

Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. 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>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate</i>	Zhong, Zeng, Liu & Luo (2006a)	10.1107/S1600536806041122	KERQEE
<i>cis-Dichlorobis(1,10-phenanthroline)cobalt(II)</i>	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
<i>Tris(quinolin-8-olato-κ<sup>2</sup>N,O)cobalt(III) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2006b)	10.1107/S1600536806050240	MEQHEW
<i>(8-Quinololinol-κ<sup>2</sup>N,O)bis(8-quinolinolato-κ<sup>2</sup>N,O)nickel(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate</i>	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
<i>(8-Quinololinol-κ<sup>2</sup>N,O)-bis(8-quinolinolato-κ<sup>2</sup>N,O)zinc(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
<i>(Dimethylglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')nickel(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007a)	10.1107/S1600536807004102	YEYGOZ
<i>(Dimethylglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')zinc(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007b)	10.1107/S1600536807004096	YEYGUF
<i>Chloridobis(1,10-phenanthroline-κN,N')copper(I) hexahydrate</i>	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)</i>	Zhong, Zeng, Yang & Luo (2007a)	10.1107/S1600536807017461	ITPCOO1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)</i>	Zhong, Zeng, Yang & Luo (2007b)	10.1107/S160053680701879X	AVUJEG02
<i>Tetrakis(nitrato-κ<sup>2</sup>O,O')bis(4-phenylpyridine-κN)cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007c)	10.1107/S1600536807018831	CICDOI
<i>Bis(4,4'-bipyridine-κ<sup>2</sup>N,N')tetrakis(nitrato-κ<sup>2</sup>O,O')cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007d)	10.1107/S1600536807021502	YIDNEF
<i>(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)</i>	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
<i>(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)</i>	Zhong, Yang, Luo & Xu (2007a)	10.1107/S1600536807028061	EDUTUT
<i>(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)</i>	Zhong, Yang, Luo & Xu (2007b)	10.1107/S1600536807028693	RIGQEE
<i>(1,10-Phenanthroline-κ<sup>2</sup>N,N')tris(phenoxyacetato)-κO;κO;κO,O'-neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007c)	10.1107/S1600536807030371	UDUMEM
<i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(thiocyanato-κN)nickel(II)</i>	Zhong, Yang, Luo & Xu (2007d)	10.1107/S1600536807031613	YEJGOJ01
<i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(isothiocyanato-κN)copper(II)</i>	Zhong, Yang, Luo & Xu (2007e)	10.1107/S1600536807033181	UFAPOH
<i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(thiocyanato-κN)zinc(II)</i>	Zhong, Yang, Luo & Xu (2007f)	10.1107/S1600536807035337	TIGFAR
<i>(1,10-Phenanthroline-κ<sup>2</sup>N,N')tris(3-phenylpropanoato-κO)neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007g)	10.1107/S1600536807035350	TIGFEV
<i>2-Fluoro-3,5-dinitrobenzamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007j)	10.1107/S1600536807038676	VIKGAY
<i>2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007k)	10.1107/S1600536807039724	KILKIA
<i>1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007l)	10.1107/S1600536807040779	AFETAH
<i>N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007m)	10.1107/S160053680704086X	AFINAF
<i>catena-Poly[[bis(μ-anilinoacetato-κ<sup>2</sup>O:O')bis(μ-anilinoacetato-κ<sup>2</sup>O:O')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')samarium(III)]-μ-anilinoacetato-κ<sup>2</sup>O:O']</i>	Zhong, Yang, Xie & Luo (2007a)	10.1107/S1600536807043528	PILDAQ
<i>2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate</i>	Zhong, Yang, Xie & Luo (2007n)	10.1107/S1600536807045199	XILWIZ
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007b)	10.1107/S1600536807048489	WIMWEV
<i>Hexaaquacopper(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007c)	10.1107/S1600536807049525	TOLSCV01

