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catena-Poly[[aquamanganese(II)]-di-μ-4-pyridylthioacetato-κ^6*O*,*O*′:*N*;*N*:*O*,*O*′]

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The Mn atom and the coordinated water molecule in the title compound, $[Mn(C_7H_6NO_2S)_2(H_2O)]_n$, lie on a twofold axis; the Mn atom is chelated by the carboxyl $-CO_2$ units and is also coordinated by the pyridyl N atoms of two adjacent anionic groups in a seven-coordinate *trans*-pentagonal bipyramidal geometry. The polymeric chain runs in a zigzag manner along the *c* axis, and neighboring chains are linked into a hydrogen-bonded layer structure.

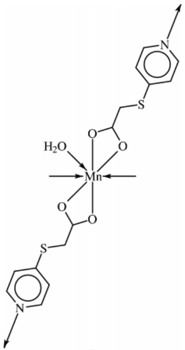
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.054
wR factor = 0.131
Data-to-parameter ratio = 15.2

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

Comment

The reaction of a divalent transition metal ion with the anion of 4-pyridylthioacetic acid affords different products depending on the reaction conditions and the nature of the metal ion. Under hydrothermal conditions, the reaction with Zn^{2+} affords polymeric $[Zn(C_7H_6NO_2S)_2]_n$ in which the metal atom is four-coordinate in a tetrahedral environment, the metal atom being linked to two N and two O atoms (Zhang *et al.*, 2003). On the other hand, the Ni^{II} derivative exists as a zwitterionic compound, $[Ni(C_7H_6NO_2S)_2(H_2O)_4]$, in which the metal atom is coordinated by four water molecules and the pyridyl N atom of the anionic group; the metal atom exists in an all-*trans* octahedral geometry (Zhang *et al.*, 2004). In the present study, the Mn^{II} derivative is coordinated by only one water molecule, but the coordination number is seven as the two carboxyl $-CO_2$ units behave in a chelating mode; the donor set is completed by the pyridyl N atoms of two adjacent anions (Fig. 1) that occupy the apical sites of the pentagonal bipyramidal polyhedron. Bridging gives rise to the formation of a linear zigzag chain that runs along the *c* axis (Fig. 2); adjacent chains are linked by a hydrogen bond [$O1w\cdots O1^{i}$ = 2.781 (4) Å; symmetry code: (i) $-x, y-1, \frac{1}{2}-z$] into layers.



(I)

Seven-coordinate Mn complexes are relatively less common than six-coordinate Mn complexes; in fact, there appears to be only one example of an MnN_2O_5 fragment in which four of the O atoms belong to a pair of carboxyl $-CO_2$ units. The dinuc-

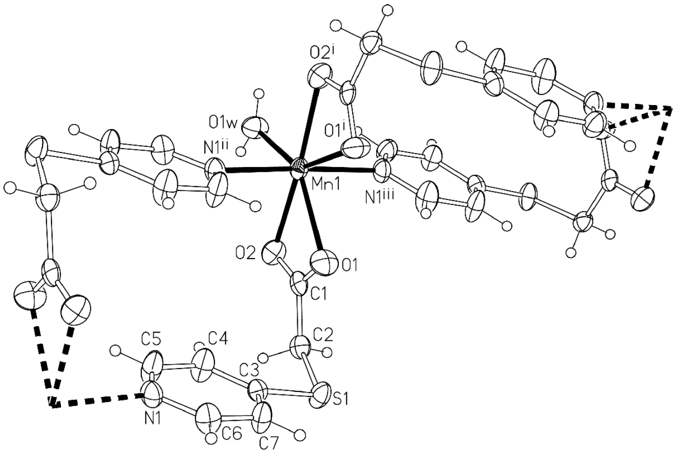


Figure 1
*ORTEP*II (Johnson, 1976) plot of a fragment of the $[Mn(C_7H_6NO_2S)_2(H_2O)]_n$ chain, with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

