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Poly[[[(1,10-phenanthroline)manganese(II)]-μ_3-2-nitrobenzene-1,4-dicarboxylato] monohydrate]

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Key indicators

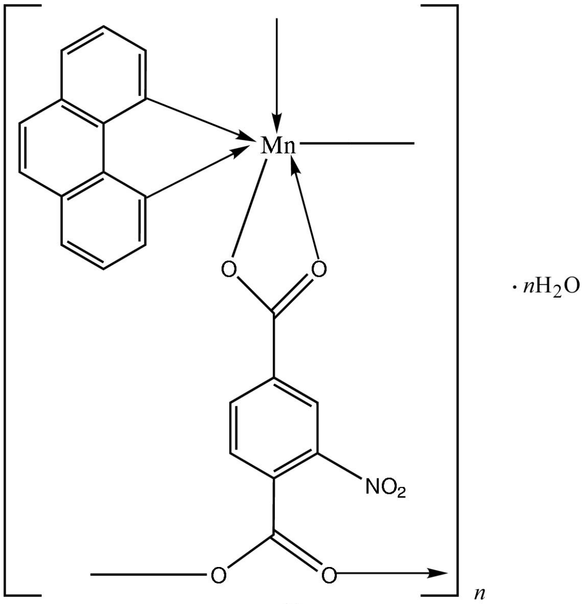
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.063
wR factor = 0.142
Data-to-parameter ratio = 11.2

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

In the title polymeric structure, $\{[Mn(C_8H_3NO_6)(C_{12}H_8N_2)]\cdot H_2O\}_n$, the Mn atom adopts an octahedral geometry. The 2-nitrobenzene-1,4-dicarboxylate ligand is in a chelating–bridging mode and its two carboxylate groups are approximately perpendicular to each other. The crystal structure can be described as layers formed by a two-dimensional network of hydrogen bonds.

Comment

Metal complexes of 2-nitrobenzene-1,4-dicarboxylate (nbdc) have shown interesting architectures compared with benzene-1,4-dicarboxylate complexes (Ma *et al.*, 2003, 2005; Zhu *et al.*, 2004; Ma & Zhu, 2004; He *et al.*, 2005). As part of a series of investigations of the nbdc metal complexes, the title manganese(II) compound, (I), was prepared.



(I)

The metal atom has an octahedral geometry defined by two N donors from one 1,10-phenanthroline and four carboxyl O atoms from three nbdc ligands (Fig. 1 and Table 1). One carboxylate group of the nbdc ligand is in a chelating mode and the other in a μ_2-bridging mode. The μ_2-bridging carboxylate group is approximately perpendicular to the benzene ring, with a dihedral angle of 73.7 (3)°, and connects two Mn^{II} atoms with a separation of 6.357 (1) Å. The structure is extended by the μ_2-bridging carboxylate group into a two-dimensional network (Fig. 2). The layered structure is formed by hydrogen bonds between uncoordinated water molecules and carboxylate O atoms.

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Experimental

A mixture of manganese acetate tetrahydrate (0.055 g, 0.22 mmol), 2-nitrobenzene-1,4-dicarboxylic acid (0.051 g, 0.24 mmol), 1,10-phenanthroline (0.049 g, 0.25 mmol) and water (15 ml) was heated at 423 K for 24 h in a 30 ml Teflon-lined stainless steel autoclave. After cooling, pale yellow block-shaped crystals of (I) were obtained.

Crystal data

$[Mn(C_8H_3NO_6)(C_{12}H_8N_2)]\cdot H_2O$
$M_r = 462.27$
Monoclinic, $I2/a$
$a = 18.515\ (3)$ Å
$b = 9.927\ (2)$ Å
$c = 20.948\ (3)$ Å
$\beta = 94.659\ (3)^\circ$
$V = 3837\ (1)$ Å^3
$Z = 8$

$D_x = 1.600$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3483 reflections
$\theta = 2.2$–26.6°
$\mu = 0.74$ mm^{-1}
$T = 295\ (2)$ K
Block, pale yellow
0.28 × 0.18 × 0.16 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.820$, $T_{\max} = 0.891$
7693 measured reflections