**Table 1 (continued)**

Title	Reference	DOI	Refcode
<i>catena-Poly[[tetra-<math>\mu</math>-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-<math>\mu</math>-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007d)	10.1107/S1600536807051240	GIMZEI
<i>Hexaaquachromium(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007e)	10.1107/S1600536807051227	GIMZIM
<i>Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007f)	10.1107/S1600536807052051	QUKQES01
<i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')cobalt(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>	Zhong, Yang, Xie & Luo (2007g)	10.1107/S1600536807053494	NIQLAB
<i>Hexaaquanickel(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007a)	10.1107/S1600536807054372	HIPZOW
<i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')copper(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>	Zhong, Yang, Xie & Luo (2007h)	10.1107/S160053680705622X	XIRGOV
<i>Hexaaquazinc(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007b)	10.1107/S1600536807056498	XIRJEO
<i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')nickel(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>	Zhong, Yang, Xie & Luo (2007i)	10.1107/S1600536807058540	HIQJOH
<i>Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
<i>catena-Poly[[tetra-<math>\mu</math>-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-<math>\mu</math>-anilinoacetato]</i>	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
<i>(Dimethylglyoxime-<math>\kappa^2</math>N,N')bis(1,10-phenanthroline-<math>\kappa^2</math>N,N')copper(II) dinirate dihydrate</i>	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
<i>catena-Poly[(1,10-phenanthroline-<math>\kappa^2</math>N,N')praseodymium(III)]-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^4</math>O:O'-[(1,10-phenanthroline-<math>\kappa^2</math>N,N')praseodymium(III)]-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^4</math>O:O'-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^3</math>O,O':<math>\kappa^3</math>O:O,O']</i>	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

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## Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)

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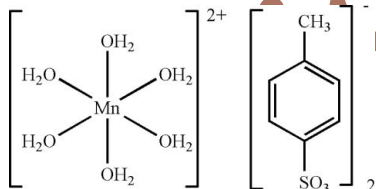
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Key indicators: single-crystal X-ray study;  $T = 273$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.041;  $wR$  factor = 0.117; data-to-parameter ratio = 13.4.

The asymmetric unit of the title compound,  $[\text{Mn}(\text{H}_2\text{O})_6] \cdot (\text{C}_7\text{H}_7\text{O}_3\text{S})_2$ , contains one half-cation and one anion; the Mn atom lies on an inversion centre. In the crystal structure, intermolecular  $\text{O}-\text{H} \cdots \text{O}$  and  $\text{O}-\text{H} \cdots \text{S}$  hydrogen bonds result in the formation of a supramolecular network structure; an intramolecular  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bond is also present.

## Related literature

For a related structure, see: Zhong *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



## Experimental

## Crystal data

$[\text{Mn}(\text{H}_2\text{O})_6] \cdot (\text{C}_7\text{H}_7\text{O}_3\text{S})_2$   
 $M_r = 505.41$   
Monoclinic,  $P2_1/n$   
 $a = 7.002$  (2) Å  
 $b = 6.0153$  (17) Å  
 $c = 24.9011$  (11) Å  
 $\beta = 90.997$  (5)°

$V = 1048.7$  (4) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.89$  mm<sup>-1</sup>  
 $T = 273$  (2) K  
 $0.48 \times 0.37 \times 0.20$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.673$ ,  $T_{\max} = 0.845$

6632 measured reflections  
2110 independent reflections  
1829 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.118$   
 $S = 1.00$   
2110 reflections  
158 parameters  
9 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.41$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.46$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Mn1—O1	2.046 (2)	Mn1—O3	2.027 (2)
Mn1—O2	1.944 (2)		
O1 <sup>i</sup> —Mn1—O1	180	O2—Mn1—O2 <sup>i</sup>	180
O1—Mn1—O2	89.54 (11)	O2—Mn1—O3 <sup>i</sup>	89.97 (11)
O1 <sup>i</sup> —Mn1—O2	90.46 (11)	O2—Mn1—O3	90.03 (11)
O1 <sup>i</sup> —Mn1—O3	87.34 (14)	O3 <sup>i</sup> —Mn1—O3	180
O1—Mn1—O3	92.66 (14)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C3—H3 <sup>⋯</sup> O5	0.93	2.56	2.894 (5)	102
O3—H3A <sup>⋯</sup> S1 <sup>ii</sup>	0.853 (19)	3.00 (3)	3.798 (3)	157 (3)
O1—H1B <sup>⋯</sup> O5 <sup>ib</sup>	0.84 (4)	1.95 (2)	2.781 (3)	170 (5)
O1—H1B <sup>⋯</sup> S1 <sup>iii</sup>	0.84 (4)	2.98 (2)	3.779 (3)	158 (3)
O2—H2B <sup>⋯</sup> O6 <sup>iv</sup>	0.87 (4)	1.92 (3)	2.724 (3)	154 (5)
O3—H3B <sup>⋯</sup> O5 <sup>iv</sup>	0.865 (19)	1.90 (2)	2.756 (3)	171 (4)
O1—H1A <sup>⋯</sup> O4 <sup>v</sup>	0.814 (18)	1.861 (18)	2.674 (3)	177 (4)
O2—H2A <sup>⋯</sup> O4 <sup>iii</sup>	0.877 (19)	1.90 (2)	2.770 (3)	173 (4)
O3—H3A <sup>⋯</sup> O6 <sup>ii</sup>	0.853 (19)	1.84 (2)	2.669 (3)	164 (4)

