

## Retraction of articles

## IUCr Editorial Office

5 Abbey Square, Chester CH1 2HU, England

This article reports the retraction of 11 articles published in *Acta Crystallographica Section E* between 2005 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), 11 additional articles are retracted by the authors or by the journal as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

**Table 1**

Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
[ <i>N,N'</i> -Bis(2-hydroxynaphthylmethylene)-1,2-ethanediaminato]zinc(II)	Chen <i>et al.</i> (2005)	10.1107/S1600536805026796	YAWZOM
Diazidobis(2,2'-biimidazole)copper(II)	Liu <i>et al.</i> (2007)	10.1107/S1600536807047873	SILZIX
Dichlorido(1,10-phenanthroline)copper(II)	Liu (2007)	10.1107/S1600536807056735	MISSAJ
Diazidobis(2,2'-biimidazole)cobalt(II)	Li <i>et al.</i> (2008)	10.1107/S1600536807062873	MIRYAO
Diazidobis(2,2'-biimidazole)manganese(II)	Zhang <i>et al.</i> (2008)	10.1107/S1600536808017984	MODBUD
Diazidobis(2,2'-biimidazole)iron(II)	Hao <i>et al.</i> (2008a)	10.1107/S1600536808018539	MODFOB
Bis(pentane-2,4-dionato)bis[2-(4-pyridyl)-4,4,5,5-tetramethylimidazole-1-oxyl 3-oxide]nickel(II)	Hao <i>et al.</i> (2008b)	10.1107/S1600536808018552	MODFUH
Bis(pentane-2,4-dionato- $\kappa^2 O, O'$ )bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazole-1-oxyl 3-oxide- $\kappa^2 N^2$ ]manganese(II)	Liu, Zhang <i>et al.</i> (2008)	10.1107/S1600536808022952	MODLUN
Bis[2,4-pentanedionato(1-)]bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazole-1-oxyl 3-oxide]manganese(II)	Liu, He <i>et al.</i> (2008)	10.1107/S1600536808038440	MODLUN01
Di- $\mu$ -chlorido-bis[chlorido(1,10-phenanthroline- $\kappa^2 N, N'$ )zinc(II)]	Yang <i>et al.</i> (2009)	10.1107/S1600536809014482	JOLBOC
Tris(ethylenediamine)manganese(II) sulfate	Lu (2009)	10.1107/S1600536809034874	YUCZEC

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- Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* **E66**, e1–e2.
- Li, S., Wang, S.-B., Zhang, F.-L. & Tang, K. (2008). *Acta Cryst.* **E64**, m76.
- Liu, Y.-Q. (2007). *Acta Cryst.* **E63**, m2991.
- Liu, Y., Dou, J., Li, D. & Zhang, X. (2007). *Acta Cryst.* **E63**, m2661.
- Liu, Y., He, Q., Zhang, X., Xue, Z. & Lv, C. (2008). *Acta Cryst.* **E64**, m1604.
- Liu, Y., Zhang, X., Xue, Z., He, Q. & Zhang, Y. (2008). *Acta Cryst.* **E64**, m1077.
- Lu, J. (2009). *Acta Cryst.* **E65**, m1187.
- Yang, X.-M., Leng, Q.-B., Chen, Y., He, Y.-G. & Luo, S.-W. (2009). *Acta Cryst.* **E65**, m567.
- Zhang, X., Wei, P. & Li, B. (2008). *Acta Cryst.* **E64**, m934.

## Tris(ethylenediamine)manganese(II) sulfate

Jing Lu

School of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, People's Republic of China  
Correspondence e-mail: lujing@luc.edu.cn

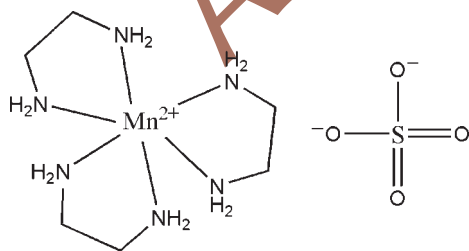
Received 21 August 2009; accepted 31 August 2009

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.011$  Å; disorder in main residue;  $R$  factor = 0.058;  $wR$  factor = 0.159; data-to-parameter ratio = 9.1.

