

Yi-Min Zhu, Kai-Long Zhong and  
Wen-Jie Lu\*Department of Chemical and Environmental  
Engineering, Wuyi University, Jiangmen,  
Guangdong Province, People's Republic  
of ChinaCorrespondence e-mail:  
wjlu\_56@yahoo.com.cn

## Key indicators

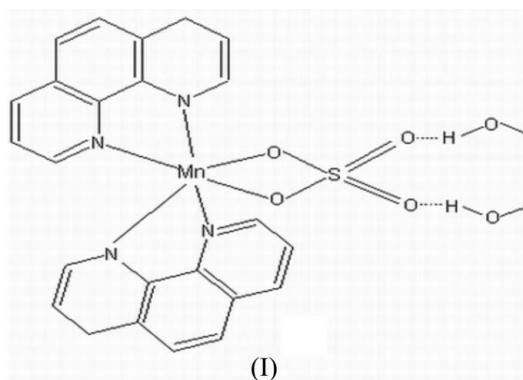
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
Disorder in solvent or counterion  
 $R$  factor = 0.040  
 $wR$  factor = 0.112  
Data-to-parameter ratio = 12.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis(1,10-phenanthroline- $\kappa^2N,N'$ )(sulfato- $\kappa^2O,O'$ )-  
manganese(II) ethene-1,2-diol solvate

In the title compound,  $[\text{Mn}(\text{SO}_4)(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot \text{C}_2\text{H}_6\text{O}_2$ , the Mn atom has a distorted octahedral coordination composed of four N atoms from two phenanthroline groups and two O atoms from a bidentate sulfate ligand. The formula unit lies on a special position of site symmetry 2. Intermolecular O—H $\cdots$ O hydrogen bonds help to stabilize the structure.

Received 14 September 2006  
Accepted 18 September 2006

## Comment

Mn–phen complexes with monodentate sulfate ligands (Zheng & Lin, 2001; Zheng *et al.* 2002), and with bidentate bridging sulfate ligands (Zheng & Lin, 2003) have been synthesized and characterized structurally by X-ray diffraction. The title complex, (I), which is isomorphous with the recently reported cobalt(II) and cadmium(II) structures (Zhong *et al.*, 2006; Lu *et al.*, 2006), represents another such complex. A twofold rotation axis passes through the Mn and S atoms, and through the mid-point of the solvent C—C bond. In the complex molecule, each Mn<sup>II</sup> centre has a distorted octahedral coordination composed of four N atoms from two phenanthroline groups and two O atoms from a bidentate sulfate ligand (Table 1). The geometry of the phen and sulfate ligands is in good agreement with those reported in the two isomorphous complexes  $[\text{Co}(\text{SO}_4)(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot \text{C}_2\text{H}_6\text{O}_2$  (Zhong *et al.*, 2006) and  $[\text{Cd}(\text{SO}_4)(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot \text{C}_2\text{H}_6\text{O}_2$  (Lu *et al.*, 2006).



A pair of symmetry-related intermolecular O—H $\cdots$ O hydrogen bonds stabilizes the structure (Table 2 and Fig. 1).

## Experimental

Compound (I), as pale-red block-shaped crystals, was obtained by a procedure similar to that described previously by Zhong *et al.* (2006), using  $\text{MnSO}_4 \cdot \text{H}_2\text{O}$  instead of  $\text{CoSO}_4 \cdot 7\text{H}_2\text{O}$ .

## Crystal data

[Mn(SO<sub>4</sub>)(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>]-C<sub>2</sub>H<sub>6</sub>O<sub>2</sub> $M_r = 573.48$ Monoclinic,  $C2/c$  $a = 18.480$  (2) Å $b = 12.0337$  (13) Å $c = 12.9824$  (14) Å $\beta = 120.094$  (2)° $V = 2497.9$  (5) Å<sup>3</sup> $Z = 4$  $D_x = 1.525$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation $\mu = 0.66$  mm<sup>-1</sup> $T = 293$  (2) K

Block, pale red

 $0.33 \times 0.30 \times 0.21$  mm

## Data collection

Bruker SMART CCD 1K area-detector diffractometer

 $\varphi$  and  $\omega$  scans

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

 $T_{\min} = 0.811$ ,  $T_{\max} = 0.873$ 

6594 measured reflections

2204 independent reflections

1761 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.034$  $\theta_{\text{max}} = 25.0^\circ$ 