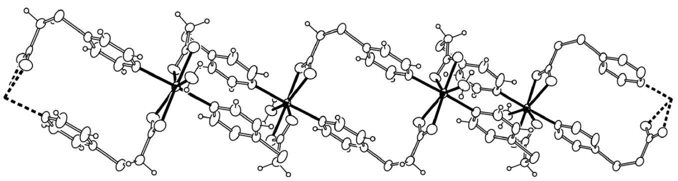


Figure 2
*ORTEP*II (Johnson, 1976) plot of the pyridyl-bridged zigzag $[Mn(C_7H_6NO_2S)_2(H_2O)]_n$ chain. The chains are linked by hydrogen bonds into layers.

lear 2,2′-bipyridine-chelated bicyclo[2.2.1]hept-5-ene-2-*exo*,3-*exo*-dicarboxylate also features a coordinated water molecule [Mn—O$_{water}$ = 2.208 (1) Å]; the N atoms of the chelating ligand occupy adjacent sites of the pentagonal plane (Baumeister & Hartung, 1997).

Experimental

A mixture of manganese acetate tetrahydrate (0.25 g, 1 mmol), 4-pyridylthioacetic acid (0.20 g, 1.2 mmol) and imidazole (0.03, 0.5 mmol) in water (7 ml) was treated with several drops of 2 N sodium hydroxide to a pH of approximately 6. The solution was placed in a 15 ml Teflon-lined stainless-steel bomb, which was heated at 433 K for 96 h. Colorless crystals of the title compound were obtained in about 40% yield; the imidazole component was not incorporated into the molecule.

Crystal data

$[Mn(C_7H_6NO_2S)_2(H_2O)]$
$M_r = 409.33$
Monoclinic, $C2/c$
$a = 21.595$ (3) Å
$b = 6.4904$ (8) Å
$c = 15.611$ (2) Å
$\beta = 132.774$ (1)°
$V = 1606.1$ (3) Å^3
$Z = 4$
$D_x = 1.693$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 950 reflections
$\theta = 2.5$–24.7°
$\mu = 1.11$ mm^{-1}
$T = 298$ (2) K
Block, colorless
0.09 × 0.08 × 0.06 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.525$, $T_{max} = 0.936$
4507 measured reflections
1692 independent reflections
1419 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.0°$
$h = -27 \rightarrow 27$
$k = -8 \rightarrow 5$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.131$
$S = 1.12$
1692 reflections
111 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.9714P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.378 (3)	Mn1—N1^{i}	2.276 (3)
Mn1—O2	2.280 (2)	Mn1—N1^{ii}	2.276 (3)
Mn1—O1*w*	2.218 (4)		
O1—Mn1—O1^{iii}	74.5 (1)	O2—Mn1—O2^{iii}	173.3 (1)
O1—Mn1—O2	56.1 (1)	O2—Mn1—O1*w*	86.7 (1)
O1—Mn1—O2^{iii}	130.6 (1)	O2—Mn1—N1^{i}	90.1 (1)
O1—Mn1—O1*w*	142.8 (1)	O2—Mn1—N1^{ii}	90.2 (1)
O1—Mn1—N1^{i}	88.0 (1)	O1*w*—Mn1—N1^{i}	92.6 (1)
O1—Mn1—N1^{ii}	87.9 (1)	N1^{i}—Mn1—N1^{ii}	174.9 (2)

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

A dimensionless value $\mu \times 2r = 0.10$ was used in the absorption correction. The H atoms were placed at calculated positions in the riding-model approximation, with C—H = 0.98 Å for aliphatic H atoms, C—H = 0.93 Å for aromatic H atoms and O—H = 0.82 Å; the displacement parameters were tied to those (U_{eq}) of the parent atoms by a factor of 1.2. The H atom belonging to the O1*w* water molecule, which lies on the twofold axis, was generated by the HFIX 147 instruction in *SHELXL*97 (Sheldrick, 1997).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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