In the title compound,  $[\text{Mn}(\text{C}_2\text{H}_8\text{N}_2)_3]\text{SO}_4$ , the metal atom (site symmetry 3.2) is coordinated by six N atoms from three ethylenediamine (en) ligands in a slightly distorted octahedral geometry. The en ligands are generated from one half-molecule in the asymmetric unit. The O atoms of the sulfate anion (S site symmetry 3.2) are disordered over four orientations in a 0.220 (12):0.210 (13):0.203 (14):0.10 (2) ratio, with one of the O atoms having site symmetry 3. In the crystal, the ions are connected by  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, forming a three-dimensional network.

### Related literature

For a structure containing  $\text{Mn}^{\text{II}}$  and aromatic amine ligands, see: Shang *et al.* (2009). For other compounds containing transition metals coordinated by ethylenediamine, see: Cullen & Lingafelter (1970); Daniels *et al.* (1995); Jameson *et al.* (1982).



### Experimental

#### Crystal data

$[\text{Mn}(\text{C}_2\text{H}_8\text{N}_2)_3]\text{SO}_4$   
 $M_r = 331.31$   
Trigonal,  $P\bar{3}1c$   
 $a = 8.9460$  (13) Å  
 $c = 9.6230$  (19) Å  
 $V = 666.96$  (19) Å<sup>3</sup>

$Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 1.17$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.35 \times 0.30 \times 0.28$  mm

#### Data collection

Bruker SMART CCD diffractometer  
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)  
 $T_{\text{min}} = 0.686$ ,  $T_{\text{max}} = 0.736$

2640 measured reflections  
402 independent reflections  
386 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$   
 $wR(F^2) = 0.159$   
 $S = 1.55$   
402 reflections  
44 parameters

2 restraints  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.72$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.63$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Mn1—N1	2.125 (6)
N1 <sup>i</sup> —Mn1—N1	81.6 (3)
Symmetry code: (i) $-x + y, -y, -z + \frac{3}{2}$ .	

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N1—H1A <sup>i</sup> ⋯O1 <sup>ii</sup>	0.90	2.28	3.16 (3)	166
N1—H1A <sup>i</sup> ⋯O1 <sup>iii</sup>	0.90	2.43	3.15 (3)	138
N1—H1B <sup>i</sup> ⋯O1 <sup>iv</sup>	0.90	2.17	3.06 (2)	170
N1—H1B <sup>i</sup> ⋯O2 <sup>iv</sup>	0.90	2.11	3.00 (2)	167
N1—H1A <sup>i</sup> ⋯O2 <sup>v</sup>	0.90	2.14	2.95 (5)	148
N1—H1A <sup>i</sup> ⋯O3 <sup>ii</sup>	0.90	1.92	2.80 (3)	166
N1—H1B <sup>i</sup> ⋯O3 <sup>iv</sup>	0.90	2.15	2.96 (3)	150
N1—H1B <sup>i</sup> ⋯O3 <sup>vi</sup>	0.90	2.36	3.18 (3)	152
N1—H1B <sup>i</sup> ⋯O4 <sup>vii</sup>	0.90	2.15	2.94 (7)	146

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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*.

This work was supported by the National Natural Science Foundation of China (No. 20671048) and the Doctoral Foundation of Liaocheng University (No. 31805).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5060).

### References

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**supplementary materials**

**Article retracted**

*Acta Cryst.* (2009). E65, m1187 [ doi:10.1107/S1600536809034874 ]

## Tris(ethylenediamine)manganese(II) sulfate

J. Lu

### Comment

Ethylenediamine (en) ligand has been seen in a number of coordination compound (Cullen *et al.*, 1970; Daniels *et al.*, 1995 and Jameson *et al.*, 1982), because it can not only chelate metal center by two nitrogen atoms, but also offer hydrogen atoms to form N—H $\cdots$ X hydrogen bonds. In this paper, we report the structure of the title compound, (I).

