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catena-Poly[[*cis*-diaqua(2,2′-bipyridine)-manganese(II)]-μ-5-sulfonatosalicylato]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.091
Data-to-parameter ratio = 12.3

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

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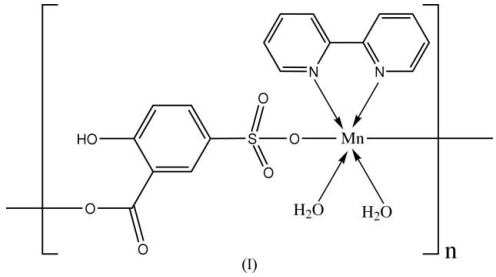
In the title polymeric compound, $[Mn(C_7H_4O_6S)(C_{10}H_8N_2)(H_2O)_2]_n$, the octahedral coordination geometry of each Mn^{II} atom comprises two N-atom donors of one 2,2′-bipyridine ligand, two O atoms, one from a carboxylate and one from a sulfonate group of two 5-sulfonatosalicylate ligands, and two further O atoms from two water molecules. The molecules, bridged by 5-sulfonatosalicylate ligands, form a one-dimensional polymeric chain. Intermolecular O—H···O hydrogen bonds between the chains generate a two-dimensional hydrogen-bonded layer.

Comment

Recently, the M^{2+}/2,2′-bipy/H_3ssal system (2,2′-bipy = 2,2′-bipyridine and H_3ssal = 5-sulfosalicylic acid) has been extensively studied in our laboratory and three complexes with the formula $[M(Hssal)(2,2'\text{-bipy})(H_2O)_2]_n$ [$M = Cu^{2+}$ for (II), Co^{2+} for (III) and Zn^{2+} for (IV)] were reported (Fan *et al.*, 2005, 2005*a*,*b*). These three complexes were synthesized by a one-pot solution method. However, for the system Mn^{2+}/2,2′-bipy/H_3ssal, the one-pot solution method did not produce the above-mentioned complex, while the hydrothermal synthesis (Fan *et al.*, 2005*c*) yielded a monomer, $[Mn(Hssal)(2,2'\text{-bipy})_2(H_2O)]\cdot 2H_2O$. To investigate systematically the complexes of type $[M(Hssal)(2,2'\text{-bipy})(H_2O)_2]_n$, a two-step reaction method was developed and successfully applied to the synthesis of the title polymeric complex, (I).



(I)

In (I), each Mn^{II} atom adopts an octahedral geometry completed by two N atoms from one 2,2′-bipy, two O atoms from two 5-sulfonatosalicylate ligands, and two *cis*-arranged water molecules (Fig. 1 and Table 1). The 5-sulfonatosalicylate dianion acts as a μ_2-bridging ligand, linking two Mn^{II} atoms by its carboxylate and sulfonate groups and forming a one-dimensional polymeric chain. In the chain, two types of hydrogen bonds (Table 2) are formed, between the water molecule and the uncoordinated carboxylate O atom, and between the hydroxyl group and the coordinated carboxylate O atom. Moreover, the water molecules and sulfonate O atoms are engaged in hydrogen bonds (Table 2), which link the

chains into a two-dimensional hydrogen-bonded layer (Fig. 2) and stabilize the crystal packing.

A comparison of (I) with the three isostructural complexes (II)–(IV) indicates that the geometry around the Cu^{II} atom in (II) is distorted octahedral, due to the Jahn–Teller effect, while the geometries around the Mn^{II}, Co^{II} and Zn^{II} atoms are regular octahedral.

Experimental

A mixture of $Mn(CH_3COO)_2{\cdot}4H_2O$ (0.124 g, 0.50 mmol) and 5-sulfosalicylic acid dihydrate (0.127 g, 0.50 mmol) in water (15 ml) was stirred at room temperature for 24 h. 2,2′-Bipyridine (0.077 g, 0.50 mmol) was added with stirring. The resulting solution was set aside and the solvent allowed to evaporate. After two weeks, pale-yellow block-shaped crystals of (I) were obtained by suction filtration.