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Siemens, 1996); 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: HK2348).

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**supplementary materials**

**Article retracted**

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## Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)

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### Comment

The crystal structure of hexaaquacopper(II) bis(4-methylbenzenesulfonate), (II), has previously been reported (Zhong *et al.*, 2007). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We report herein the crystal structure of (I).

The asymmetric unit of the title compound, (I), (Fig. 1) contains one half-cation and one anion; the Mn atom lies on an inversion centre, as in (II). The bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987).

In the crystal structure, intermolecular O—H $\cdots$ O and O—H $\cdots$ S hydrogen bonds (Fig. 2 and Table 2) result in the formation of a supramolecular network structure; an intramolecular C—H $\cdots$ O hydrogen bond is also present, as in (II).

The both compounds, (I) and (II), are isostructural.

### Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Lanthanum (III) nitrate hexahydrate (216.4 mg, 0.5 mmol), manganous nitrate hexahydrate (143.5 mg, 0.5 mmol), 4-methylbenzenesulfonic acid (344.4 mg, 2 mmol), ammonia (0.5 mol/l, 4 ml) and distilled water (10 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

### Refinement

H atoms (for H<sub>2</sub>O) were located in difference syntheses and refined isotropically [O—H = 0.814 (18)–0.877 (19) Å and  $U_{\text{iso}}(\text{H}) = 0.065 (10) - 0.11 (2) \text{Å}^2$ ]. The remaining H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å, for aromatic and methyl H atoms and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$ , where  $x = 1.2$  for aromatic H and  $x = 1.5$  for methyl H atoms.

### Figures

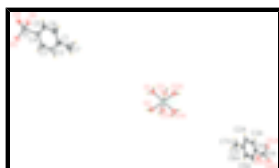


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A):  $3/2 - x, 1/2 - y, 1/2 - z$ ].

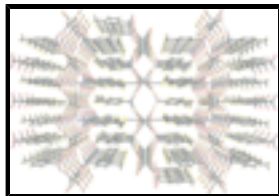


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

**Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)**

*Crystal data*

$[\text{Mn}(\text{H}_2\text{O})_6](\text{C}_7\text{H}_7\text{O}_3\text{S})_2$

$M_r = 505.41$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2yn$

$a = 7.002\ (2)\ \text{\AA}$

$b = 6.0153\ (17)\ \text{\AA}$

$c = 24.9011\ (11)\ \text{\AA}$

$\beta = 90.997\ (5)^\circ$

$V = 1048.7\ (4)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 526$

$D_x = 1.601\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5239 reflections

$\theta = 2.5\text{--}27.8^\circ$

$\mu = 0.89\ \text{mm}^{-1}$

$T = 273\ (2)\ \text{K}$

Prism, colorless

$0.48 \times 0.37 \times 0.20\ \text{mm}$

*Data collection*

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273\ (2)\ \text{K}$

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\text{min}} = 0.673$ ,  $T_{\text{max}} = 0.845$

6632 measured reflections

2110 independent reflections

1829 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\text{max}} = 26.5^\circ$

