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catena-Poly[bis[(2,2′-bipyridine-κ^2N,N')-manganese(II)]-di-μ-4-hydroxyisophthalato]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.039
wR factor = 0.118
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.

The two Mn atoms in the crystal structure of the title compound, $[Mn_2(C_8H_4O_5)_2(C_{10}H_8N_2)_2]_n$, are each chelated by the bipyridine heterocycle as well as by the carboxyl group of the dianionic ligand. Each Mn atom is covalently linked to the singly bonded carboxylate O atom of a second dianion and is datively linked to the carbonyl O atom of a third dianion. The Mn atoms exist in octahedral geometries in the linear polymeric chain.

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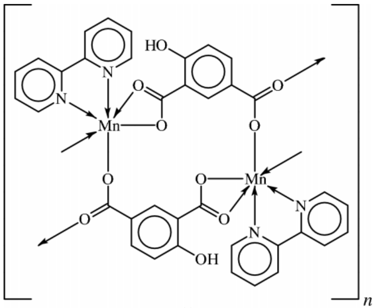
Comment

Whereas the isophthalate dianion in its metal complexes adopts several coordination modes, the 4-hydroxy-substituted analog displays more possibilities that arise from the extra hydroxy unit (Zhang *et al.*, 2003). The 2,2′-bipyridine-coordinated Co, Zn and Cd complexes of the isophthalate dianion adopt layer structures in which the hydroxy O atom of one polymeric chain binds to the metal atom of an adjacent chain (Zhang *et al.*, 2004). The present Mn complex of the 4-hydroxy-substituted analog, (I), which was synthesized under somewhat more acidic conditions in a hydrothermal reaction, adopts a chain motif in which the hydroxy O atom is not involved in bonding.



(I)

The asymmetric unit (Fig. 1) consists of two bipyridine-chelated Mn atoms and two hydroxyisophthalate dianions; for both dianions, one carboxyl group is bonded through the singly bonded O atom to one Mn atom whereas the other chelates to the second Mn atom. The doubly bonded atom O9 interacts across a center of inversion (symmetry code: $1 - x$, $1 - y$, $1 - z$) to form an eight-membered → Mn—O═C—O—Mn—O—C═O→ ring. Similarly, the other doubly bonded atom, O4, interacts across another inversion center. The bridging mode of the two carboxyl groups gives rise to the formation of a chain structure (Fig. 2). The hydroxyl group is only involved in intra-anion hydrogen bonding. The structure of the parent carboxylic acid has been recently reported (Cox & Murphy, 2003).

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Experimental

A mixture of manganese diacetate tetrahydrate (0.25 g, 1.0 mmol), 4-hydroxyisophthalic acid (0.09 g, 0.5 mmol) and 2,2′-bipyridine (0.08 g, 0.5 mmol) in water (10 ml) was treated with aqueous sodium hydroxide to a pH of 5. The solution was placed in a 23 ml Teflon-lined stainless-steel bomb, which was then heated to 433 K for 120 h. After cooling to room temperature, pale-yellow prisms were obtained in 50% yield. Elemental analysis found: C 54.69, H 3.18, N 7.13%; calculated for $C_{36}H_{24}Mn_2N_4O_{10}$: C 55.26, H 3.09, N 7.16%.

Crystal data

$[Mn_2(C_{10}H_8N_2)_2(C_8H_4O_5)_2]$
$M_r = 782.47$
Triclinic, $P\bar{1}$
$a = 9.473$ (1) Å
$b = 10.694$ (1) Å
$c = 17.900$ (2) Å
$\alpha = 79.413$ (2)°
$\beta = 86.879$ (3)°
$\gamma = 64.923$ (2)°
$V = 1613.9$ (3) Å^3

$Z = 2$
$D_x = 1.610$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 883 reflections
$\theta = 2.6$–26.6°
$\mu = 0.85$ mm^{-1}
$T = 298$ (2) K
Prism, pale yellow
0.50 × 0.24 × 0.14 mm

Data collection

Bruker AXS SMART 1K area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.789$, $T_{max} = 0.890$
8340 measured reflections