Crystal data

$[Mn(C_7H_4O_6S)(C_{10}H_8N_2)(H_2O)_2]$	D_x = 1.611 Mg m^{-3}
M_r = 463.32	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 5941 reflections
a = 14.5715 (7) Å	θ = 2.3–28.2°
b = 7.7080 (4) Å	μ = 0.85 mm^{-1}
c = 18.3799 (9) Å	T = 295 (2) K
β = 112.291 (1)°	Block, pale yellow
V = 1910.11 (16) Å^3	0.49 × 0.28 × 0.19 mm
Z = 4	

Data collection

Bruker SMART APEX area-detector diffractometer	3395 independent reflections
φ and ω scans	3219 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	R_{int} = 0.018
T_{min} = 0.681, T_{max} = 0.855	θ_{max} = 25.1°
9655 measured reflections	$h = -17 \rightarrow 17$
	$k = -9 \rightarrow 9$
	$l = -18 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.9958P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.091	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
S = 1.07	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
3395 reflections	
277 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Mn1—O3	2.1905 (15)	Mn1—N2	2.2309 (19)
Mn1—O6^{i}	2.1144 (15)	S1—O1	1.4614 (15)
Mn1—O7	2.2448 (17)	S1—O2	1.4492 (15)
Mn1—O8	2.1213 (16)	S1—O3	1.4585 (15)
Mn1—N1	2.2592 (19)		
O6^{i}—Mn1—O8	97.35 (7)	N2—Mn1—O7	88.99 (7)
O6^{i}—Mn1—O3	81.05 (6)	O6^{i}—Mn1—N1	171.93 (7)
O8—Mn1—O3	88.38 (6)	O8—Mn1—N1	90.41 (7)
O6^{i}—Mn1—N2	99.57 (8)	O3—Mn1—N1	97.04 (6)
O8—Mn1—N2	162.91 (8)	N2—Mn1—N1	72.59 (8)
O3—Mn1—N2	91.96 (7)	O7—Mn1—N1	93.56 (6)
O6^{i}—Mn1—O7	88.13 (6)	O2—S1—O3	113.92 (10)
O8—Mn1—O7	93.88 (6)	O2—S1—O1	112.43 (9)
O3—Mn1—O7	169.15 (6)	O3—S1—O1	109.26 (9)

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

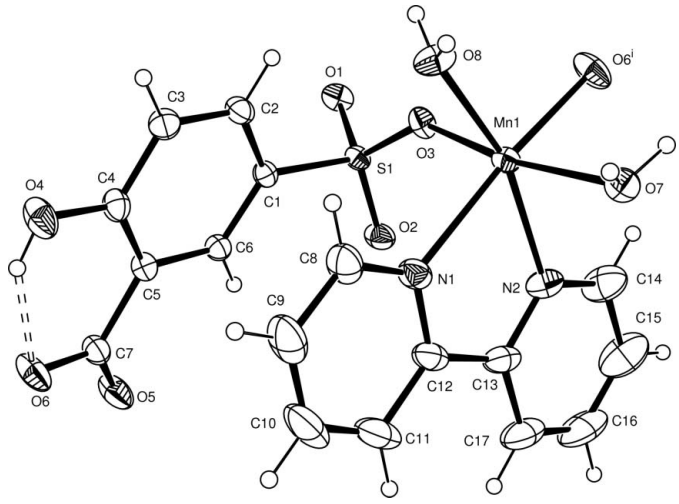


Figure 1
ORTEP-3 (Farrugia, 1997) view of (I). Displacement ellipsoids are drawn at the 40% probability level. The intramolecular hydrogen bond is shown as a double dashed line [symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$].

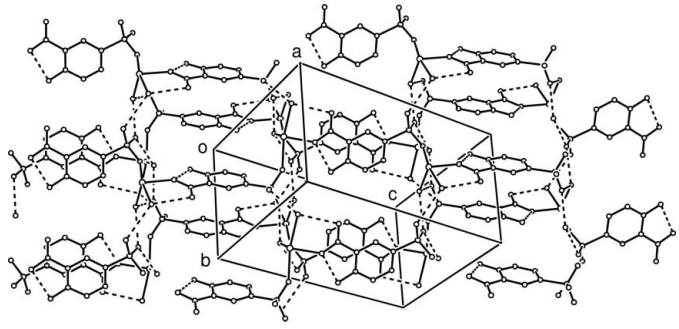


Figure 2
A view of the two-dimensional hydrogen-bonded (dashed lines) network in (I). The 2,2′-bipyridine ligands and H atoms have been omitted for clarity.

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O6	0.843 (10)	1.820 (17)	2.575 (2)	148 (3)
O7—H7B···O5^{i}	0.853 (9)	1.907 (11)	2.726 (2)	160 (2)
O7—H7A···O2^{ii}	0.846 (9)	2.003 (10)	2.821 (2)	162 (2)
O8—H8B···O1^{iii}	0.85 (3)	1.89 (3)	2.727 (2)	170 (3)
O8—H8A···O1^{ii}	0.844 (9)	1.871 (10)	2.713 (2)	176 (3)

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

The aromatic H atoms were placed in calculated positions (C—H = 0.93 Å) and included in the refinement in the riding-model approximation with the constraint U_{iso}(H) = 1.2U_{eq}(carrier). The water H atoms and hydroxyl H atom were found in a difference Fourier map and refined with a distance restraint of O—H = 0.85 (1) Å and with U_{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).

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