In the title compound (Fig. 1), [Mn(C<sub>2</sub>H<sub>8</sub>N<sub>2</sub>)<sub>3</sub>]SO<sub>4</sub>, the cation and anion are situated on a sixfold rotation axis. The Mn(II) is coordinated by six N atoms from three en ligands in a distorted octahedral geometry. The Mn—N bond length is 2.129 Å, which is shorter than the distance between Mn(II) and aromatic nitrogen atom (Shang *et al.*, 2009). The O atoms of the sulfate anions are disordered. The disordered anions hydrogen bond with the coordination cations by N—H $\cdots$ O hydrogen bonds, forming three-dimensional supramolecular network. The hydrogen bond is listed in table 1.

### Experimental

Manganese sulfate (0.2 mmol) and malic acid (0.4 mmol) were added to water (15 ml). The pH value was adjusted to 9 by en. Violet blocks of (I) were obtained after several days in 30% yield. Elemental analysis, Found: C, 21.73; H, 7.24; N, 25.35%. Calc. for C<sub>6</sub>H<sub>24</sub>N<sub>6</sub>MnSO<sub>4</sub>: C, 21.20; H, 7.00; N, 24.93%.

### Refinement

All H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H 0.970 and N—H 0.900 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ . The O atoms are resolved into four positions by PART instructions. The geometries and anisotropic displacement parameters of disordered atoms were refined with soft restraints using the *SHELXL* commands SUMP, SIMU and EADP.

### Figures

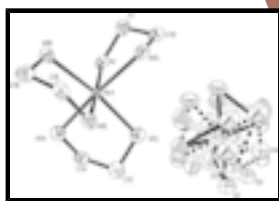


Fig. 1. The molecular structure of (I) with 50% probability displacement ellipsoids. The symmetry codes for N and C atoms: A  $-y+1, x-y+1, z$ ; B  $-x+y, -x+1, z$ ; C  $-y+1, -x+1, -z+3/2$ ; D  $-x+y, y, -z+3/2$ ; E  $x, x-y+1, -z+3/2$ .

## Tris(ethylenediamine)manganese(II) sulfate

### Crystal data

[Mn(C<sub>2</sub>H<sub>8</sub>N<sub>2</sub>)<sub>3</sub>]SO<sub>4</sub>

Z = 2

## supplementary materials

$M_r = 331.31$	$F_{000} = 350$
Trigonal, $P\bar{3}1c$	$D_x = 1.650 \text{ Mg m}^{-3}$
$a = 8.9460 (13) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$b = 8.9460 (13) \text{ \AA}$	Cell parameters from 2640 reflections
$c = 9.6230 (19) \text{ \AA}$	$\theta = 2.6\text{--}25.0^\circ$
$\alpha = 90^\circ$	$\mu = 1.17 \text{ mm}^{-1}$
$\beta = 90^\circ$	$T = 293 \text{ K}$
$\gamma = 120^\circ$	Block, violet
$V = 666.96 (19) \text{ \AA}^3$	$0.35 \times 0.30 \times 0.28 \text{ mm}$

### Data collection

Bruker SMART CCD diffractometer	402 independent reflections
Radiation source: fine-focus sealed tube	386 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.031$
$T = 293 \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
$\omega$ scans	$\theta_{\text{min}} = 2.6^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2003)	$h = -8 \rightarrow 10$
$T_{\text{min}} = 0.686$ , $T_{\text{max}} = 0.736$	$k = -10 \rightarrow 4$
2640 measured reflections	$l = -11 \rightarrow 11$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.058$	H-atom parameters constrained
$wR(F^2) = 0.159$	$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 1.2291P]$
$S = 1.55$	where $P = (F_o^2 + 2F_c^2)/3$
402 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
44 parameters	$\Delta\rho_{\text{max}} = 0.72 \text{ e \AA}^{-3}$
2 restraints	$\Delta\rho_{\text{min}} = -0.63 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXS97 (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.051 (15)