$\theta_{\text{min}} = 3.3^\circ$

$h = -8 \rightarrow 8$

$k = -6 \rightarrow 7$

$l = -31 \rightarrow 30$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.118$

$S = 1.01$

2110 reflections

158 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 0.7242P]$

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

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

$\Delta\rho_{\text{max}} = 0.41\ \text{e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.46\ \text{e \AA}^{-3}$

9 restraints

Extinction correction: none

Primary atom site location: structure-invariant direct methods

*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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.5000	0.0000	0.0000	0.03519 (19)
S1	-0.01448 (10)	0.60823 (11)	0.90523 (3)	0.0493 (2)
O1	0.7232 (4)	-0.1027 (4)	0.04798 (13)	0.0811 (8)
O2	0.5084 (3)	0.2890 (4)	0.03489 (11)	0.0634 (6)
O3	0.3032 (4)	-0.1043 (4)	0.05314 (13)	0.0820 (8)
O4	0.1537 (4)	0.5144 (3)	0.93043 (10)	0.0625 (6)
O5	-0.0142 (3)	0.8389 (4)	0.90908 (9)	0.0620 (6)
O6	-0.1915 (4)	0.5171 (3)	0.92383 (10)	0.0633 (6)
C1	0.0132 (6)	0.4349 (8)	0.72946 (15)	0.0735 (10)
C2	-0.0456 (6)	0.6327 (8)	0.74479 (16)	0.0821 (11)
H2	-0.0830	0.7356	0.7188	0.099*
C3	-0.0533 (6)	0.6926 (7)	0.79872 (15)	0.0717 (9)
H3	-0.0932	0.8344	0.8083	0.086*
C4	-0.0031 (4)	0.5457 (5)	0.83685 (13)	0.0539 (7)
C5	0.0530 (6)	0.3421 (6)	0.82199 (14)	0.0675 (9)
H5	0.0860	0.2363	0.8478	0.081*
C6	0.0614 (6)	0.2917 (8)	0.76891 (16)	0.0795 (11)
H6	0.1027	0.1505	0.7593	0.095*
C7	0.0320 (8)	0.3697 (11)	0.67176 (17)	0.1042 (16)
H7A	-0.0156	0.4874	0.6492	0.156*
H7B	-0.0403	0.2368	0.6649	0.156*
H7C	0.1640	0.3432	0.6642	0.156*
H1A	0.762 (5)	-0.228 (3)	0.0533 (13)	0.065 (10)*
H2A	0.616 (4)	0.343 (7)	0.0478 (17)	0.088 (13)*
H3A	0.258 (5)	-0.236 (3)	0.0545 (18)	0.100 (15)*
H1B	0.804 (5)	-0.022 (5)	0.0643 (17)	0.088 (14)*
H2B	0.432 (5)	0.385 (8)	0.049 (2)	0.11 (2)*
H3B	0.204 (4)	-0.030 (5)	0.0628 (19)	0.093 (15)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mn1	0.0354 (3)	0.0223 (3)	0.0479 (3)	0.00068 (18)	0.0018 (2)	0.00160 (19)
S1	0.0511 (4)	0.0356 (4)	0.0614 (4)	0.0005 (3)	0.0032 (3)	-0.0004 (3)
O1	0.0832 (17)	0.0386 (13)	0.120 (2)	0.0051 (12)	-0.0439 (16)	0.0007 (13)
O2	0.0578 (13)	0.0417 (12)	0.0908 (17)	-0.0012 (10)	0.0045 (12)	-0.0127 (11)
O3	0.0897 (18)	0.0395 (13)	0.119 (2)	0.0000 (12)	0.0508 (16)	0.0046 (13)
O4	0.0699 (14)	0.0449 (12)	0.0722 (14)	0.0046 (10)	-0.0104 (11)	-0.0025 (10)
O5	0.0668 (13)	0.0354 (10)	0.0839 (15)	-0.0008 (9)	0.0060 (11)	-0.0021 (10)
O6	0.0673 (14)	0.0443 (12)	0.0788 (15)	-0.0044 (9)	0.0176 (11)	-0.0028 (10)
C1	0.065 (2)	0.094 (3)	0.061 (2)	-0.008 (2)	0.0023 (16)	0.0021 (19)
C2	0.083 (3)	0.095 (3)	0.069 (2)	0.008 (2)	0.0002 (19)	0.022 (2)
C3	0.076 (2)	0.066 (2)	0.074 (2)	0.0121 (17)	0.0065 (17)	0.0151 (18)
C4	0.0478 (15)	0.0483 (16)	0.0657 (18)	-0.0001 (12)	0.0015 (13)	0.0049 (13)
C5	0.087 (2)	0.0522 (19)	0.0629 (18)	0.0116 (17)	-0.0012 (16)	-0.0034 (15)
C6	0.086 (3)	0.077 (3)	0.076 (2)	0.008 (2)	0.0029 (19)	-0.017 (2)
C7	0.097 (3)	0.146 (5)	0.069 (2)	-0.005 (3)	0.008 (2)	-0.007 (3)

