)
O8—Mn1—O1	88.47 (6)	C3—C2—H2A	125.3
O7—Mn1—O1	85.33 (7)	N1—C2—H2A	125.3
N1—Mn1—O1	89.68 (7)	C2—C3—N2	106.71 (19)
O6—Mn1—O1	174.81 (6)	C2—C3—H3A	126.6
C1—N1—C2	105.20 (17)	N2—C3—H3A	126.6
C1—N1—Mn1	123.33 (14)	N3—C4—N2	111.86 (17)
C2—N1—Mn1	131.33 (14)	N3—C4—H4A	109.2
C1—N2—C3	106.80 (17)	N2—C4—H4A	109.2
C1—N2—C4	125.85 (19)	N3—C4—H4B	109.2
C3—N2—C4	127.36 (19)	N2—C4—H4B	109.2

supplementary materials

N4—N3—C5	110.75 (18)	H4A—C4—H4B	107.9
N4—N3—C4	119.50 (19)	N3—C5—C6	133.4 (2)
C5—N3—C4	129.72 (19)	N3—C5—C10	103.5 (2)
N5—N4—N3	108.1 (2)	C6—C5—C10	123.0 (2)
N4—N5—C10	109.1 (2)	C7—C6—C5	115.2 (2)
S1—O1—Mn1	134.35 (9)	C7—C6—H6A	122.4
Mn1—O5—H1W	123.1	C5—C6—H6A	122.4
Mn1—O5—H2W	106.7	C6—C7—C8	122.1 (3)
H1W—O5—H2W	113.6	C6—C7—H7A	119.0
Mn1—O6—H3W	114.6	C8—C7—H7A	119.0
Mn1—O6—H4W	121.6	C9—C8—C7	122.2 (2)
H3W—O6—H4W	100.5	C9—C8—H8A	118.9
Mn1—O7—H5W	121.8	C7—C8—H8A	118.9
Mn1—O7—H6W	118.3	C8—C9—C10	117.3 (2)
H5W—O7—H6W	105.2	C8—C9—H9A	121.4
Mn1—O8—H7W	127.1	C10—C9—H9A	121.4
Mn1—O8—H8W	123.0	N5—C10—C5	108.5 (2)
H7W—O8—H8W	105.9	N5—C10—C9	131.3 (2)
H9W—O9—H10W	109.6	C5—C10—C9	120.2 (2)
O5—Mn1—N1—C1	42.94 (17)	N1—C2—C3—N2	0.0 (3)
O7—Mn1—N1—C1	-134.43 (17)	C1—N2—C3—C2	-0.1 (3)
O6—Mn1—N1—C1	135.13 (17)	C4—N2—C3—C2	-179.8 (2)
O1—Mn1—N1—C1	-49.16 (17)	N4—N3—C4—N2	82.7 (3)
O5—Mn1—N1—C2	-142.02 (19)	C5—N3—C4—N2	-99.3 (3)
O7—Mn1—N1—C2	40.6 (2)	C1—N2—C4—N3	-91.1 (3)
O6—Mn1—N1—C2	-49.82 (19)	C3—N2—C4—N3	88.5 (3)
O1—Mn1—N1—C2	125.89 (19)	N4—N3—C5—C6	176.6 (2)
C5—N3—N4—N5	0.4 (3)	C4—N3—C5—C6	-1.5 (4)
C4—N3—N4—N5	178.76 (19)	N4—N3—C5—C10	-0.6 (2)
N3—N4—N5—C10	0.0 (3)	C4—N3—C5—C10	-178.7 (2)
O5—Mn1—O1—S1	-2.77 (13)	N3—C5—C6—C7	-178.3 (2)
O8—Mn1—O1—S1	-92.36 (13)	C10—C5—C6—C7	-1.6 (3)
O7—Mn1—O1—S1	-179.05 (13)	C5—C6—C7—C8	0.7 (4)
N1—Mn1—O1—S1	84.92 (13)	C6—C7—C8—C9	0.5 (4)
Mn1—O1—S1—O2	-118.40 (14)	C7—C8—C9—C10	-0.8 (4)
Mn1—O1—S1—O3	0.99 (17)	N4—N5—C10—C5	-0.3 (3)
Mn1—O1—S1—O4	122.26 (14)	N4—N5—C10—C9	-178.4 (2)
C2—N1—C1—N2	-0.2 (2)	N3—C5—C10—N5	0.5 (2)
Mn1—N1—C1—N2	175.94 (13)	C6—C5—C10—N5	-177.0 (2)
C3—N2—C1—N1	0.2 (2)	N3—C5—C10—C9	178.9 (2)
C4—N2—C1—N1	179.91 (18)	C6—C5—C10—C9	1.4 (3)
C1—N1—C2—C3	0.1 (3)	C8—C9—C10—N5	177.8 (3)
Mn1—N1—C2—C3	-175.60 (16)	C8—C9—C10—C5	-0.1 (4)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H1W \cdots O10	0.85	1.79	2.634 (2)	173.
O5—H2W \cdots O3	0.85	1.92	2.729 (3)	159.

