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Aquabis(1,10-phenanthroline)(3-sulfonatobenzoato)manganese(II) tetrahydrate

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Key indicators

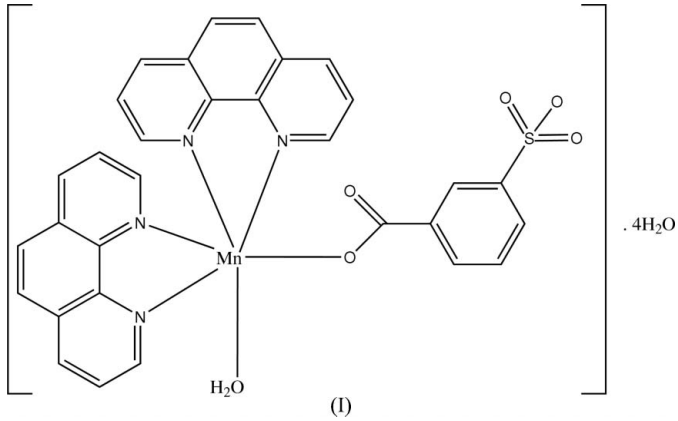
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.065
wR factor = 0.145
Data-to-parameter ratio = 12.6

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

The title compound, $[Mn(C_7H_4O_5S)(C_{12}H_8N_2)_2(H_2O)]\cdot 4H_2O$, which was obtained by the reaction of $MnCl_2$ with sodium hydrogen 3-sulfobenzoate and 1,10-phenanthroline, is a monomer. The coordination polyhedron of the Mn atom is a distorted octahedron. π–π Interactions between neighboring monomers and extensive hydrogen bonding consolidate the stability of the crystal structure.

Comment

Recently, 12 3-sulfobenzoate compounds have been synthesized in our laboratory and by other groups. These compounds include one organic complex (Adrabinska *et al.*, 2001) and 11 metal complexes in which the metal atoms include lead (Ying & Mao, 2004; Ma *et al.*, 2005; Zhu & Xiao, 2005), barium (Gao *et al.*, 2005), zinc (Li *et al.*, 2005; Zhang & Zhu, 2005), cadmium (Chen *et al.*, 2005; Miao & Zhu, 2006) and copper (Cai *et al.*, 2005; Cai & Zhu, 2005; Miao *et al.*, 2005). As part of an investigation on 3-sulfobenzoate metal complexes, a manganese 1,10-phenanthroline compound has been prepared, (I).



(I)

Compound (I) is a monomer, in which the Mn atom adopts a distorted octahedral geometry completed by four N-atom donors from two 1,10-phenanthroline, one O atom from one 3-sulfonatobenzoato, and one O atom from a water molecule (Fig. 1 and Table 1). The 3-sulfonatobenzoate ligand coordinates to the Mn atom in a monodentate manner *via* one O atoms of the carboxylate group. The carboxylate group is nearly coplanar with the benzene ring to which it is attached, forming a dihedral angle of 2.1 (3)°.

In neighboring monomers, there is a strong π–π interaction between 1,10-phenanthroline ligands, with a centroid-to-centroid distance of 3.497 (2) Å. Extensive hydrogen bonding between water molecules, and between water molecules and

sulfonyl groups, give rise to a three-dimensional network (Fig. 2).

Experimental

A mixture of $MnCl_2$ (0.032 g, 0.25 mmol), sodium hydrogen 3-sulfobenzoate (0.056 g, 0.25 mmol) and 1,10-phenanthroline (0.051 g, 0.25 mmol) in aqueous solution (20 ml) was stirred for 1 h and then filtered. The resulting solution was allowed to evaporate at room temperature. After 2 d, pale-yellow crystals were filtered off and washed with water.

Crystal data

$[Mn(C_7H_4O_5S)(C_{12}H_8N_2)_2(H_2O)]\cdot 4H_2O$
$M_r = 705.59$
Monoclinic, $C2/c$
$a = 33.549$ (7) Å
$b = 8.1406$ (15) Å
$c = 23.584$ (4) Å
$\beta = 90.032$ (8)°
$V = 6441$ (2) Å^3
$Z = 8$
$D_x = 1.455$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.54$ mm^{-1}
$T = 295$ (2) K
Block, pale yellow
0.33 × 0.21 × 0.14 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.843$, $T_{max} = 0.929$
16479 measured reflections
5733 independent reflections
5039 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.145$
$S = 1.16$
5733 reflections
454 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 13.5505P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.095 (2)	Mn1—N1	2.295 (3)
Mn1—O6	2.165 (3)	S1—O4	1.411 (4)
Mn1—N2	2.245 (3)	S1—O3	1.431 (4)
Mn1—N3	2.258 (3)	S1—O5	1.441 (3)
Mn1—N4	2.270 (3)		
O1—Mn1—O6	85.45 (10)	N3—Mn1—N4	73.34 (11)
O1—Mn1—N2	160.12 (10)	O1—Mn1—N1	89.09 (10)
O6—Mn1—N2	88.33 (11)	O6—Mn1—N1	99.37 (12)
O1—Mn1—N3	86.42 (10)	N2—Mn1—N1	73.31 (10)
O6—Mn1—N3	164.10 (12)	N3—Mn1—N1	94.13 (10)
N2—Mn1—N3	103.66 (11)	N4—Mn1—N1	162.41 (11)
O1—Mn1—N4	102.08 (10)	O4—S1—O3	113.3 (3)
O6—Mn1—N4	95.06 (12)	O4—S1—O5	112.8 (3)
N2—Mn1—N4	97.25 (10)	O3—S1—O5	111.4 (2)

H atoms bonded to C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}$(parent). The water H atoms were located in difference Fourier maps and refined with restraints for O—H distances [0.85 (1) Å] and with $U_{iso}(H) = 0.08$ Å^2.

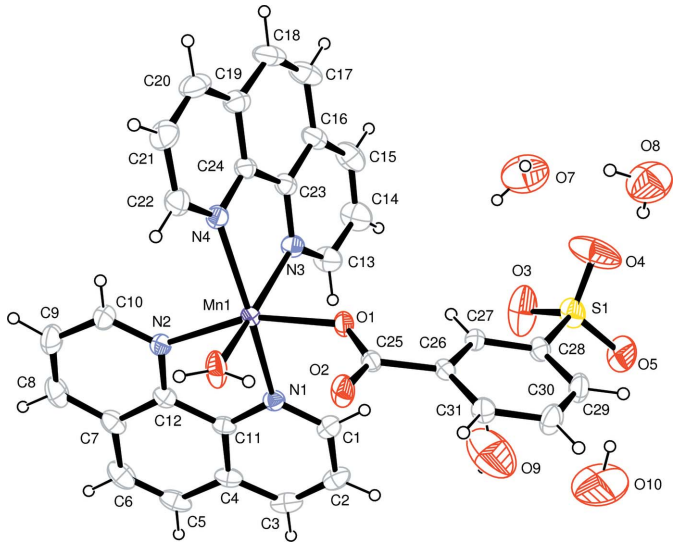


Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 40% probability level.

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).

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