### 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Mn1	0.3333	0.6667	0.7500	0.0200 (8)	
S1	0.3333	0.6667	0.2500	0.0332 (10)	
O1	0.489 (3)	0.813 (4)	0.186 (2)	0.051 (4)	0.220 (12)
O2	0.489 (3)	0.721 (6)	0.163 (3)	0.051 (4)	0.210 (13)
O3	0.373 (6)	0.799 (3)	0.146 (3)	0.051 (4)	0.203 (14)
O4	0.3333	0.6667	0.114 (9)	0.051 (4)	0.10 (2)
N1	0.3136 (7)	0.4590 (8)	0.8712 (6)	0.0427 (14)	
H1A	0.4072	0.4479	0.8581	0.051*	
H1B	0.3070	0.4791	0.9621	0.051*	
C1	0.1570 (9)	0.3007 (9)	0.8275 (8)	0.0491 (18)	
H1C	0.0561	0.2960	0.8692	0.059*	
H1D	0.1626	0.2002	0.8578	0.059*	

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mn1	0.0208 (9)	0.0208 (9)	0.0184 (12)	0.0104 (5)	0.000	0.000
S1	0.0327 (13)	0.0327 (13)	0.034 (2)	0.0163 (7)	0.000	0.000
O1	0.045 (8)	0.042 (12)	0.047 (7)	0.008 (10)	0.007 (6)	0.000 (8)
O2	0.045 (8)	0.042 (12)	0.047 (7)	0.008 (10)	0.007 (6)	0.000 (8)
O3	0.045 (8)	0.042 (12)	0.047 (7)	0.008 (10)	0.007 (6)	0.000 (8)
O4	0.045 (8)	0.042 (12)	0.047 (7)	0.008 (10)	0.007 (6)	0.000 (8)
N1	0.041 (3)	0.051 (3)	0.040 (3)	0.026 (3)	0.008 (2)	0.000 (2)
C1	0.051 (4)	0.053 (4)	0.054 (4)	0.035 (3)	0.002 (3)	-0.006 (3)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Mn1—N1 <sup>i</sup>	2.125 (6)	S1—O2 <sup>iii</sup>	1.48 (3)
Mn1—N1 <sup>ii</sup>	2.125 (6)	S1—O2 <sup>vii</sup>	1.48 (3)
Mn1—N1 <sup>iii</sup>	2.125 (6)	S1—O2 <sup>viii</sup>	1.48 (3)
Mn1—N1 <sup>iv</sup>	2.125 (6)	S1—O2 <sup>ii</sup>	1.48 (3)
Mn1—N1 <sup>v</sup>	2.125 (6)	O1—O1 <sup>viii</sup>	1.74 (5)
Mn1—N1	2.125 (6)	O2—O2 <sup>viii</sup>	1.72 (6)
S1—O4	1.30 (9)	O3—O3 <sup>iii</sup>	1.82 (4)
S1—O4 <sup>vi</sup>	1.30 (9)	O3—O3 <sup>ii</sup>	1.82 (4)
S1—O3 <sup>vii</sup>	1.45 (3)	N1—C1	1.471 (9)
S1—O3 <sup>iii</sup>	1.45 (3)	N1—H1A	0.9000
S1—O3	1.45 (3)	N1—H1B	0.9000
S1—O3 <sup>vi</sup>	1.45 (3)	C1—C1 <sup>iv</sup>	1.496 (15)
S1—O3 <sup>ii</sup>	1.45 (3)	C1—H1C	0.9700

