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Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
 Disorder in solvent or counterion
 R factor = 0.052
 wR factor = 0.125
 Data-to-parameter ratio = 11.9

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

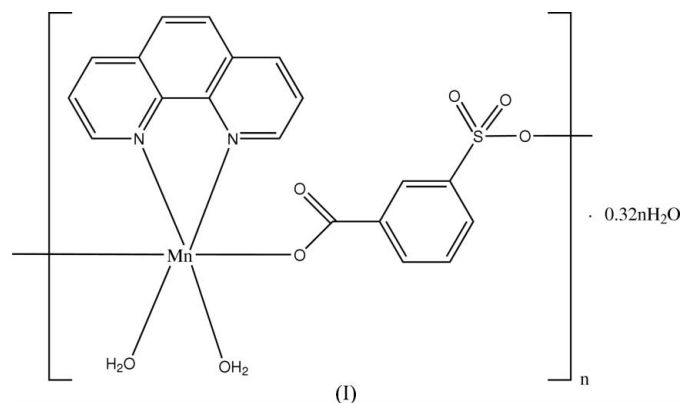
catena-Poly[[[*cis*-diaqua(1,10-phenanthroline- κ^2N,N')manganese(II)]- μ_2 -3-sulfonatobenzoato- $\kappa^2O:O'$] 0.32-hydrate]

In the title polymeric compound, $[\text{Mn}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2] \cdot 0.32\text{H}_2\text{O}$, which was synthesized by a combination of hydrothermal reaction and solution evaporation, each Mn^{II} ion approximates an octahedral geometry and each 3-sulfonatobenzoate ligand links two metal atoms in a μ_2 mode. Extensive hydrogen bonds between water molecules and sulfonate groups give rise to a three-dimensional network in the crystal structure.

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Comment

Very recently, a monomeric 3-sulfonatobenzoato (3-sb) Mn^{II} compound with the 1,10-phenanthroline (phen) ligand, $[\text{Mn}(3\text{-sb})(\text{phen})_2(\text{H}_2\text{O})] \cdot 4\text{H}_2\text{O}$, (II), was synthesized in our laboratory by a combination of hydrothermal synthesis and solution evaporation (Yang *et al.*, 2006). Further exploration on this system indicates that the monomer can be converted into a polymeric compound, (I), which is structurally similar to a Cd^{II} analogous polymer including 2,2'-bipyridine in place of 1,10-phenanthroline (Miao & Zhu, 2006).



The structure of (I) is formed by a one-dimensional chain where each Mn^{II} ion approximates an octahedral geometry completed by two N donors from one phen ligand, two O atoms from one 3-sb ligand and two O atoms from two water molecules (Fig.1 and Table 1). The 3-sb ligand acts as a linker in μ_2 mode, using its sulfonate and carboxylate groups, extending the structure into a one-dimensional chain. The carboxylate group C13/O1/O2 makes a dihedral angle of $22.7(3)^\circ$ with the benzene ring of 3-sb, an angle significantly larger than that observed in (II). In the chain, the coordinated water molecule O6 forms hydrogen bonds with the uncoordinated carboxylate atom O1. Moreover, hydrogen bonds between the coordinated water molecules (O6 and O7) and sulfonate functionality extend the chains into a three-dimensional hydrogen-bonding network (Table 2).

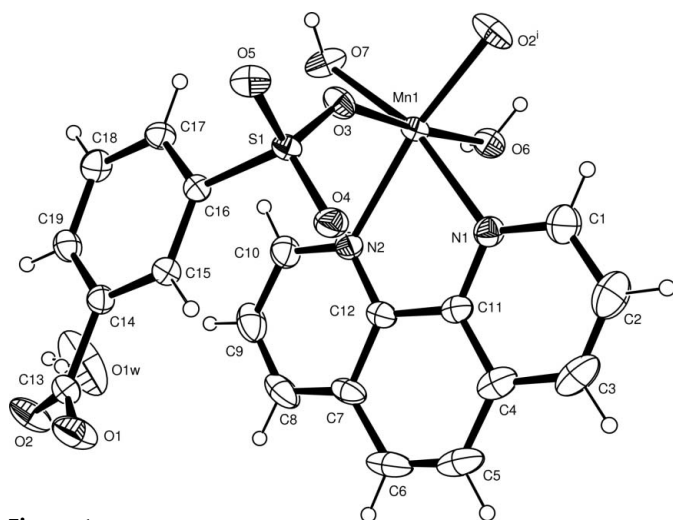


Figure 1
Part of the polymeric chain structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$.]

