Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

catena-Poly[[*cis*-diaqua(1,10-phenanthroline-κ^2N,N')-manganese(II)]-μ_2-5-sulfonatosalicylato-κ^2O:O']

Sai-Rong Fan and Long-Guan Zhu*

Department of Chemistry, Zhejiang University, Hangzhou 310027, People's Republic of China

Correspondence e-mail: chezlg@zju.edu.cn

Received 31 May 2005
Accepted 6 June 2005
Online 10 June 2005

Key indicators

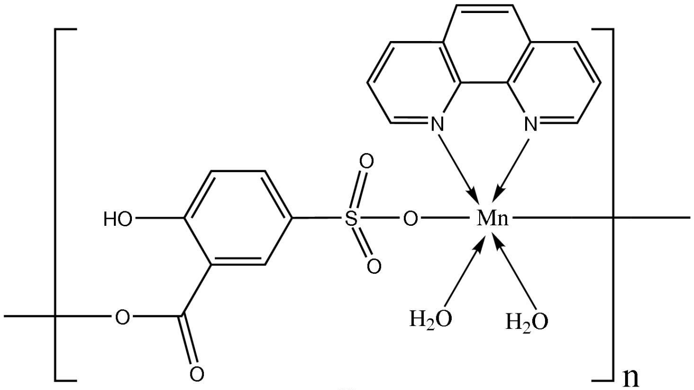
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.084
Data-to-parameter ratio = 13.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title complex, $[Mn(C_7H_4O_6S)(C_{12}H_8N_2)(H_2O)_2]_n$, comprises a one-dimensional chain in which each Mn atom displays a distorted octahedral geometry. Hydrogen-bonding interactions between chains generate a two-dimensional architecture.

Comment

Recently, much attention has been paid to metal complexes of 5-sulfosalicylic acid (H_3ssal) because of the structural diversity and biological interest of this ligand (Fan, Cai *et al.*, 2005; Gao *et al.*, 2005; Fan, Zhu *et al.*, 2005*a*). In our previous work on the manganese(II) 1,10-phenanthroline (phen) complex $[Mn(phen)_2(H_2O)_2](Hssal)\cdot 4H_2O$, (II), the doubly deprotonated 5-sulfosalicylate does not coordinate to the metal atom (Fan, Zhu *et al.*, 2005*b*), partly because the phen ligand can strongly chelate to the metal atom. Therefore, a new synthetic procedure, a two-step reaction method, was introduced to the Mn^{2+}/H_3ssal/phen system and, as expected, the $Hssal^{2-}$ coordinated complex, (I), was synthesized.



(I)

In the title complex, the Mn^{II} atom adopts a distorted octahedral geometry defined by two N donors from one phen ligand, two O atoms from two *cis* water molecules and two O atoms, one from a sulfonyl and one from a carboxyl group of two different $Hssal^{2-}$ ligands (Fig. 1 and Table 1). The Mn—N and Mn—O*w* distances are similar to those of (II). The 5-sulfonatosalicylate ligand acts as a linker using one sulfonyl and one carboxyl O atom to extend the structure into a one-dimensional chain (Fig. 2). Hydroxy and uncoordinated carboxyl O atoms form intrachain hydrogen bonds with a carboxyl group and a water molecule, respectively. Between chains, water molecules and sulfonyl O atoms form intermolecular hydrogen bonds, generating a two-dimensional hydrogen-bonding network (Fig. 3 and Table 2).

Comparison of (II), $[Mn(phen)_2(H_2O)_2]^{2+}$, with (I), $[Mn(phen)(H_2O)_2(Hssal)]$, shows that one phen ligand in II is replaced by an $Hssal^{2-}$ ligand in (I). Two such diverse structures were constructed by different synthetic procedures. For (II), a one-pot synthesis was used, while for (I), a two-step reaction method was used, *i.e.* phen was added after the metal salt had completely reacted with 5-sulfosalicylic acid in the presence of a weak base. Therefore, multi-step reactions are very useful in the construction of different architectures.

Experimental

A mixture of $MnCl_2·4H_2O$ (0.199 g, 1.0 mmol), 5-sulfosalicylic acid dihydrate (0.050 g, 0.20 mmol), and 4% pyridine (2 ml) in water (20 ml) was stirred for 17 h. 1,10-Phenanthroline (0.040 g, 0.20 mmol) was then added. The resulting solution was put aside and the solvent was allowed to evaporate at room temperature. After three weeks, pale-yellow block-shaped crystals were obtained.

Crystal data

$[Mn(C_7H_4O_6S)(C_{12}H_8N_2)(H_2O)_2]$
$M_r = 487.34$
Monoclinic, $P2_1/c$
$a = 14.4166$ (9) Å
$b = 7.7234$ (5) Å
$c = 18.6868$ (11) Å
$\beta = 107.421$ (1)°
$V = 1985.2$ (2) Å^3
$Z = 4$

$D_x = 1.631$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5871 reflections
$\theta = 2.3$–28.2°
$\mu = 0.82$ mm^{-1}
$T = 295$ (2) K
Block, pale yellow
0.43 × 0.25 × 0.16 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.719$, $T_{max} = 0.880$
10821 measured reflections

