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Aquabis(1,10-phenanthroline-κ^2N,N')(2-sulfobenzoato-κO)manganese(II) trihydrate

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In the title compound, $[Mn(C_7H_4O_5S)(C_{12}H_8N_2)_2(H_2O)]\cdot 3H_2O$, the Mn^{II} atom displays an octahedral MnN_4O_2 configuration, defined by four N atoms from two 1,10-phenanthroline ligands, one carboxyl O atom belonging to a 2-sulfobenzoate dianion and one aqua O atom. O—H···O hydrogen bonds involving 2-sulfobenzoate dianions, aqua ligands and uncoordinated water molecules link the mononuclear units into a three-dimensional network structure.

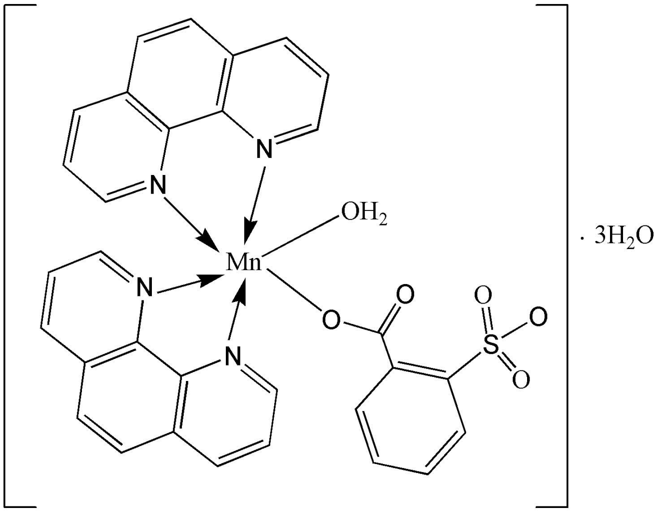
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.073
wR factor = 0.154
Data-to-parameter ratio = 12.7

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

Comment

The sulfonate group can exhibit very different coordination behaviour compared with the carboxyl group, in the construction of metal–organic coordination polymers (Fan *et al.*, 2004; Wang *et al.*, 2004; Zheng *et al.*, 2003). The 2-sulfobenzoic acid (o-H_2sb) ligand, containing one sulfonate group and one carboxyl group, is a good ligand for the preparation of metal–organic coordination polymers (Li & Yang, 2004; Su *et al.*, 2005; Xiao *et al.*, 2005). The title compound, (I) or $[Mn(phen)_2(o\text{-sb})(H_2O)]\cdot 3H_2O$ (phen is 1,10-phenanthroline and o-sb^{2-} is the 2-sulfobenzoate dianion), is an example of this.



(I)

In the molecule of (I), the Mn^{II} atom displays an octahedral MnN_4O_2 configuration, defined by four N atoms from two 1,10-phenanthroline ligands, one carboxyl O atom belonging to a 2-sulfobenzoate dianion and one aqua O atom (Fig. 1). The o-sb ligand coordinates to the Mn^{II} centre in monodentate mode. The dihedral angle between the planes of the o-sb ring and its carboxylate group is 126.8 (3)°, which is much larger than in the previously reported compound [Ni(o-sb)(bpe)-

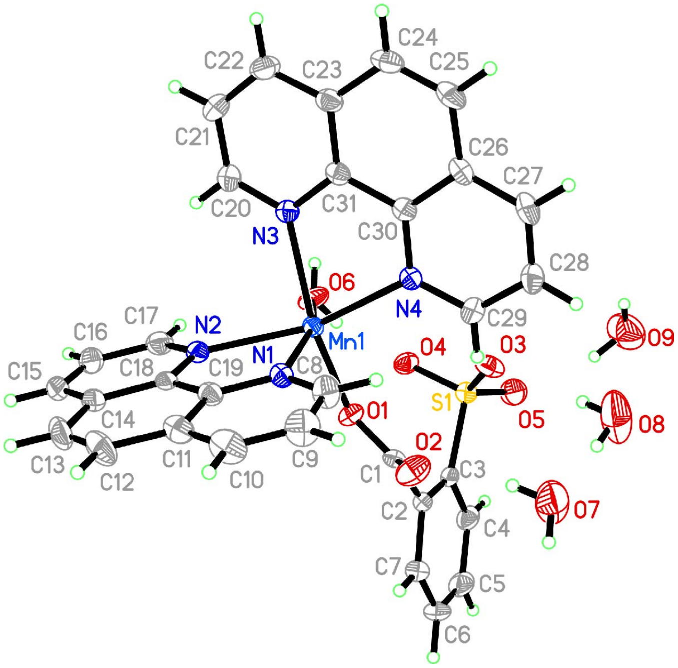


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

$(H_2O)_2]\cdot0.25H_2O$ [bpe = 1,2-bis(4-pyridyl)ethylene; Xiao *et al.*, 2005]. The dihedral angles between the benzene ring (C2–C7) of the *o*-sb ligand and the two phen ring systems are 87.7 (3) (C8–C19/N1/N2) and 93.4 (2)° (C20–C31/N3/N4), respectively. This indicates that the ring of the *o*-sb ligand is amost perpendicular to the two phen ligands.

