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catena-Poly[[aqua(2,2′-bipyridine-κ^2N,N')manganese(II)]-μ-4-carboxylatophenoxyacetato-$\kappa^3O,O':O''$]

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In the title coordination polymer, $[Mn(4\text{-}CPOA)(2,2'\text{-}bipy)(H_2O)]_n$ [where 4-CPOA^{2-} is 4-carboxylatophenoxyacetate ($C_9H_6O_5$) and 2,2′-bipy is 2,2′-bipyridine ($C_{10}H_8N_2$)], each Mn^{II} ion displays a distorted octahedral coordination configuration, defined by three carboxyl O atoms from two different 4-CPOA^{2-} groups, two N atoms from the 2,2′-bipyridine ligand and one water molecule. Adjacent Mn^{II} ions are linked by carboxylate groups into a one-dimensional chain structure with a shortest Mn···Mn distance of 9.771 (3) Å. A two-dimensional supramolecular network is constructed through O—H···O intermolecular hydrogen bonds and π–π stacking interactions.

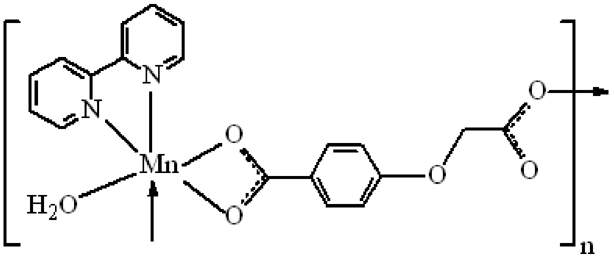
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.007 Å
R factor = 0.066
wR factor = 0.146
Data-to-parameter ratio = 16.0

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

Comment

4-Carboxyphenoxyacetic acid (4-CPOAH$_2$), with its multiple coordination sites and the capability of participating in hydrogen bonding as both a donor and an acceptor, represents an excellent candidate for the construction of supramolecular complexes (Gao, Li *et al.*, 2004; Gao, Huo *et al.*, 2004). Recently, we reported the structure of the Zn^{II} polymer, $[Zn(4\text{-}CPOA)(2,2'\text{-}bipy)(H_2O)]_n$, in which the Zn^{II} ion has an octahedral coordination geometry with the 4-CPOA^{2-} and 2,2′-bipyridine ligands (Gao, Gu *et al.*, 2004). The present Mn^{II} complex, $[Mn(4\text{-}CPOA)(2,2'\text{-}bipy)(H_2O)]_n$ (where 4-CPOA^{2-} is 4-carboxylatophenoxyacetate and 2,2′-bipy is 2,2′-bipyridine), (I), is isostructural with the Zn^{II} analogue. The structural features discussed for the Zn^{II} analogue in the previous paper are applicable to the present complex.



(I)

As shown in Fig. 1, the Mn^{II} centre is in a distorted octahedral coordination environment, defined by three carboxyl O atoms from two different 4-CPOA^{2-} groups, two N atoms from one 2,2′-bipyridine ligand and one water molecule. Atoms O1, O2, N1 and O1W constitute the equatorial plane, with an r.m.s. deviation of 0.13 (4) Å, the Mn^{II} atom being displaced from the plane by 0.17 (4) Å. Atoms N2 and O5^i [symmetry code: (i) $x+\frac{1}{2}, y+\frac{1}{2}, z$] occupy the axial sites, with an angle of 165.06 (13)°.

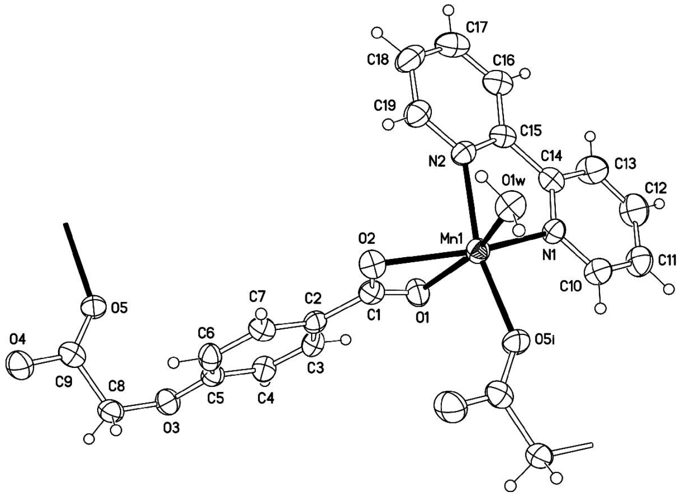


Figure 1

ORTEP plot (Johnson, 1976) showing part of the one-dimensional chain of the title complex, with displacement ellipsoids drawn at the 30% probability level [symmetry code (i): $\frac{1}{2}+x, \frac{1}{2}+y, z$].

