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catena-Poly[[aqua(2,2′-bipyridine)manganese(II)]-μ_2-5-nitrobenzene-1,3-dicarboxylato-$\kappa^3O:O',O''$]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.113
Data-to-parameter ratio = 14.6

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

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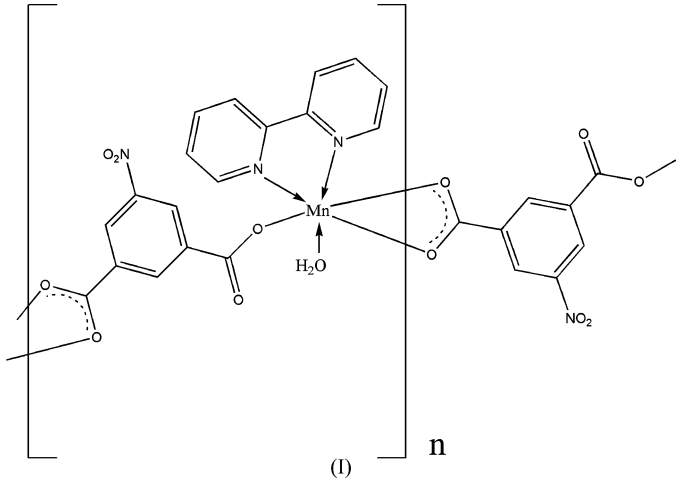
In the title compound, $[Mn(C_8H_3NO_6)(C_{10}H_8N_2)(H_2O)]_n$, the coordination polyhedron of the Mn^{II} ion is an octahedron defined by an N_2O_4 donor set. Each pair of adjacent Mn^{II} ions is bridged by a 5-nitrobenzene-1,3-dicarboxylate dianion to form a chiral helical chain running along a crystallographic 2_1 axis in the *c* direction with a long pitch of 19.04 Å. These chains are linked by $O_{water}—H\cdots O$ hydrogen bonds into a layer structure.

Comment

The 5-nitrobenzene-1,3-dicarboxylate dianion ($nmbdc^{2-}$) can act as a bridge ligand in a bis-monodentate coordination mode (Xiao *et al.*, 2005) or a bis-bridging coordination mode (He *et al.*, 2004). In the title compound, (I), the two carboxylate groups of the nmbdc ligand coordinate in different modes.



(I)

In (I), the coordination polyhedron of Mn^{II} ion is an octahedron defined by an N_2O_4 donor set (Fig. 1) formed by two N atoms from a 2,2′-bipyridine ligand, two O atoms from an nmbdc dianion, one O atom from another nmbdc dianion and one water O atom. Each pair of adjacent Mn^{II} ions is bridged by an nmbdc ligand to form a chiral helical chain running along a crystallographic 2_1 axis in the *c*-axis direction with a long pitch of 19.04 Å. Two types of coordination mode of each nmbdc ligand are observed; one carboxylate group is monodentate and the other is bidentate. These chains are linked by $O_{water}—H\cdots O$ hydrogen bonds into a layer structure (Fig. 2 and Fig. 3).

Experimental

A mixture of manganese acetate tetrahydrate (0.062 g, 0.25 mmol), 5-nitroisophthalic acid (0.053 g, 0.25 mmol), 2,2′-bipyridine (0.039 g,

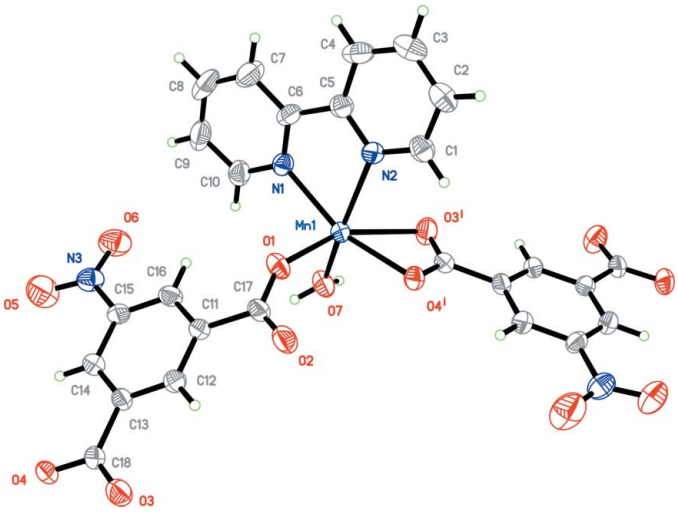


Figure 1
The structure of the title complex, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms as spheres of arbitrary radii [symmetry code: (i) $\frac{3}{2}-x, 2-y, \frac{1}{2}+z$].