O—H···O hydrogen bonds involving 2-sulfobenzoate dianions, aqua ligands and uncoordinated water molecules link the mononuclear units into a three-dimensional network structure (Table 1 and Fig. 2). These intermolecular hydrogen-bond interactions enhance the stability of the structure.

Experimental

The title compound was synthesized by the hydrothermal method from a mixture of 2-sulfobenzoic acid (0.5 mmol, 0.101 g), $Mn(CH_3COO)_2\cdot4H_2O$ (0.5 mmol, 0.125 g), 1,10-phenanthroline (1.0 mmol, 0.180 g) and water (8.0 ml) in a 15 ml Teflon-lined stainless steel reactor. The solution was heated at 423 K for 5 d. After completion of the reaction, the system was slowly cooled to room temperature and yellow crystals of (I) were collected.

Crystal data

$[Mn(C_7H_4O_5S)(C_{12}H_8N_2)_2(H_2O)]\cdot3H_2O$
$M_r = 687.57$
Triclinic, $P\overline{1}$
$a = 10.2204$ (11) Å
$b = 12.4047$ (13) Å
$c = 13.7842$ (15) Å
$\alpha = 106.505$ (2)°
$\beta = 94.417$ (2)°
$\gamma = 110.455$ (2)°
$V = 1539.4$ (3) Å^3
$Z = 2$
$D_x = 1.483$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1690 reflections
$\theta = 2.2$–21.1°
$\mu = 0.56$ mm^{-1}
$T = 298$ (2) K
Rod, yellow
0.39 × 0.18 × 0.16 mm

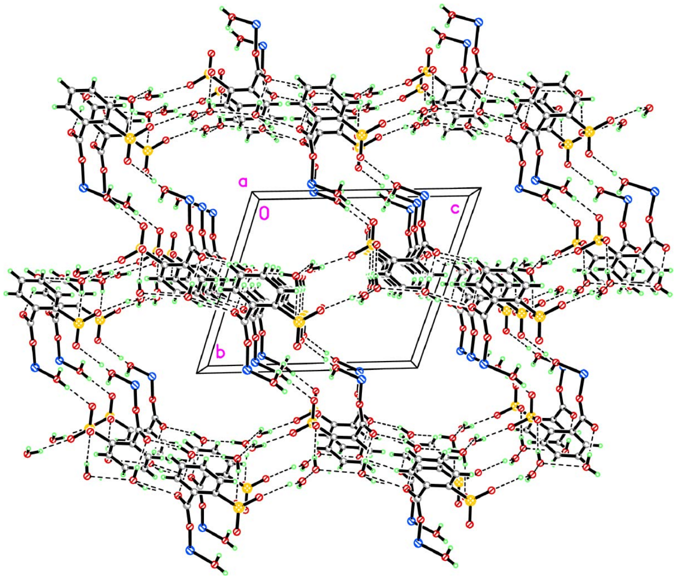


Figure 2
A view showing the hydrogen-bonding network structure of (I). For clarity, the 1,10-phenanthroline ligands have been omitted.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.812$, $T_{max} = 0.916$
11 511 measured reflections
5575 independent reflections
4185 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 25.3°$
$h = -12 \rightarrow 12$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.073$
$wR(F^2) = 0.154$
$S = 1.12$
5575 reflections
439 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.7094P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O9—H9B···O5	0.88 (4)	1.95 (4)	2.832 (6)	176 (4)
O9—H9A···O8^{i}	0.91 (4)	2.08 (3)	2.822 (8)	137 (4)
O8—H8B···O3	0.84 (4)	2.12 (2)	2.955 (6)	171 (5)
O8—H8A···O7	0.85 (2)	1.98 (2)	2.809 (7)	167 (5)
O7—H7B···O2	0.84 (2)	1.97 (3)	2.757 (6)	157 (5)
O7—H7A···O2^{ii}	0.85 (2)	2.05 (3)	2.858 (6)	158 (5)
O6—H6B···O4^{iii}	0.84 (2)	1.93 (2)	2.770 (4)	177 (5)
O6—H6A···O4	0.83 (4)	1.98 (2)	2.798 (4)	167 (5)

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

The H atoms of the water molecules were located in a difference map and were refined isotropically, with O—H distances restrained to 0.85 (5) Å and H···H distances to 1.39 (1) Å. H atoms attached to C atoms were introduced in calculated positions (C—H = 0.93 Å) and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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: *XP* in *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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