## supplementary materials

S1—O3 <sup>viii</sup>	1.45 (3)	C1—H1D	0.9700
N1 <sup>i</sup> —Mn1—N1 <sup>ii</sup>	81.6 (3)	O3 <sup>ii</sup> —S1—O2 <sup>iii</sup>	99.3 (13)
N1 <sup>i</sup> —Mn1—N1 <sup>iii</sup>	93.5 (3)	O3 <sup>viii</sup> —S1—O2 <sup>iii</sup>	170.3 (17)
N1 <sup>ii</sup> —Mn1—N1 <sup>iii</sup>	92.7 (2)	O4—S1—O2 <sup>vii</sup>	124.3 (10)
N1 <sup>i</sup> —Mn1—N1 <sup>iv</sup>	92.7 (2)	O4 <sup>vi</sup> —S1—O2 <sup>vii</sup>	55.7 (10)
N1 <sup>ii</sup> —Mn1—N1 <sup>iv</sup>	93.5 (3)	O3 <sup>vii</sup> —S1—O2 <sup>vii</sup>	62.4 (15)
N1 <sup>iii</sup> —Mn1—N1 <sup>iv</sup>	171.8 (3)	O3 <sup>iii</sup> —S1—O2 <sup>vii</sup>	97 (2)
N1 <sup>i</sup> —Mn1—N1 <sup>v</sup>	92.7 (2)	O3—S1—O2 <sup>vii</sup>	94 (3)
N1 <sup>ii</sup> —Mn1—N1 <sup>v</sup>	171.8 (3)	O3 <sup>vi</sup> —S1—O2 <sup>vii</sup>	30.1 (12)
N1 <sup>iii</sup> —Mn1—N1 <sup>v</sup>	81.6 (3)	O3 <sup>ii</sup> —S1—O2 <sup>vii</sup>	170.3 (17)
N1 <sup>iv</sup> —Mn1—N1 <sup>v</sup>	92.7 (2)	O3 <sup>viii</sup> —S1—O2 <sup>vii</sup>	99.3 (13)
N1 <sup>i</sup> —Mn1—N1	171.8 (3)	O2 <sup>iii</sup> —S1—O2 <sup>vii</sup>	71 (2)
N1 <sup>ii</sup> —Mn1—N1	92.7 (2)	O4—S1—O2 <sup>viii</sup>	124.3 (11)
N1 <sup>iii</sup> —Mn1—N1	92.7 (2)	O4 <sup>vi</sup> —S1—O2 <sup>viii</sup>	55.7 (10)
N1 <sup>iv</sup> —Mn1—N1	81.6 (3)	O3 <sup>vii</sup> —S1—O2 <sup>viii</sup>	30.1 (12)
N1 <sup>v</sup> —Mn1—N1	93.5 (3)	O3 <sup>iii</sup> —S1—O2 <sup>viii</sup>	170.3 (18)
O4—S1—O4 <sup>vi</sup>	180.000 (19)	O3—S1—O2 <sup>viii</sup>	97 (2)
O4—S1—O3 <sup>vii</sup>	133.7 (10)	O3 <sup>vi</sup> —S1—O2 <sup>viii</sup>	99.3 (13)
O4 <sup>vi</sup> —S1—O3 <sup>vii</sup>	46.3 (10)	O3 <sup>iv</sup> —S1—O2 <sup>viii</sup>	94 (3)