3197 independent reflections
2021 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.064$
$\theta_{\max} = 25.0^\circ$
$h = -21 \rightarrow 22$
$k = -11 \rightarrow 8$
$l = -24 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.142$
$S = 1.02$
3197 reflections
286 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.35$ e Å^{-3}
$\Delta\rho_{\min} = -0.37$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.301 (3)	Mn1—O4^{ii}	2.102 (3)
Mn1—O2	2.223 (3)	Mn1—N1	2.260 (4)
Mn1—O3^{i}	2.134 (3)	Mn1—N2	2.260 (4)
O4^{ii}—Mn1—O3^{i}	102.0 (1)	O2—Mn1—N1	164.8 (1)
O4^{ii}—Mn1—O2	104.0 (1)	N2—Mn1—N1	73.4 (1)
O3^{i}—Mn1—O2	86.4 (1)	O4^{ii}—Mn1—O1	94.4 (1)
O4^{ii}—Mn1—N2	159.2 (1)	O3^{i}—Mn1—O1	143.6 (1)
O3^{i}—Mn1—N2	89.1 (1)	O2—Mn1—O1	58.0 (1)
O2—Mn1—N2	94.2 (1)	N2—Mn1—O1	86.5 (1)
O4^{ii}—Mn1—N1	86.9 (1)	N1—Mn1—O1	111.3 (1)
O3^{i}—Mn1—N1	102.0 (1)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
OW1—H1W1···O3^{i}	0.86 (4)	2.15 (3)	2.949 (6)	156 (5)

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

The aromatic H atoms were positioned geometrically and were included in the refinement in the riding-model approximation [C—H = 0.93 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C)]. The water H atoms were located in a difference Fourier map and were refined with a distance restraint of O—H = 0.85 (1) Å and with fixed isotropic displacement parameters of $U_{\rm iso}$(H) = 0.08 Å^2. The data completeness is only 94.6% due to the low quality of the crystal.

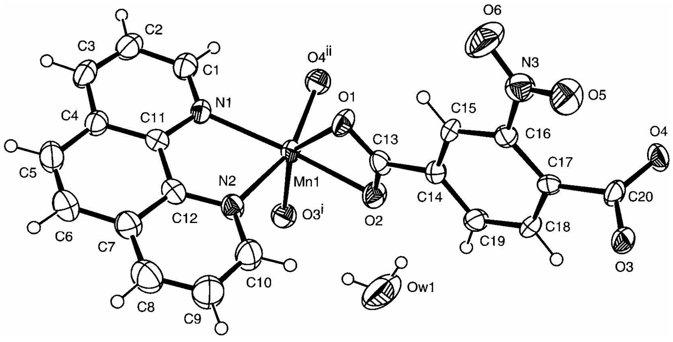

Figure 1
ORTEP-3 view (Farrugia, 1997) of a portion of the title compound. Displacement ellipsoids are drawn at the 40% probability level. [Symmetry codes: (i) $-\frac{1}{2} + x, -y, z$; (ii): $\frac{1}{2} - x, -\frac{1}{2} - y, \frac{1}{2} - z$.]

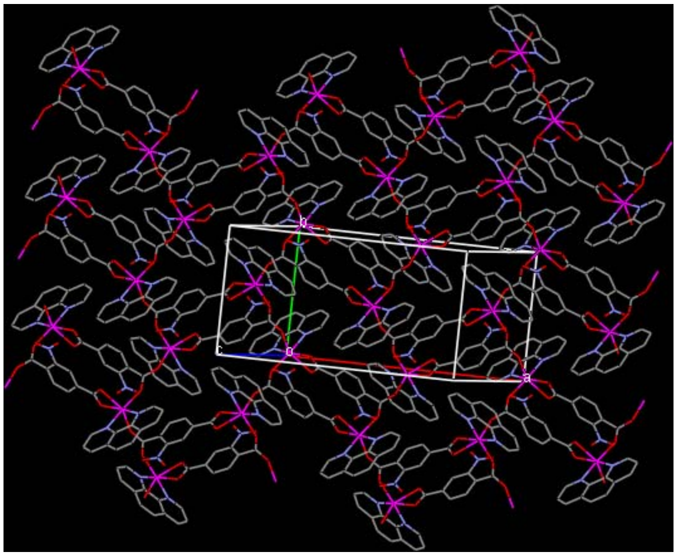

Figure 2
View of the two-dimensional network of the title compound. H atoms and uncoordinated water molecules have been omitted for clarity.

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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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