5605 independent reflections
4418 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 25.0°$
$h = -11 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.118$
$S = 1.04$
5605 reflections
471 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2 + 0.961P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.23$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.344 (2)	Mn2—O4^{ii}	2.093 (2)
Mn1—O2	2.280 (2)	Mn2—O5	2.062 (3)
Mn1—O9^{i}	2.096 (2)	Mn2—O6	2.336 (2)
Mn1—O10	2.088 (2)	Mn2—O7	2.339 (3)
Mn1—N1	2.235 (3)	Mn2—N3	2.277 (3)
Mn1—N2	2.261 (3)	Mn2—N4	2.248 (2)
O1—Mn1—O2	56.5 (1)	O4^{ii}—Mn2—O5	109.1 (1)
O1—Mn1—O9^{i}	142.7 (1)	O4^{ii}—Mn2—O6	139.6 (1)
O1—Mn1—O10	83.0 (1)	O4^{ii}—Mn2—O7	83.9 (1)
O1—Mn1—N1	84.7 (1)	O4^{ii}—Mn2—N3	87.7 (1)
O1—Mn1—N2	121.8 (1)	O4^{ii}—Mn2—N4	99.4 (1)
O2—Mn1—O9^{i}	87.1 (1)	O5—Mn2—O6	84.7 (1)
O2—Mn1—O10	96.4 (1)	O5—Mn2—O7	101.0 (1)
O2—Mn1—N1	100.8 (1)	O5—Mn2—N3	90.6 (1)
O2—Mn1—N2	173.1 (1)	O5—Mn2—N4	145.9 (1)
O9^{i}—Mn1—O10	111.5 (1)	O6—Mn2—O7	56.0 (1)
O9^{i}—Mn1—N1	95.8 (1)	O6—Mn2—N3	131.0 (1)
O9^{i}—Mn1—N2	93.3 (1)	O6—Mn2—N4	85.6 (1)
O10—Mn1—N1	148.4 (1)	O7—Mn2—N3	167.4 (1)
O10—Mn1—N2	89.9 (1)	O7—Mn2—N4	100.4 (1)
N1—Mn1—N2	72.3 (1)	N3—Mn2—N4	71.7 (1)

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

H atoms were placed at calculated positions in the riding-model approximation (O—H = 0.82 Å and C—H = 0.93 Å), and their isotropic displacement parameters were set to $1.2U_{eq}$ of the parent atoms. The final difference Fourier map had a large peak (1.23 e Å^{-3}) at about 0.5 Å from atom H5 but was otherwise featureless.

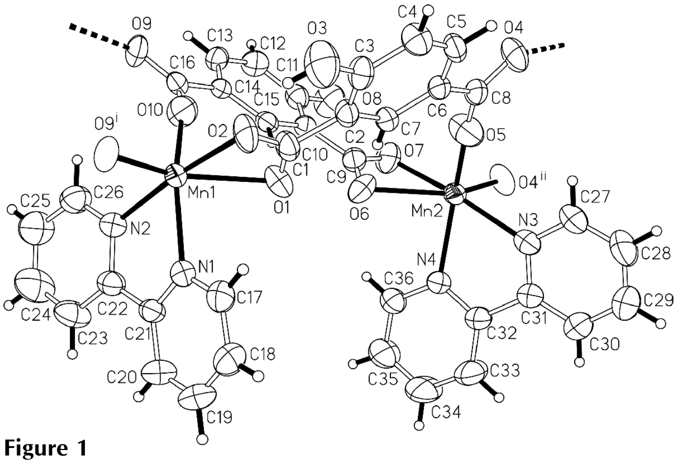

Figure 1
*ORTEP*II (Johnson, 1976) plot of the asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Symmetry codes: (i) $1 - x$, $1 - y$, $1 - z$; (ii) $1 - x$, $-y$, $2 - z$.]

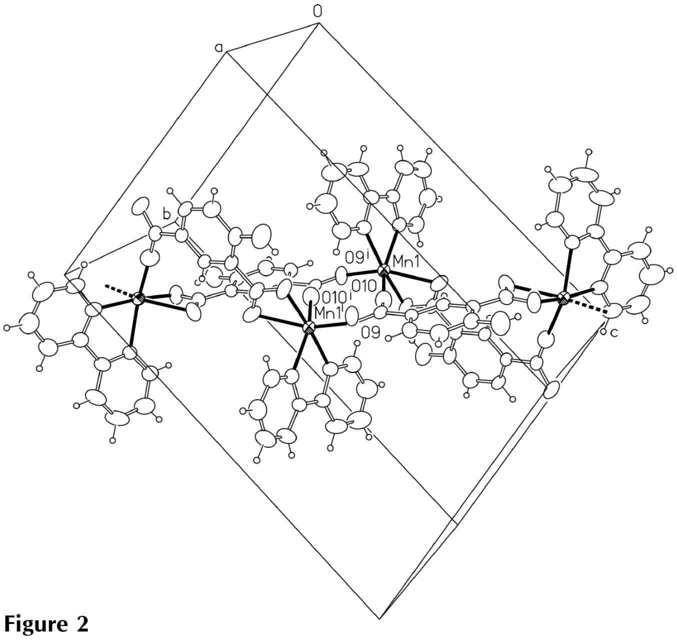

Figure 2
*ORTEP*II (Johnson, 1976) plot, illustrating the linear chain structure. [Symmetry code: (i) $1 - x$, $1 - y$, $1 - z$.]

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); 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.

References

Bruker (1999). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cox, P. J. & Murphy, M. T. (2003). *Acta Cryst.* E**59**, o1108–o1110.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Zhang, X.-M., Chen, J.-S., Xu, K.-Y., Ding, C.-R., She, W.-L. & Chen, X.-M. (2004). *Inorg. Chim. Acta.* In the press.

Zhang, L.-Y., Liu, G.-F., Zheng, S.-L., Ye, B.-H., Zhang, X.-M. & Chen, X.-M. (2003). *Eur. J. Inorg. Chem.* pp. 2965–2971.