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

**Ying Wang[a]* and Ying-Ying Sun[b]**

[a]Department of Geriatrics, The First Affiliated Hospital, Zhengzhou University, Zhengzhou 450000, People's Republic of China, and [b]Department 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

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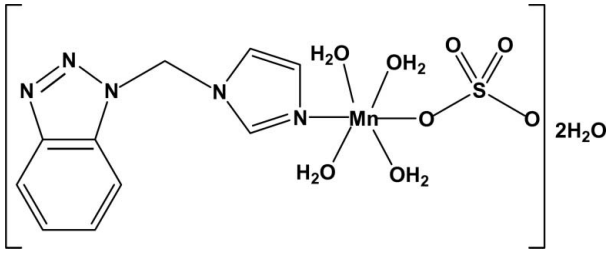
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.038; $wR$ factor = 0.087; data-to-parameter ratio = 17.8.

In the title complex, $[Mn(SO_4)(C_{10}H_9N_5)(H_2O)_4]\cdot 2H_2O$, 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 O—H···O and O—H···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

$[Mn(SO_4)(C_{10}H_9N_5)(H_2O)_4]\cdot 2H_2O$
$M_r$ = 458.32
Triclinic, $P\overline{1}$
$a$ = 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) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.89 mm$^{-1}$
$T$ = 293 K
0.20 × 0.18 × 0.15 mm

### Data collection

Rigaku Saturn diffractometer
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 $I > 2\sigma(I)$
$R_{int}$ = 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, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H1*W*···O10 | 0.85 | 1.79 | 2.634 (2) | 173 |
| O5—H2*W*···O3 | 0.85 | 1.92 | 2.729 (3) | 159 |
| O9—H9*W*···O4 | 0.85 | 2.02 | 2.843 (3) | 163 |
| O6—H3*W*···O9$^{i}$ | 0.85 | 1.98 | 2.824 (2) | 170 |
| O8—H8*W*···O1$^{i}$ | 0.85 | 2.04 | 2.885 (2) | 176 |
| O7—H6*W*···O4$^{i}$ | 0.85 | 2.03 | 2.855 (3) | 163 |
| O6—H4*W*···O4$^{ii}$ | 0.85 | 1.96 | 2.805 (2) | 173 |
| O7—H5*W*···O9$^{ii}$ | 0.85 | 1.99 | 2.813 (2) | 162 |
| O8—H7*W*···O2$^{iii}$ | 0.85 | 1.87 | 2.712 (2) | 172 |
| O10—H11*W*···O2$^{iii}$ | 0.85 | 2.08 | 2.842 (3) | 150 |
| O10—H12*W*···N5$^{iv}$ | 0.85 | 1.99 | 2.840 (3) | 173 |
| O9—H10*W*···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/MSC, 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/MSC (2006). *CrystalClear*. Rigaku/MSC 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.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2011). E**67**, m920 [doi:10.1107/S1600536811022197]

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

**Ying Wang and Ying-Ying Sun**

## S1. 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, $[Mn(SO_4)(C_{10}H_9N_5)(H_2O)_4](H_2O)_2$, 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).

## S2. 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.

## S3. Refinement

H atoms are positioned geometrically and refined as riding atoms, with C-H = 0.93 (aromatic) and 0.97 ($CH_2$) Å and O-H = 0.85 Å, and with $U_{iso}(H) = 1.2\ U_{eq}(C,O)$.