O4—S1—O3 <sup>iii</sup>	46.3 (10)	O3 <sup>viii</sup> —S1—O2 <sup>viii</sup>	62.4 (15)
O4 <sup>vi</sup> —S1—O3 <sup>iii</sup>	133.7 (10)	O2 <sup>iii</sup> —S1—O2 <sup>viii</sup>	116 (3)
O3 <sup>vii</sup> —S1—O3 <sup>iii</sup>	156 (4)	O2 <sup>vii</sup> —S1—O2 <sup>viii</sup>	91.3 (15)
O4—S1—O3	46.3 (10)	O4—S1—O2 <sup>ii</sup>	55.7 (10)
O4 <sup>vi</sup> —S1—O3	133.7 (10)	O4 <sup>vi</sup> —S1—O2 <sup>ii</sup>	124.3 (10)
O3 <sup>vii</sup> —S1—O3	90 (2)	O3 <sup>vii</sup> —S1—O2 <sup>ii</sup>	170.3 (17)
O3 <sup>iii</sup> —S1—O3	77.5 (15)	O3 <sup>iii</sup> —S1—O2 <sup>ii</sup>	30.1 (12)
O4—S1—O3 <sup>vi</sup>	133.7 (10)	O3—S1—O2 <sup>ii</sup>	99.3 (13)
O4 <sup>vi</sup> —S1—O3 <sup>vi</sup>	46.3 (10)	O3 <sup>vi</sup> —S1—O2 <sup>ii</sup>	97 (2)
O3 <sup>vii</sup> —S1—O3 <sup>vi</sup>	77.5 (15)	O3 <sup>ii</sup> —S1—O2 <sup>ii</sup>	62.4 (15)
O3 <sup>iii</sup> —S1—O3 <sup>vi</sup>	90 (2)	O3 <sup>viii</sup> —S1—O2 <sup>ii</sup>	94 (3)
O3—S1—O3 <sup>vi</sup>	121 (3)	O2 <sup>iii</sup> —S1—O2 <sup>ii</sup>	91.3 (15)
O4—S1—O3 <sup>ii</sup>	46.3 (10)	O2 <sup>vii</sup> —S1—O2 <sup>ii</sup>	116 (3)
O4 <sup>vi</sup> —S1—O3 <sup>ii</sup>	133.7 (10)	O2 <sup>viii</sup> —S1—O2 <sup>ii</sup>	147 (4)
O3 <sup>vii</sup> —S1—O3 <sup>ii</sup>	121 (3)	S1—O1—O1 <sup>viii</sup>	54.1 (11)
O3 <sup>iii</sup> —S1—O3 <sup>ii</sup>	77.5 (15)	S1—O2—O2 <sup>viii</sup>	54.5 (12)
O3—S1—O3 <sup>ii</sup>	77.5 (15)	S1—O3—O3 <sup>iii</sup>	51.2 (7)
O3 <sup>vi</sup> —S1—O3 <sup>ii</sup>	156 (4)	S1—O3—O3 <sup>ii</sup>	51.2 (7)
O4—S1—O3 <sup>viii</sup>	133.7 (10)	O3 <sup>iii</sup> —O3—O3 <sup>ii</sup>	60.000 (1)
O4 <sup>vi</sup> —S1—O3 <sup>viii</sup>	46.3 (10)	C1—N1—Mn1	107.9 (4)
O3 <sup>vii</sup> —S1—O3 <sup>viii</sup>	77.5 (15)	C1—N1—H1A	110.1