Adjacent Mn^{II} atoms are linked by carboxylate groups through both mono- and bidentate chelating modes, forming a zigzag chain structure along [110] and [$\overline{1}$10]. Within a chain, the shortest Mn$\cdots$Mn distance is 9.771 (3) Å. In the crystal structure, the polymeric chains are assembled to form a two-dimensional supramolecular network (Table 2) *via* O—H$\cdots$O hydrogen-bonding and π–π stacking interactions between adjacent nitrogen heterocyclic rings of 2,2′-bipy [centroid–centroid distance = 3.585 (3) Å].

Experimental

The title complex was prepared by the addition of $MnCl_2 \cdot 6H_2O$ (4.68 g, 20 mmol) and 2,2′-bipy (3.12 g, 20 mmol) to a hot aqueous solution of 4-$CPOAH_2$ (3.92 g, 20 mmol); the pH was adjusted to 6 with 0.2 *M* NaOH solution. The solution was allowed to evaporate at room temperature, and yellow prism-shaped single crystals were obtained at room temperature over several days. Analysis calculated for $C_{19}H_{16}O_6MnN_2$: C 53.91, H 3.81, N 6.62%; found: C 54.07, H 3.85, N 6.59%.

Crystal data

$[Mn(C_9H_6O_5)(C_{10}H_8N_2)(H_2O)]$
$M_r = 423.28$
Monoclinic, $C2/c$
$a = 14.379$ (2) Å
$b = 13.234$ (2) Å
$c = 19.705$ (3) Å
$\beta = 104.00$ (3)°
$V = 3638.3$ (10) Å^3
$Z = 8$
$D_x = 1.545$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6068 reflections
$\theta = 3.0$–27.4°
$\mu = 0.77$ mm^{-1}
$T = 296$ (2) K
Prism, yellow
0.32 × 0.24 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.792$, $T_{max} = 0.874$
6190 measured reflections
4139 independent reflections
2578 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 27.4°$
$h = -18 \rightarrow 18$
$k = -17 \rightarrow 16$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.146$
$S = 1.04$
4139 reflections
259 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

Mn1—N1	2.220 (4)	Mn1—O1*W*	2.136 (4)
Mn1—N2	2.284 (4)	O1—C1	1.257 (5)
Mn1—O1	2.274 (3)	O2—C1	1.268 (5)
Mn1—O2	2.251 (3)	O4—C9	1.242 (5)
Mn1—O5^{i}	2.124 (3)	O5—C9	1.232 (5)
N1—Mn1—N2	72.33 (14)	O2—Mn1—O1	58.08 (11)
N1—Mn1—O1	94.28 (12)	O5^{i}—Mn1—O2	102.48 (12)
N1—Mn1—O2	148.19 (12)	O5^{i}—Mn1—O1*W*	92.08 (13)
O1—Mn1—N2	92.72 (12)	O1*W*—Mn1—N1	103.37 (13)
O5^{i}—Mn1—N1	93.22 (13)	O1*W*—Mn1—N2	87.76 (13)
O5^{i}—Mn1—N2	165.06 (13)	O1*W*—Mn1—O1	161.60 (12)
O5^{i}—Mn1—O1	92.11 (13)	O1*W*—Mn1—O2	103.51 (12)
O2—Mn1—N2	92.06 (13)		

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

Table 2

Hydrogen-bonding geometry (Å, °).

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O1*W*—H1*W*1$\cdots$O2^{ii}	0.85 (3)	1.94 (2)	2.732 (4)	155 (5)
O1*W*—H1*W*2$\cdots$O4^{iii}	0.85 (3)	1.78 (2)	2.609 (5)	162 (6)

Symmetry codes: (ii) $\frac{3}{2}-x, \frac{3}{2}-y, 1-z$; (iii) $1-x, 1-y, 1-z$.

C-bound H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and were refined in the riding-model approximation. The H atoms of water molecules were located in a difference map and refined with O—H and H$\cdots$H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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