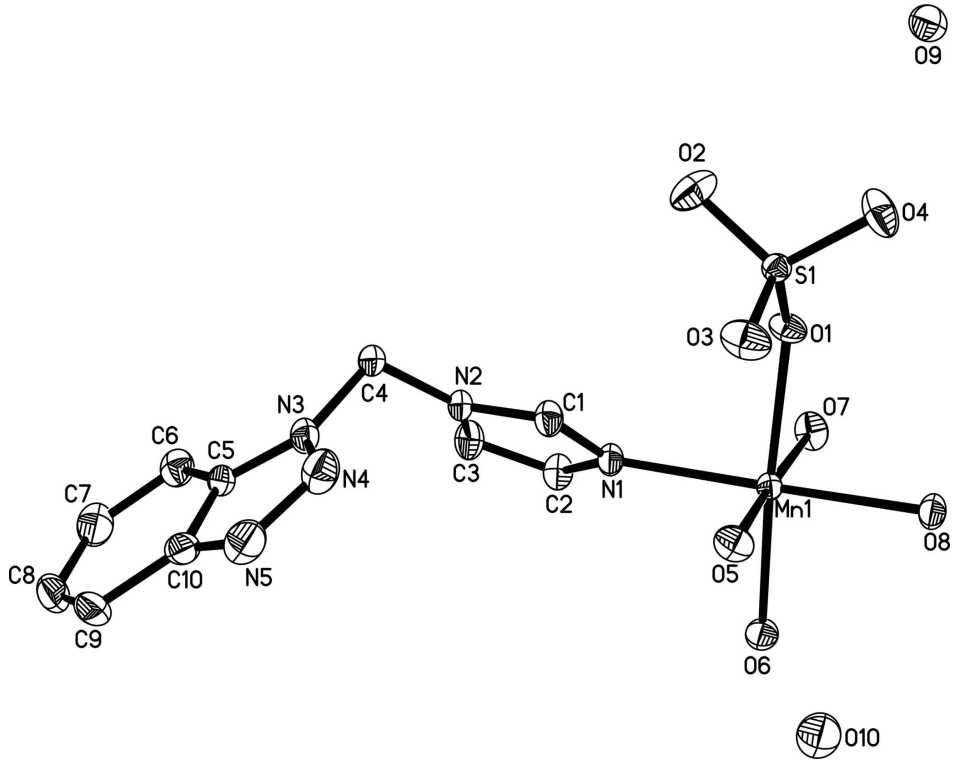



**Figure 1**

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

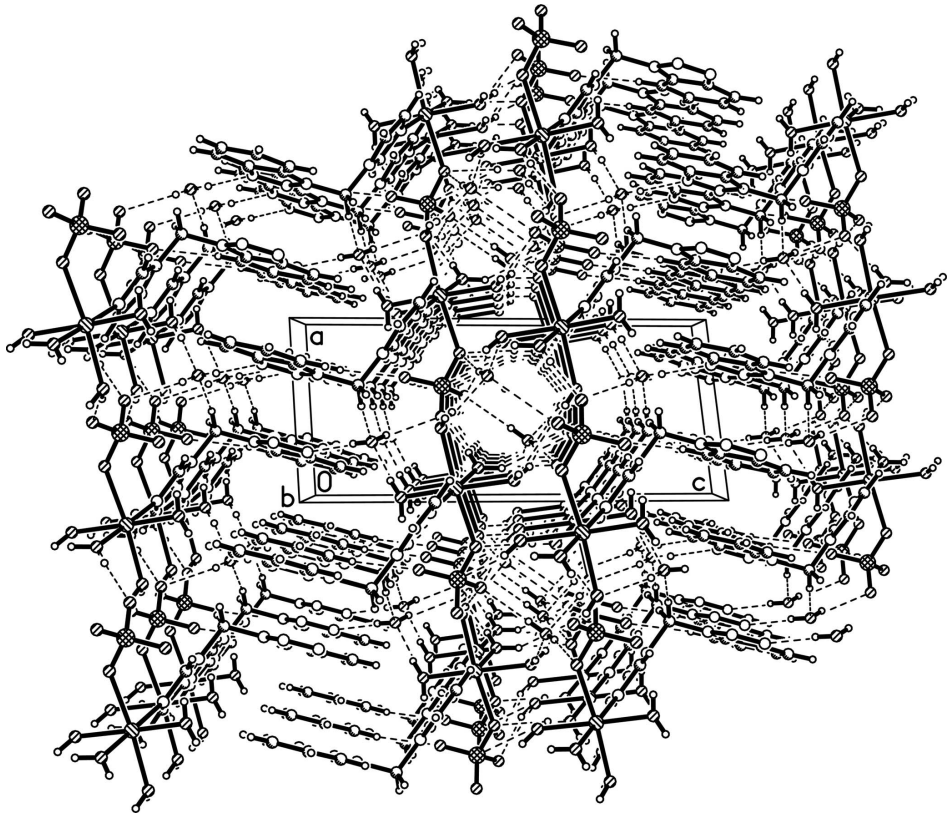



**Figure 2**

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*

$[Mn(SO_4)(C_{10}H_9N_5)(H_2O)_4]\cdot 2H_2O$
$M_r = 458.32$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.5824\ (15)$ Å
$b = 8.5237\ (17)$ Å
$c = 15.972\ (3)$ Å
$\alpha = 98.33\ (3)°$
$\beta = 91.11\ (3)°$
$\gamma = 115.21\ (3)°$
$V = 920.3\ (3)$ Å$^3$
$Z = 2$
$F(000) = 474$
$D_x = 1.654$ 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 × 0.18 × 0.15 mm

*Data collection*

Rigaku Saturn diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 28.5714 pixels mm$^{-1}$
$\omega$ 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 $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.6°$
$h = -9\rightarrow 9$
$k = -9\rightarrow 11$
$l = -20\rightarrow 20$

*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
244 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
$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.6298P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.88$ e Å$^{-3}$
$\Delta\rho_{min} = -0.42$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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) |
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) |

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| 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 |
| 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) |

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| 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) |

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|---|---|---|---|
| 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 (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H1*W*···O10 | 0.85 | 1.79 | 2.634 (2) | 173 |
| O5—H2*W*···O3 | 0.85 | 1.92 | 2.729 (3) | 159 |
| O9—H9*W*···O4 | 0.85 | 2.02 | 2.843 (3) | 163 |
| O6—H3*W*···O9$^{i}$ | 0.85 | 1.98 | 2.824 (2) | 170 |
| O8—H8*W*···O1$^{i}$ | 0.85 | 2.04 | 2.885 (2) | 176 |
| O7—H6*W*···O4$^{i}$ | 0.85 | 2.03 | 2.855 (3) | 163 |
| O6—H4*W*···O4$^{ii}$ | 0.85 | 1.96 | 2.805 (2) | 173 |
| O7—H5*W*···O9$^{ii}$ | 0.85 | 1.99 | 2.813 (2) | 162 |
| O8—H7*W*···O2$^{iii}$ | 0.85 | 1.87 | 2.712 (2) | 172 |
| O10—H11*W*···O2$^{iii}$ | 0.85 | 2.08 | 2.842 (3) | 150 |
| O10—H12*W*···N5$^{iv}$ | 0.85 | 1.99 | 2.840 (3) | 173 |
| O9—H10*W*···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.