O3 <sup>iii</sup> —S1—O3 <sup>viii</sup>	121 (3)	Mn1—N1—H1A	110.1
O3—S1—O3 <sup>viii</sup>	156 (4)	C1—N1—H1B	110.1
O3 <sup>vi</sup> —S1—O3 <sup>viii</sup>	77.5 (15)	Mn1—N1—H1B	110.1
O3 <sup>ii</sup> —S1—O3 <sup>viii</sup>	90 (2)	H1A—N1—H1B	108.4
O4—S1—O2 <sup>iii</sup>	55.7 (10)	N1—C1—C1 <sup>iv</sup>	108.9 (5)
O4 <sup>vi</sup> —S1—O2 <sup>iii</sup>	124.3 (10)	N1—C1—H1C	109.9
O3 <sup>vii</sup> —S1—O2 <sup>iii</sup>	97 (2)	C1 <sup>iv</sup> —C1—H1C	109.9
O3 <sup>iii</sup> —S1—O2 <sup>iii</sup>	62.4 (15)	N1—C1—H1D	109.9
O3—S1—O2 <sup>iii</sup>	30.1 (12)	C1 <sup>iv</sup> —C1—H1D	109.9
O3 <sup>vi</sup> —S1—O2 <sup>iii</sup>	94 (3)	H1C—C1—H1D	108.3
O4—S1—O1—O1 <sup>vii</sup>	-129 (2)	O3 <sup>vii</sup> —S1—O3—O3 <sup>iii</sup>	-159 (3)
O4 <sup>vi</sup> —S1—O1—O1 <sup>viii</sup>	51 (2)	O3 <sup>vi</sup> —S1—O3—O3 <sup>iii</sup>	-83 (2)
O3 <sup>vii</sup> —S1—O1—O1 <sup>viii</sup>	65.8 (19)	O3 <sup>ii</sup> —S1—O3—O3 <sup>iii</sup>	79.8 (10)
O3 <sup>iii</sup> —S1—O1—O1 <sup>viii</sup>	-140 (3)	O3 <sup>viii</sup> —S1—O3—O3 <sup>iii</sup>	141.8 (18)
O3—S1—O1—O1 <sup>viii</sup>	179 (3)	O2 <sup>iii</sup> —S1—O3—O3 <sup>iii</sup>	-55 (3)
O3 <sup>vi</sup> —S1—O1—O1 <sup>viii</sup>	100 (3)	O2 <sup>vii</sup> —S1—O3—O3 <sup>iii</sup>	-96 (3)
O3 <sup>ii</sup> —S1—O1—O1 <sup>viii</sup>	-77 (2)	O2 <sup>viii</sup> —S1—O3—O3 <sup>iii</sup>	172 (3)
O3 <sup>viii</sup> —S1—O1—O1 <sup>viii</sup>	0(2)	O2 <sup>ii</sup> —S1—O3—O3 <sup>iii</sup>	20.9 (16)
O2 <sup>iii</sup> —S1—O1—O1 <sup>viii</sup>	171 (2)	O4—S1—O3—O3 <sup>ii</sup>	-39.9 (5)
O2 <sup>vii</sup> —S1—O1—O1 <sup>viii</sup>	112.2 (18)	O4 <sup>vi</sup> —S1—O3—O3 <sup>ii</sup>	140.1 (5)
O2 <sup>viii</sup> —S1—O1—O1 <sup>viii</sup>	34.5 (19)	O3 <sup>vii</sup> —S1—O3—O3 <sup>ii</sup>	122 (4)
O2 <sup>ii</sup> —S1—O1—O1 <sup>viii</sup>	-108 (3)	O3 <sup>iii</sup> —S1—O3—O3 <sup>ii</sup>	-79.8 (10)
O4—S1—O2—O2 <sup>viii</sup>	163 (4)	O3 <sup>vi</sup> —S1—O3—O3 <sup>ii</sup>	-163 (2)
O4 <sup>vi</sup> —S1—O2—O2 <sup>viii</sup>	-17 (4)	O3 <sup>viii</sup> —S1—O3—O3 <sup>ii</sup>	62 (2)
O3 <sup>vii</sup> —S1—O2—O2 <sup>viii</sup>	20 (2)	O2 <sup>iii</sup> —S1—O3—O3 <sup>ii</sup>	-135 (3)
O3 <sup>iii</sup> —S1—O2—O2 <sup>viii</sup>	179 (4)	O2 <sup>vii</sup> —S1—O3—O3 <sup>ii</sup>	-176 (3)
O3—S1—O2—O2 <sup>viii</sup>	109 (4)	O2 <sup>viii</sup> —S1—O3—O3 <sup>ii</sup>	92 (3)
O3 <sup>vi</sup> —S1—O2—O2 <sup>viii</sup>	-3(22)	O2 <sup>ii</sup> —S1—O3—O3 <sup>ii</sup>	-58.9 (16)
O3 <sup>ii</sup> —S1—O2—O2 <sup>viii</sup>	-136 (5)	N1 <sup>i</sup> —Mn1—N1—C1	32.2 (4)
O3 <sup>viii</sup> —S1—O2—O2 <sup>viii</sup>	-58 (2)	N1 <sup>ii</sup> —Mn1—N1—C1	78.5 (5)
O2 <sup>iii</sup> —S1—O2—O2 <sup>viii</sup>	117 (4)	N1 <sup>iii</sup> —Mn1—N1—C1	171.4 (4)
O2 <sup>vii</sup> —S1—O2—O2 <sup>viii</sup>	61 (2)	N1 <sup>iv</sup> —Mn1—N1—C1	-14.7 (3)
O2 <sup>ii</sup> —S1—O2—O2 <sup>viii</sup>	-151 (4)	N1 <sup>v</sup> —Mn1—N1—C1	-106.9 (4)
O4—S1—O3—O3 <sup>iii</sup>	39.9 (5)	Mn1—N1—C1—C1 <sup>iv</sup>	41.5 (7)
O4 <sup>vi</sup> —S1—O3—O3 <sup>iii</sup>	-140.1 (5)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ O1 <sup>ix</sup>	0.90	2.28	3.16 (3)	166

