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# *catena*-Poly[[[(1,10-phenanthroline)manganese(II)]-$\mu$-(1-hydroxybenzene-3,5-dicarboxylato)] hydrate]

**J. M. S. Skakle,* M. R. St J. Foreman and M. J. Plater**

Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland

Correspondence e-mail: j.skakle@abdn.ac.uk

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**Key indicators**

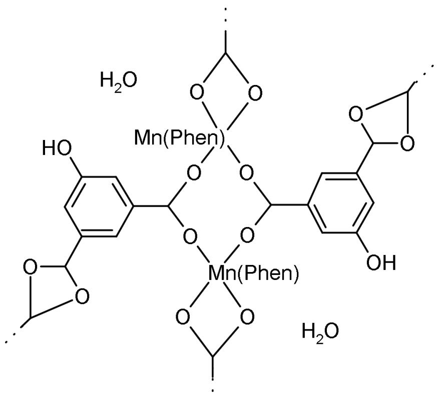
Single-crystal X-ray study
*T* = 298 K
Mean $\sigma$(C–C) = 0.003 Å
*R* factor = 0.040
*wR* factor = 0.079
Data-to-parameter ratio = 18.9

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

The title compound, $\{[Mn(C_8H_4O_5)(C_{12}H_8N_2)]\cdot H_2O\}_n$, forms a polymeric chain *via* $Mn^{2+}$–$C_8H_4O_5{}^{2-}$ (Mn–HIA) dimers which zigzag parallel to [101]. The 1,10-phenanthroline molecules are coordinated to the metal *via* the N atoms and are arranged approximately perpendicular to the Mn–HIA layers. The phenanthroline ligands are stacked parallel to one another at intervals of 3.54 Å, which is characteristic of $\pi$–$\pi$ interaction.

## Comment

The title compound, (I), was synthesized as part of a study into polymeric compounds containing metals and 5-hydroxyisophthalic acid (HIA), which may possess interesting magnetic properties.



(I)

The asymmetric unit is shown in Fig. 1. Mn is coordinated to two N and three O atoms; a fourth O, from a coordinated carboxyl group, is located at a slightly longer distance of 2.3490 (16) Å.

The structure was confirmed to be polymeric; each metal ion is bonded to three O atoms of two carboxylate groups from two distinct HIA molecules. This effectively gives a dimer of two metal and three HIA molecules, which links to form a $(Mn^{2+})_{2n}(C_8H_4O_5{}^{2-})_{2n}$ chain (Fig. 2). This chain forms a zigzag parallel to (101), as shown in Fig. 3.

The chelating phenanthroline ligand is coordinated to the metal *via* the two N atoms, and is oriented approximately perpendicular (83.7°) to the Mn–HIA network. This gives layers of Mn–HIA and phenanthroline, the layers stacking at an angle of approximately 34° to [100] (Fig. 3). The phenanthroline molecules are, on average, separated by 3.51 (5) Å, typical for $\pi$–$\pi$ stacking.

There is one free water molecule per formula unit, which is hydrogen bonded to two O atoms of the carboxylate groups of

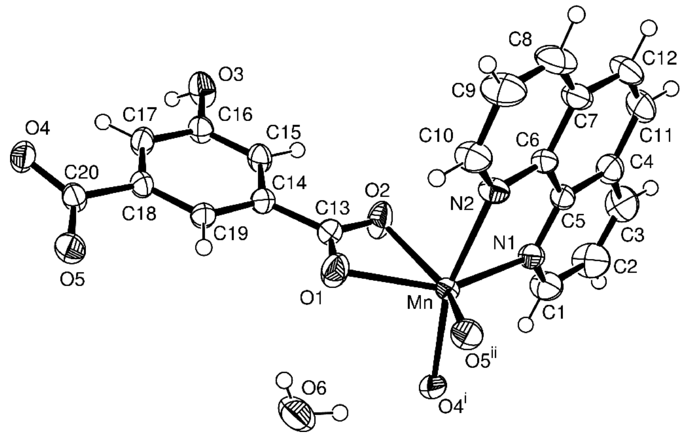


**Figure 1**
The asymmetric unit of the title compound (symmetry codes: (i) $x-\frac{1}{2}$, $-y+1$, $z-\frac{1}{2}$; (ii) $-x$, $-y+1$, $-z+2$). Ellipsoids are shown at the 50% probability level.

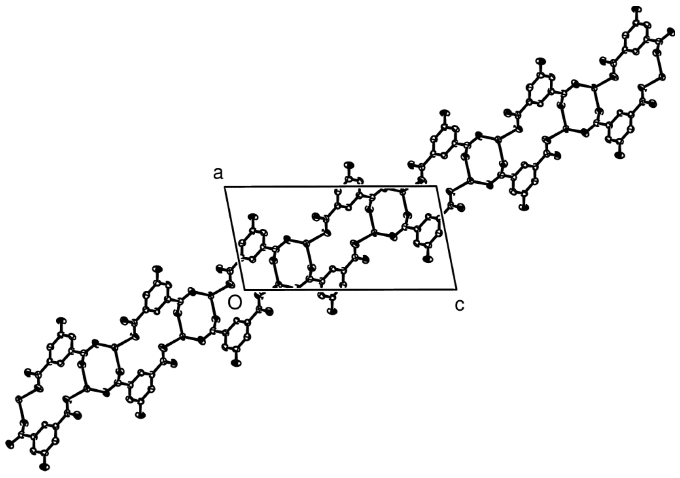


**Figure 2**
Projection of the structure down (010), showing the formation of the Mn–HIA chain along (101).

HIA, whilst the hydroxyl is hydrogen bonded to the water.