O9—H9W…O4	0.85	2.02	2.843 (3)	163.
O6—H3W…O9 ⁱ	0.85	1.98	2.824 (2)	170.
O8—H8W…O1 ⁱ	0.85	2.04	2.885 (2)	176.
O7—H6W…O4 ⁱ	0.85	2.03	2.855 (3)	163.
O6—H4W…O4 ⁱⁱ	0.85	1.96	2.805 (2)	173.
O7—H5W…O9 ⁱⁱ	0.85	1.99	2.813 (2)	162.
O8—H7W…O2 ⁱⁱⁱ	0.85	1.87	2.712 (2)	172.
O10—H11W…O2 ⁱⁱⁱ	0.85	2.08	2.842 (3)	150.
O10—H12W…N5 ^{iv}	0.85	1.99	2.840 (3)	173.
O9—H10W…O1 ^v	0.85	2.24	3.083 (2)	173.

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

Fig. 1

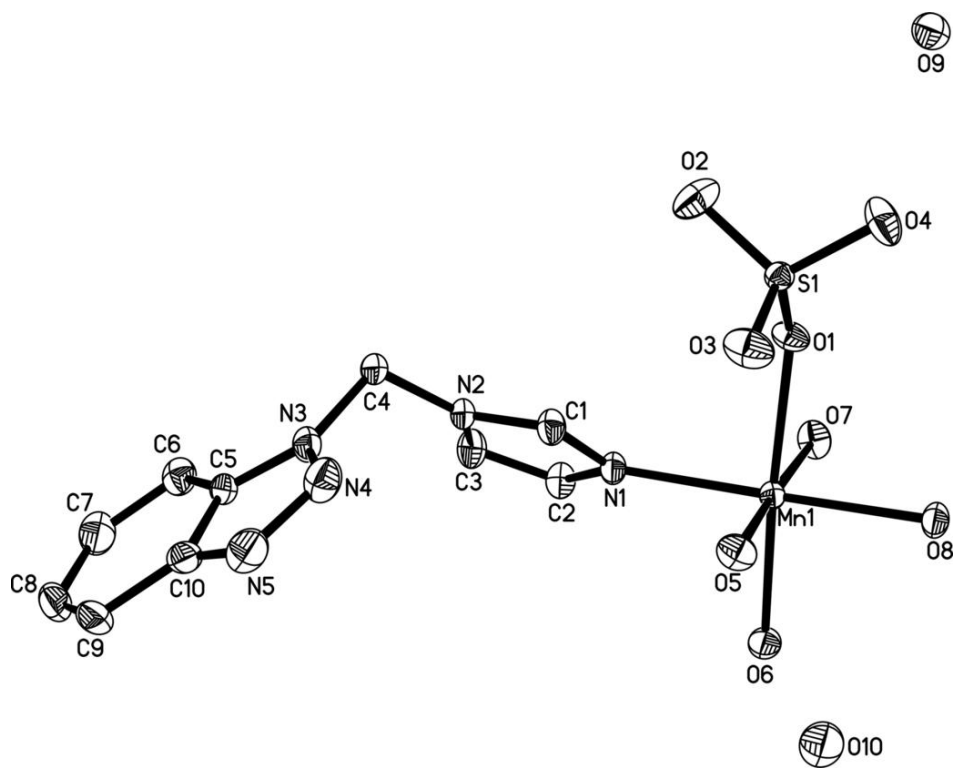


Fig. 2

