Bis(μ-3-sulfonatobenzoato)bis[bis(2,2′-bipyridine)-manganese(II)] dihydrate

Xiao-He Miao and Long-Guan Zhu*

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

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

The title centrosymmetric dimer, $[Mn_2(C_7H_4O_5S)_2(C_{10}H_8N_2)_4]\cdot 2H_2O$, was obtained by hydrothermal synthesis. The coordination geometry of the Mn^{II} atom is distorted octahedral, defined by four N atoms from two 2,2′-bipyridine ligands and two O atoms from two carboxylate groups of two μ-3-sulfonatobenzoate ligands. In the crystal structure, Mn^{II} complex molecules are linked, through water molecules, by intermolecular O—H···O hydrogen bonds, forming extended one-dimensional chains along $[1\bar{1}1]$.

Comment

Recently, sulfobenzoate–metal complexes have received much attention due to their interesting coordination modes and structural topologies (Ying & Mao, 2004; Miao & Zhu, 2006; Zhang, Zhu & Xiao, 2005; Zhang, Wang et al., 2005). The 4-sulfobenzoate(4-sb)/Mn^{II}/2,2′-bipyridine system produces a monomer, $[Mn(4\text{-sb})(2,2'\text{-bipy})(H_2O)_3]\cdot H_2O$, (II) (Zhang & Zhu, 2005), in which the carboxylate group acts in a chelating mode. Here, we present the dimeric manganese(II) complex with 3-sulfobenzoate (3-sb) as a ligand, (I).

(I)
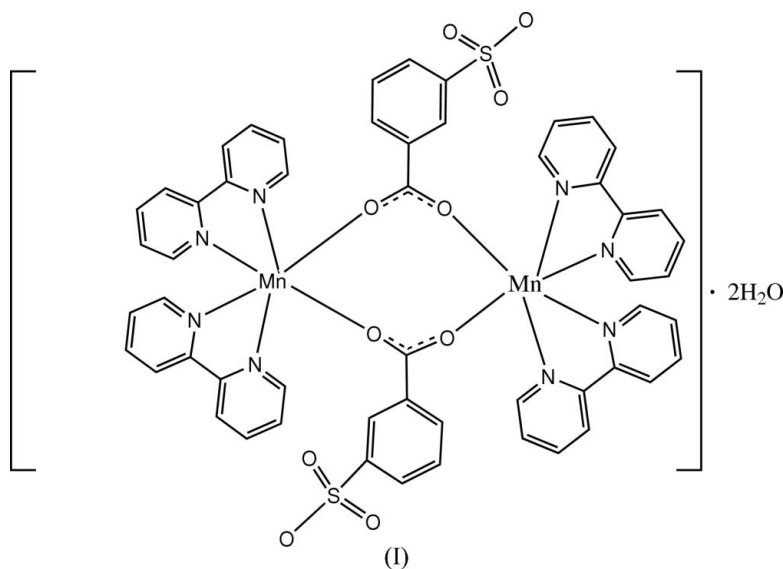
In (I), the unique Mn^{II} atom in the centrosymmetric dimer has a distorted octahedral geometry defined by two O donors from two carboxylate groups of two μ-3-sulfonatobenzoate ligands and four N atoms from two 2,2′-bipyridine ligands (Fig. 1 and Table 1). The coordination geometry of (I) is different from that of (II), in which the Mn^{II} atom adopts a seven-coordinate geometry. The Mn—O(carboxylate) and Mn—N distances in (I) (Table 1) are slightly shorter than those in (II). In the title compound, the carboxylate groups

bridge two Mn^{II} atoms and the sulfonyl group is uncoordinated. The carboxylate group forms a dihedral angle of 11.2 (3)° with the benzene ring to which it is attached. The dihedral angles between the two pyridine rings of the 2,2′-bipyridine ligands are 7.1 (2) and 9.7 (3)° for the ligands containing N1/N2 and N3/N4, respectively. In the crystal structure, dimeric complex molecules are linked, through water molecules, by intermolecular O—H···O hydrogen bonds, forming extended one-dimensional chains along [1$\bar{1}$1] (Fig. 2 and Table 2).

Experimental

A mixture of Mn(CH$_3$COO)$_2$·4H$_2$O (0.122 g, 0.5 mmol), sodium hydrogen 3-sulfobenzoate (0.112 g, 0.5 mmol), 2,2′-bipyridine (0.079 g, 0.5 mmol), and water (30 ml) was stirred and filtered; pale-yellow block crystals were obtained from the filtrate after one day.