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

Mn1—O1	2.046 (2)	O3—H3B	0.865 (19)
Mn1—O2	1.944 (2)	C1—C2	1.318 (6)
Mn1—O3	2.027 (2)	C1—C6	1.345 (6)
Mn1—O2 <sup>i</sup>	1.944 (2)	C1—C7	1.497 (6)
Mn1—O3 <sup>i</sup>	2.026 (2)	C2—C3	1.392 (6)
Mn1—O1 <sup>i</sup>	2.046 (2)	C2—H2	0.9300
S1—O5	1.391 (2)	C3—C4	1.339 (5)
S1—O6	1.439 (2)	C3—H3	0.9300
S1—O4	1.440 (2)	C4—C5	1.341 (5)
S1—C4	1.747 (3)	C5—C6	1.358 (5)
O1—H1A	0.814 (18)	C5—H5	0.9300
O1—H1B	0.84 (4)	C6—H6	0.9300
O2—H2A	0.877 (19)	C7—H7A	0.9600
O2—H2B	0.87 (4)	C7—H7B	0.9600
O3—H3A	0.853 (19)	C7—H7C	0.9600
O1 <sup>i</sup> —Mn1—O1	180	H3A—O3—H3B	100 (2)
O1—Mn1—O2	89.54 (11)	C2—C1—C6	116.2 (4)
O1 <sup>i</sup> —Mn1—O2	90.46 (11)	C2—C1—C7	123.2 (4)
O1 <sup>i</sup> —Mn1—O3	87.34 (14)	C6—C1—C7	120.5 (5)
O1—Mn1—O3	92.66 (14)	C1—C2—C3	122.0 (4)
O2—Mn1—O2 <sup>i</sup>	180	C1—C2—H2	119.0
O2—Mn1—O3 <sup>i</sup>	89.97 (11)	C3—C2—H2	119.0
O2—Mn1—O3	90.03 (11)	C4—C3—C2	119.9 (4)
O3 <sup>i</sup> —Mn1—O3	180	C4—C3—H3	120.0
O2 <sup>i</sup> —Mn1—O3 <sup>i</sup>	90.03 (11)	C2—C3—H3	120.0



O1 <sup>i</sup> —Mn1—O2 <sup>i</sup>	89.54 (11)	C3—C4—C5	118.8 (3)
O1 <sup>i</sup> —Mn1—O3 <sup>i</sup>	92.66 (14)	C3—C4—S1	122.2 (3)
O5—S1—O6	110.95 (14)	C5—C4—S1	119.0 (3)
O5—S1—O4	111.15 (14)	C4—C5—C6	119.3 (3)
O6—S1—O4	114.40 (15)	C4—C5—H5	120.3
O5—S1—C4	106.39 (15)	C6—C5—H5	120.3
O6—S1—C4	106.60 (15)	C1—C6—C5	123.6 (4)
O4—S1—C4	106.84 (15)	C1—C6—H6	118.2
Mn1—O1—H1A	129 (2)	C5—C6—H6	118.2
Mn1—O1—H1B	127 (3)	C1—C7—H7A	109.5
H1A—O1—H1B	104 (3)	C1—C7—H7B	109.5
Mn1—O2—H2A	121 (3)	H7A—C7—H7B	109.5
Mn1—O2—H2B	140 (3)	C1—C7—H7C	109.5
H2A—O2—H2B	98 (3)	H7A—C7—H7C	109.5
Mn1—O3—H3A	125 (3)	H7B—C7—H7C	109.5
Mn1—O3—H3B	125 (3)		