## Refinement

Refinement on  $F^2$  $R[F^2 > 2\sigma(F^2)] = 0.040$  $wR(F^2) = 0.112$  $S = 1.05$ 

2204 reflections

182 parameters

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 2.7949P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} < 0.001$  $\Delta\rho_{\text{max}} = 0.53$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.32$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Mn1—O1	2.198 (2)	S1—O1	1.480 (2)
Mn1—N1	2.252 (2)	C13—O3	1.360 (6)
Mn1—N2	2.257 (2)	C13—C13 <sup>i</sup>	1.503 (5)
S1—O2	1.438 (2)		
O1—Mn1—O1 <sup>i</sup>	63.94 (11)	O1 <sup>i</sup> —S1—O1	103.71 (18)
N1—Mn1—N2	73.94 (9)	O3—C13—C13 <sup>i</sup>	112.2 (5)
O2 <sup>i</sup> —S1—O2	109.7 (2)		

Symmetry code: (i)  $-x + 1, y, -z + \frac{3}{2}$ .

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 <sup>i</sup> ···O2	0.82	2.01	2.782 (9)	157
O3 <sup>i</sup> —H3 <sup>i</sup> ···O2	0.82	2.15	2.673 (9)	122

The aromatic H atoms were positioned geometrically and allowed to ride on their parent atoms, with  $C-H = 0.93$  Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The H atoms of ethene-1,2-diol were located in a difference map and then allowed to ride on their parent atoms, with  $C-H = 0.97$  Å and  $O-H = 0.82$  Å;  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  and  $1.5U_{\text{eq}}(\text{O})$ . The ethane-1,2-diol molecule is disordered over two positions, sharing a common atom C13; O3, O3', H3 and H3' each have site occupancy factors of 0.5.

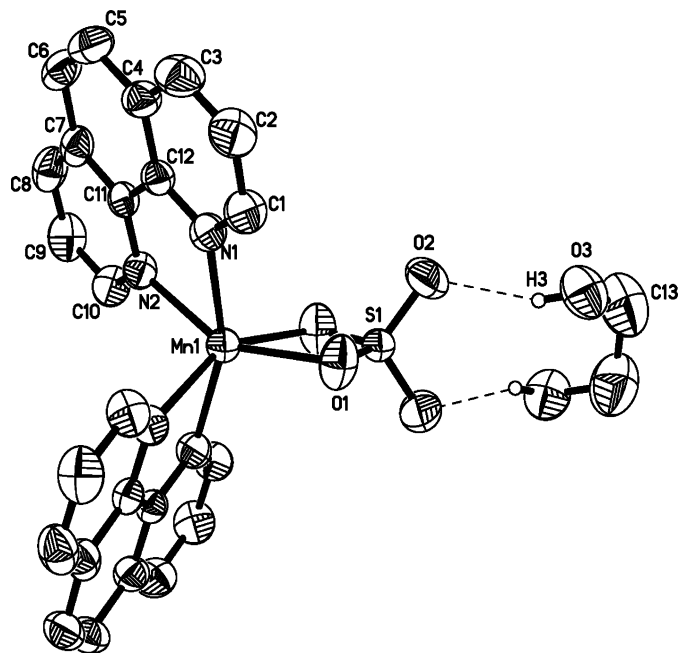


Figure 1

The molecular structure of (I), showing the atom-numbering scheme and with displacement ellipsoids drawn at the 50% probability level. The dashed lines represent  $O-H\cdots O$  interactions. H atoms not involved in hydrogen bonds have been omitted for clarity. Only one disorder is shown. [Symmetry code for unlabelled atoms:  $1 - x, y, \frac{3}{2} - z$ .]

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

X-ray data were collected at the Chinese University of Hong Kong.

## References

- Bruker (1998). SMART, SAINT and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
- Lu, W.-J., Zhong, K.-L. & Zhu, Y.-M. (2006). Acta Cryst. E62, m891–m893.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Zheng, Y. Q. & Lin, J. L. (2001). Z. Kristallogr. New Cryst. Struct. 216, 353–356.
- Zheng, Y. Q. & Lin, J. L. (2003). Z. Anorg. Allg. Chem. 629, 185–187.
- Zheng, Y. Q., Sun, J. & Lin, J. L. (2002). Z. Kristallogr. New Cryst. Struct. 217, 189–191.
- Zhong, K.-L., Zhu, Y.-M. & Lu, W.-J. (2006). Acta Cryst. E62, m631–m633.