Crystal data

[Mn$_2$(C$_7$H$_4$O$_5$S)$_2$(C$_{10}$H$_8$N$_2$)$_4$]·2H$_2$O
$M_r = 1170.97$
Triclinic, $P\bar{1}$
$a = 10.1223$ (15) Å
$b = 12.0573$ (17) Å
$c = 12.3757$ (18) Å
$\alpha = 62.927$ (2)°
$\beta = 79.505$ (2)°
$\gamma = 72.400$ (2)°

$V = 1280.2$ (3) Å^3
$Z = 1$
$D_x = 1.519$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.65$ mm^{-1}
$T = 295$ (2) K
Block, pale yellow
$0.17 \times 0.10 \times 0.10$ mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2002)
$T_{min} = 0.898$, $T_{max} = 0.938$

9370 measured reflections
4515 independent reflections
3553 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.153$
$S = 0.96$
4515 reflections
358 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0869P)^2 + 0.9109P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.97$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.104 (2)	Mn1—N4	2.262 (3)
Mn1—O2^i	2.126 (2)	S1—O3	1.422 (4)
Mn1—N1	2.268 (3)	S1—O4	1.451 (4)
Mn1—N2	2.259 (3)	S1—O5	1.428 (3)
Mn1—N3	2.304 (3)		
O1—Mn1—O2^i	101.61 (10)	N4—Mn1—N1	99.59 (11)
O1—Mn1—N2	101.14 (11)	O1—Mn1—N3	161.48 (11)
O2^i—Mn1—N2	96.64 (11)	O2^i—Mn1—N3	86.74 (11)
O1—Mn1—N4	91.86 (11)	N2—Mn1—N3	94.18 (11)
O2^i—Mn1—N4	88.72 (11)	N4—Mn1—N3	71.64 (12)
N2—Mn1—N4	164.60 (11)	N1—Mn1—N3	84.25 (11)
O1—Mn1—N1	90.50 (10)	O3—S1—O5	115.0 (3)
O2^i—Mn1—N1	165.13 (11)	O3—S1—O4	112.9 (3)
N2—Mn1—N1	72.31 (11)	O5—S1—O4	110.1 (2)

Symmetry code: (i) $-x + 1, -y + 1, -z$.
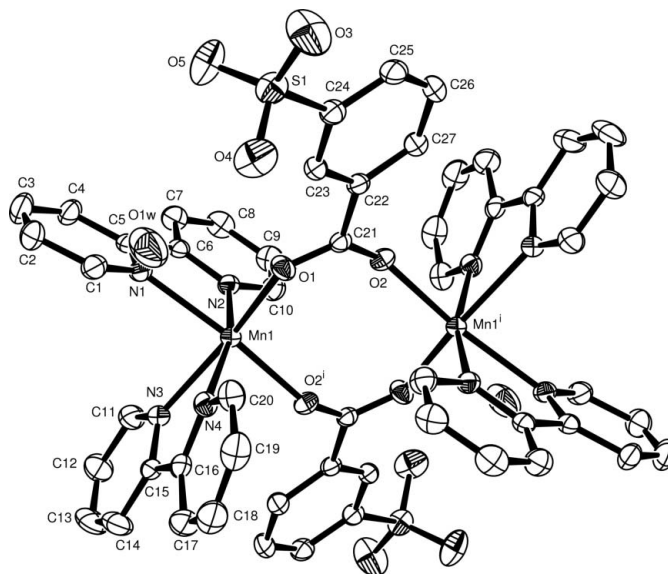
Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are omitted. [Symmetry code: (i) $1 - x, 1 - y, -z$.]
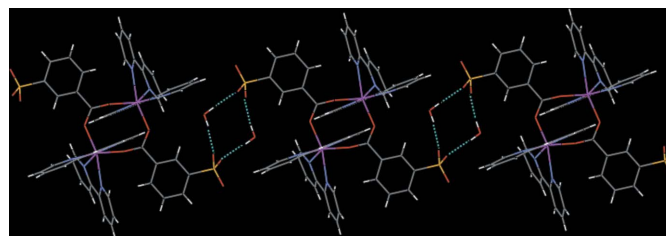
Figure 2
Part of the one-dimensional hydrogen-bonded chain of (I), propagating in the [1$\bar{1}$1] direction. Hydrogen bonds are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O4	0.85 (4)	2.13 (4)	2.956 (6)	165 (4)
O1W—H1B···O5^{ii}	0.85 (5)	1.98 (2)	2.793 (5)	161 (5)

Symmetry code: (ii) $-x + 2, -y, -z + 1$.

All C-bound H atoms were placed in calculated positions (C—H = 0.93 Å) and included in the riding-model approximation, and $U_{iso}(H) = 1.2U_{eq}(C)$. The water H atoms were located in a difference Fourier map and refined with restraints for O—H distances [0.85 (1) Å] and with $U_{iso}(H) = 0.08$ 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).

References

Bruker (2002). *SADABS* (Version 2.03), *SAINT* (Version 6.02a) and *SMART* (Version 5.618). Bruker AXS Inc., Madison, Wisconsin, USA.

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

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

Miao, X.-H. & Zhu, L.-G. (2006). *Acta Cryst.* E**62**, m548–m550.

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

Ying, S. M. & Mao, J. G. (2004). *Eur. J. Inorg. Chem.* pp. 1270–1276.

Zhang, L.-P. & Zhu, L.-G. (2005). *Acta Cryst.* E**61**, m1036–m1038.

Zhang, L.-P., Zhu, L.-G. & Xiao, H.-P. (2005). *Acta Cryst.* E**61**, m860–m862.

Zhang, W.-B., Wang, J.-G., Chen, H.-X. & Xiao, H.-P. (2005). *Acta Cryst.* E**61**, m2559–m2560.