## supplementary materials

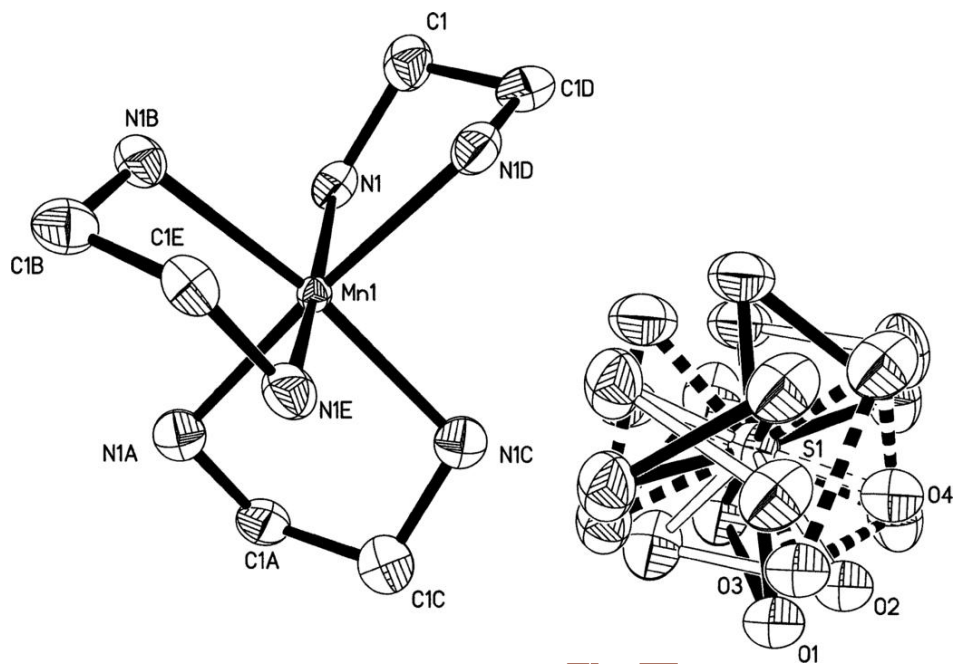
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N1—H1A···O1 <sup>x</sup>	0.90	2.43	3.15 (3)	138
N1—H1B···O1 <sup>xi</sup>	0.90	2.17	3.06 (2)	170
N1—H1B···O2 <sup>xi</sup>	0.90	2.11	3.00 (2)	167
N1—H1A···O2 <sup>xii</sup>	0.90	2.14	2.95 (5)	148
N1—H1A···O3 <sup>ix</sup>	0.90	1.92	2.80 (3)	166
N1—H1B···O3 <sup>xi</sup>	0.90	2.15	2.96 (3)	150
N1—H1B···O3 <sup>xiii</sup>	0.90	2.36	3.18 (3)	152
N1—H1B···O4 <sup>xiv</sup>	0.90	2.15	2.94 (7)	146

Symmetry codes: (ix)  $x-y+1, x, -z+1$ ; (x)  $-x+1, -x+y, z+1/2$ ; (xi)  $-x+y, -x+1, z+1$ ; (xii)  $-x+1, -y+1, -z+1$ ; (xiii)  $-y+1, x-y+1, z+1$ ; (xiv)  $x, y, z+1$ .

Article retracted

Fig. 1



Article retr