The Zn analogue was also synthesized and shown to be isostructural, but due to the poor quality of crystals and hence data, the full structure is not reported.

## Experimental

5-Hydroxyisophthalic acid (51.4 mg, 0.285 mmol), manganese acetate tetrahydrate (69.2 mg, 0.282 mmol), phenanthroline (51.1 mg, 0.284 mmol) and water (10 ml) were placed in a 23 ml Parr bomb. After sealing, the bomb was heated at 100 K h$^{-1}$ to 513 K. This temperature was maintained for 2 h, after which the bomb was cooled at 5 K h$^{-1}$ to 453 K, left for 6 h, then cooled at 4 K h$^{-1}$ to 293 K. The bomb was opened, and the product was collected by filtration, washed with water and dried in air. This method produced a mixture of yellow crystals and brown non-crystalline material.

*Crystal data*

$[Mn(C_8H_4O_5)(C_{12}H_8N_2)]\cdot H_2O$
$M_r = 433.27$
Monoclinic, $P2/n$
$a = 8.6089$ (5) Å
$b = 12.2249$ (7) Å
$c = 17.3057$ (11) Å
$\beta = 100.860$ (2)°
$V = 1788.68$ (18) Å$^3$
$Z = 4$
$D_x = 1.609$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3745 reflections
$\theta = 2.4$–29.2°
$\mu = 0.78$ mm$^{-1}$
$T = 298$ (2) K
Block, yellow
$0.3 \times 0.1 \times 0.1$ mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{\min} = 0.798$, $T_{\max} = 0.928$
15 609 measured reflections
5186 independent reflections
2944 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.059$
$\theta_{\max} = 30.0°$
$h = -12 \rightarrow 12$
$k = -16 \rightarrow 17$
$l = -24 \rightarrow 14$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.079$
$S = 0.85$
5186 reflections
274 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0291P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.33$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.43$ e Å$^{-3}$

**Table 1**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3O···O6$^{\rm i}$ | 0.82 (3) | 1.85 (3) | 2.664 (3) | 175 (3) |
| O6—H6*WA*···O1 | 0.79 (4) | 2.31 (3) | 2.874 (3) | 130 (3) |
| O6—H6*WB*···O4$^{\rm ii}$ | 0.90 (3) | 1.96 (4) | 2.837 (3) | 164 (3) |

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

In general, H atoms were placed in geometrical positions and refined using a riding model. Those for the water molecule and the hydroxyl were located from the difference map and refined freely.

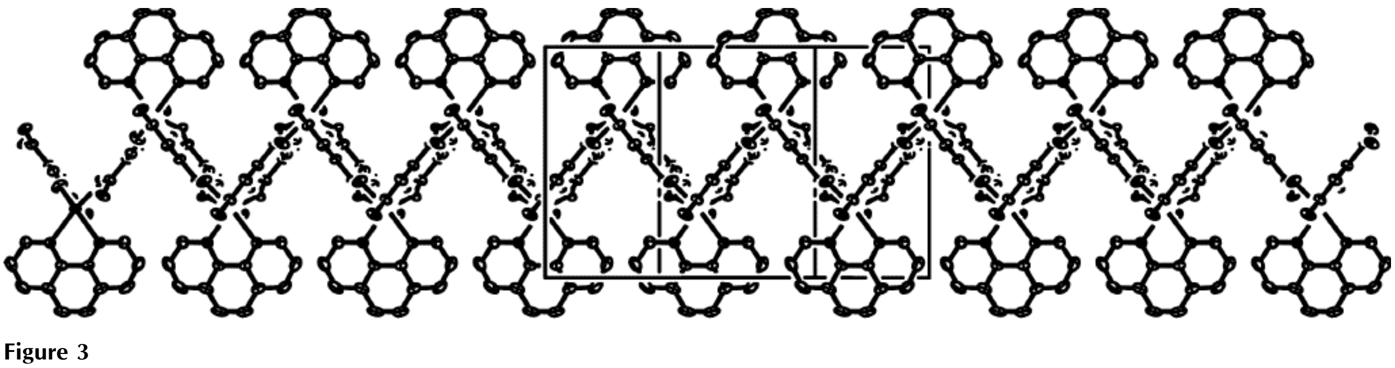


**Figure 3**
Projection of the structure showing the zigzag of the Mn–HIA dimeric chain and relative orientation of the phenanthroline molecules. The projection is offset from (100) by ~34° so that the phenanthroline molecules are superposed.

**m374** J. M. S. Skakle *et al.* • $[Mn(C_8H_4O_5)(C_{12}H_8N_2)]\cdot H_2O$ *Acta Cryst.* (2001). E**57**, m373–m375

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEX* in *OSCAIL* (McArdle, 1994), *ATOMS* (Dowty, 1999) and *ORTEP*-3 *for Windows* (Farrugia, 1997).

We wish to acknowledge the use of the EPSRC's Chemical Database Service at Daresbury (Fletcher *et al.*, 1996). JMSS would also like to thank R. A. Howie for helpful discussions.

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