3888 independent reflections
3537 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 26.0°$
$h = -14 \rightarrow 17$
$k = -9 \rightarrow 9$
$l = -23 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.084$
$S = 1.07$
3888 reflections
295 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.5664P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1*w*	2.2316 (14)	Mn1—N2	2.2447 (15)
Mn1—O2*w*	2.1255 (14)	S1—O4	1.4595 (12)
Mn1—O2^i	2.1174 (13)	S1—O5	1.4479 (13)
Mn1—O4	2.1835 (12)	S1—O6	1.4627 (12)
Mn1—N1	2.2659 (15)		
O2^i—Mn1—O1*w*	88.61 (5)	O2*w*—Mn1—O1*w*	94.12 (5)
O2^i—Mn1—O2*w*	97.59 (6)	O2*w*—Mn1—N1	88.91 (6)
O2^i—Mn1—O4	81.49 (5)	O2*w*—Mn1—N2	162.63 (6)
O2^i—Mn1—N1	173.00 (6)	N2—Mn1—N1	73.76 (6)
O2^i—Mn1—N2	99.68 (6)	O5—S1—O4	113.94 (8)
O4—Mn1—O1*w*	169.86 (5)	O5—S1—O6	112.67 (8)
O4—Mn1—N1	96.03 (5)	O4—S1—O6	109.13 (7)
O4—Mn1—N2	91.36 (5)	O5—S1—C6	107.69 (8)
O1*w*—Mn1—N1	93.55 (5)	O4—S1—C6	105.45 (7)
O1*w*—Mn1—N2	88.13 (6)	O6—S1—C6	107.50 (8)
O2*w*—Mn1—O4	89.39 (5)		

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

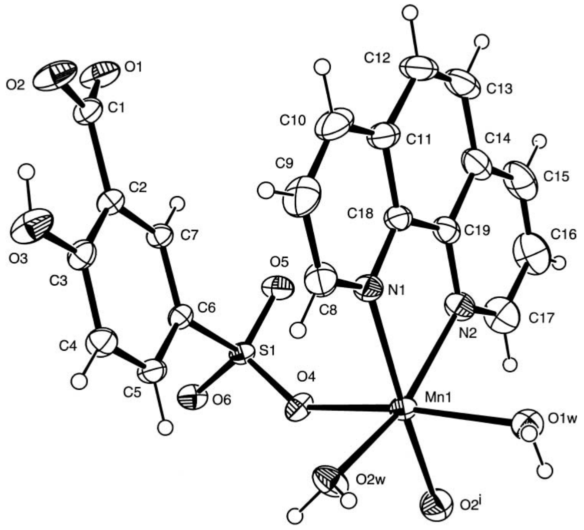


Figure 1
An *ORTEP-3* (Farrugia, 1997) view of a segment of (I). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $x, \frac{1}{2} - y, z - \frac{1}{2}$.]

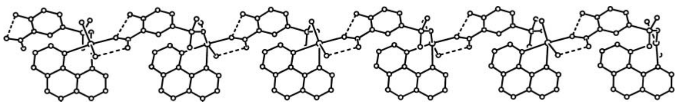


Figure 2
A view of the one-dimensional chain in (I). Hydrogen bonds are shown as dashed lines and H atoms have been omitted for clarity.

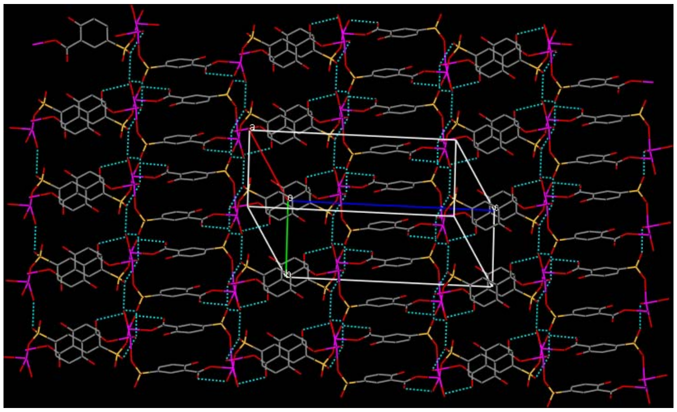


Figure 3
A view of the two-dimensional hydrogen-bonding (dashed lines) network for (I). The phen ligand and H atoms have been omitted for clarity.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*w*—H1*B*···O6^{ii}	0.84 (1)	1.89 (1)	2.7214 (18)	169 (2)
O1*w*—H1*A*···O5^{iii}	0.84 (1)	2.01 (1)	2.8233 (18)	163 (2)
O1*w*—H2*A*···O1^i	0.85 (1)	1.90 (1)	2.7076 (19)	158 (2)
O2*w*—H2*B*···O6^{iii}	0.84 (1)	1.88 (1)	2.7127 (17)	173 (2)
O3—H3*A*···O2	0.84 (1)	1.80 (1)	2.578 (2)	152 (2)

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

The aromatic H atoms were positioned geometrically, and were included in the refinement in the riding-model approximation [C—

H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C)]. The water and hydroxy H atoms were located in difference Fourier maps and were refined with a distance restraint of O—H = 0.85 (1) Å and fixed isotropic displacement parameters of $U_{\rm iso}$(H) = 0.05 Å^2.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We thank the National Natural Science Foundation of China (50073019).

References

Bruker (2002). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.

Fan, S. R., Cai, G. Q., Zhu, L. G. & Xiao, H. P. (2005). *Acta Cryst.* C**61**, m177–m179.

Fan, S. R., Zhu, L. G., Xiao, H. P. & Ng, S. W. (2005*a*). *Acta Cryst.* E**61**, m377–m378.

Fan, S. R., Zhu, L. G., Xiao, H. P. & Ng, S. W. (2005*b*). *Acta Cryst.* E**61**, m563–m565.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Gao, S., Zhu, Z. B., Huo, L. H. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m279–m281.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.