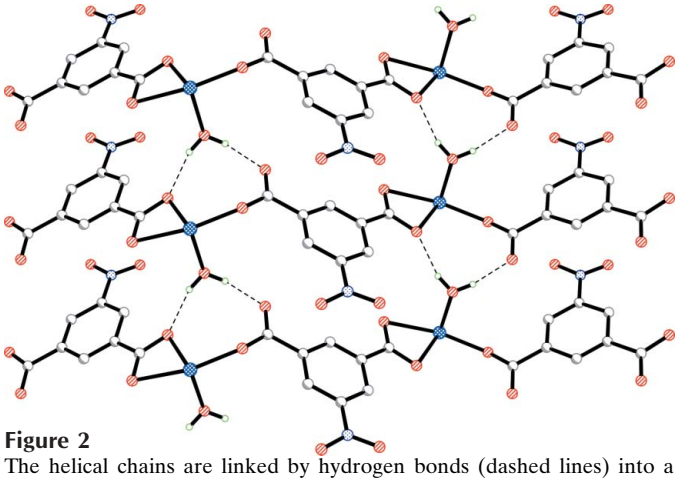


Figure 2
The helical chains are linked by hydrogen bonds (dashed lines) into a layer structure parallel to the *ac* plane. For the sake of clarity, 2,2′-bipyridine and H atoms not involved in hydrogen bonding have been omitted..

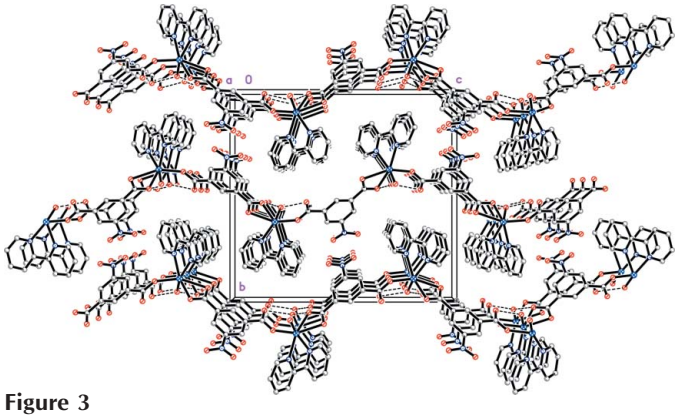


Figure 3
The layer structure of (I); for clarity, H atoms have been omitted.

0.25 mmol), sodium hydroxide (0.02 g, 0.5 mmol) and water (10 ml) was stirred in air for 5 min, then transferred and sealed in a 23 ml Teflon-lined stainless steel Parr bomb, which was heated at 433 K for 120 h and then cooled to room temperature. Colorless prismatic crystals were obtained and washed with deionized water (yield 45% based on Mn).

Crystal data

$[Mn(C_8H_3NO_6)(C_{10}H_8N_2)(H_2O)]$
M_r = 438.25
Orthorhombic, $P2_12_12_1$
a = 5.2027 (2) Å
b = 17.8203 (7) Å
c = 19.0427 (7) Å
V = 1765.52 (12) Å^3
Z = 4
D_x = 1.649 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 976 reflections
θ = 2.4–23.5°
μ = 0.80 mm^{-1}
T = 293 (2) K
Lath, colorless
0.33 × 0.13 × 0.07 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.779, T_{max} = 0.950
9400 measured reflections
3923 independent reflections
2866 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 27.6°
$h = -6 \rightarrow 6$
$k = -21 \rightarrow 23$
$l = -24 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.113
S = 1.00
3923 reflections
268 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2)]$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), 1540 Friedel pairs
Flack parameter: 0.04 (3)

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.074 (3)	Mn1—O7	2.108 (3)
Mn1—O3^{i}	2.429 (3)	Mn1—N1	2.250 (3)
Mn1—O4^{i}	2.195 (3)	Mn1—N2	2.267 (3)
O1—Mn1—O3^{i}	154.81 (10)	O7—Mn1—O3^{i}	80.59 (10)
O1—Mn1—O4^{i}	100.09 (10)	O7—Mn1—O4^{i}	95.90 (11)
O1—Mn1—O7	93.96 (11)	O7—Mn1—N1	99.45 (12)
O1—Mn1—N1	88.61 (11)	O7—Mn1—N2	157.37 (12)
O1—Mn1—N2	106.68 (11)	N1—Mn1—O3^{i}	116.50 (10)
O4^{i}—Mn1—O3^{i}	56.56 (10)	N1—Mn1—N2	72.46 (12)
O4^{i}—Mn1—N1	161.78 (11)	N2—Mn1—O3^{i}	84.30 (10)
O4^{i}—Mn1—N2	89.65 (10)		

Symmetry code: (i) $-x+\frac{3}{2}, -y+2, z+\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O4^{ii}	0.85 (2)	1.95 (2)	2.794 (4)	163 (3)
O7—H7B···O2^{iii}	0.85 (2)	1.83 (2)	2.655 (4)	169 (3)

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

H atoms attached to C atoms were positioned geometrically and refined as riding with the constraints C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The water H atoms were located in difference Fourier maps, and were refined with distance restraints of O—H = 0.85 (2) Å and H···H = 1.39 (2) Å.

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: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

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