Experimental

A mixture of manganese(II) acetate tetrahydrate (0.122 g, 0.5 mmol), sodium hydrogen 3-sulfobenzoate (0.113 g, 0.5 mmol), 1,10-phenanthroline (0.101 g, 0.5 mmol) and water (15 ml) was heated to 423 K for 3 d in a 30 ml Teflon-lined stainless steel autoclave. After cooling the autoclave, a yellow solution was obtained and, after one week, yellow crystals were grown, identified as $[\text{Mn}(3\text{-sb})(\text{phen})_2(\text{H}_2\text{O})] \cdot 4\text{H}_2\text{O}$, (II), as confirmed by IR and single-crystal X-ray analysis (Yang *et al.*, 2006). These crystals were allowed to stay in the solution until almost all the solvent had evaporated. Water (10 ml) was then added and the mixture was filtered, giving yellow block-shaped crystals of (I).

Crystal data

$[\text{Mn}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{12}\text{H}_8\text{N}_2) \cdot (\text{H}_2\text{O})_2] \cdot 0.32\text{H}_2\text{O}$

$M_r = 477.10$
Monoclinic, $P2_1/c$
 $a = 14.4739$ (11) Å
 $b = 7.6406$ (6) Å
 $c = 18.9230$ (15) Å
 $\beta = 107.413$ (1)°

$V = 1996.8$ (3) Å³
 $Z = 4$
 $D_x = 1.598$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.81$ mm⁻¹
 $T = 295$ (2) K
Block, yellow
 $0.26 \times 0.24 \times 0.21$ mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.816$, $T_{\max} = 0.848$

10076 measured reflections
3539 independent reflections
3193 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 $\theta_{\text{max}} = 25.1^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.125$
 $S = 0.99$
3539 reflections
298 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.064P)^2 + 2.9349P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.45$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.28$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Mn1—O2 ⁱ	2.083 (2)	Mn1—N2	2.270 (3)
Mn1—O7	2.146 (3)	S1—O4	1.438 (2)
Mn1—O3	2.187 (2)	S1—O3	1.454 (2)
Mn1—O6	2.232 (3)	S1—O5	1.459 (2)
Mn1—N1	2.247 (3)		
O2 ⁱ —Mn1—O7	99.86 (12)	O6—Mn1—N1	89.09 (10)
O2 ⁱ —Mn1—O3	86.10 (10)	O2 ⁱ —Mn1—N2	169.26 (12)
O7—Mn1—O3	85.74 (10)	O7—Mn1—N2	90.77 (11)
O2 ⁱ —Mn1—O6	89.31 (10)	O3—Mn1—N2	93.18 (9)
O7—Mn1—O6	93.55 (10)	O6—Mn1—N2	91.61 (10)
O3—Mn1—O6	175.16 (9)	N1—Mn1—N2	73.57 (10)
O2 ⁱ —Mn1—N1	95.75 (12)	O4—S1—O3	114.17 (15)
O7—Mn1—N1	164.20 (11)	O4—S1—O5	112.87 (15)
O3—Mn1—N1	92.89 (10)	O3—S1—O5	109.57 (14)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O6—H6B \cdots O1 ⁱ	0.850 (10)	1.887 (18)	2.696 (4)	158 (4)
O6—H6A \cdots O4 ⁱⁱⁱ	0.84 (3)	2.039 (15)	2.857 (4)	162 (4)
O7—H7A \cdots O5 ⁱⁱ	0.847 (10)	1.869 (11)	2.714 (3)	175 (4)
O7—H7B \cdots O5 ⁱⁱⁱ	0.84 (3)	1.93 (3)	2.767 (3)	175 (5)
O1W—H1WA \cdots O2	0.850 (10)	2.18 (5)	2.990 (16)	160 (14)

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

The aromatic H atoms were positioned geometrically and treated as riding, with C—H distances constrained to 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$. The water H atoms were found in a difference Fourier map and refined with O—H distances restrained to 0.85 (1) Å and $U_{\text{iso}}(\text{H}) = 0.08$ Å². The site occupation factor for the uncoordinated water molecule, O1w, was first refined and converged to 0.325 (13). In the final cycles of refinement the occupation factor for this molecule was fixed at 0.32.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); 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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