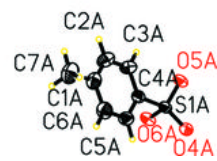
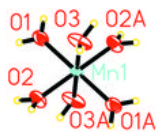
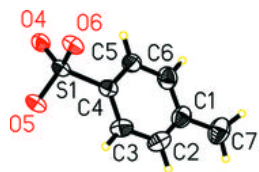
Symmetry codes: (i)  $-x+1, -y, -z$ .

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C3—H3...O5	0.93	2.56	2.894 (5)	102
O3—H3A...S1 <sup>ii</sup>	0.853 (19)	3.00 (3)	3.798 (3)	157 (3)
O1—H1B...O5 <sup>iii</sup>	0.84 (4)	1.95 (2)	2.781 (3)	170 (5)
O1—H1B...S1 <sup>iii</sup>	0.84 (4)	2.98 (2)	3.779 (3)	158 (3)
O2—H2B...O6 <sup>iv</sup>	0.87 (4)	1.92 (3)	2.724 (3)	154 (5)
O3—H3B...O5 <sup>iv</sup>	0.865 (19)	1.90 (2)	2.756 (3)	171 (4)
O1—H1A...O4 <sup>v</sup>	0.814 (18)	1.861 (18)	2.674 (3)	177 (4)
O2—H2A...O4 <sup>iii</sup>	0.877 (19)	1.90 (2)	2.770 (3)	173 (4)
O3—H3A...O6 <sup>ii</sup>	0.853 (19)	1.84 (2)	2.669 (3)	164 (4)

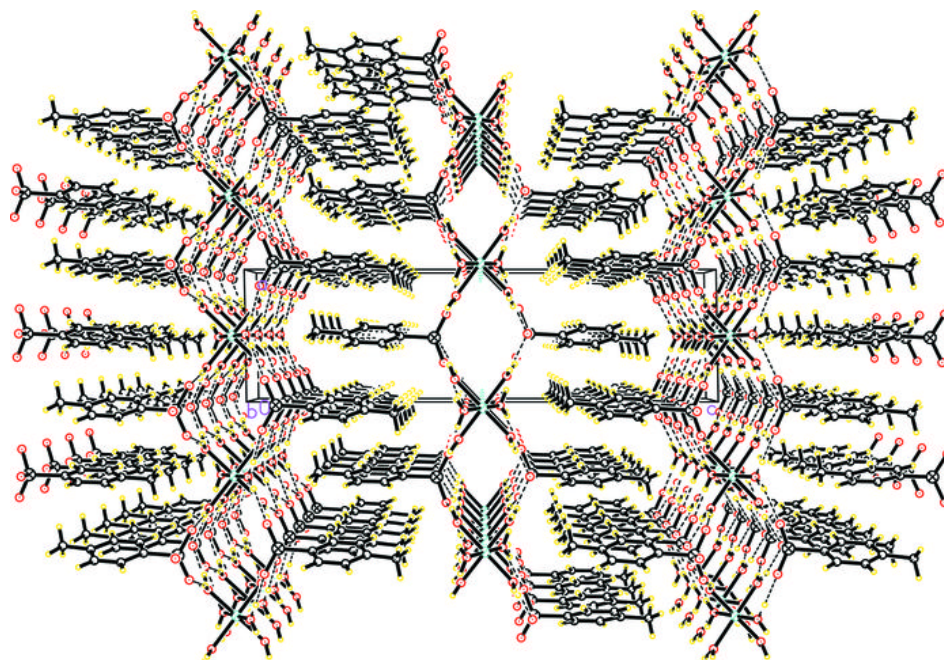
Symmetry codes: (ii)  $-x, -y, -z+1$ ; (iii)  $-x+1, -y+1, -z+1$ ; (iv)  $-x, -y+1, -z+1$ ; (v)  $-x+1, -y, -z+1$ .

Fig. 1



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Fig. 2



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