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cis-Diaqua(1,10-phenanthroline-κ^2N,N')-(pyridine-2,5-dicarboxylato-κ^2N,O)-manganese(II) monohydrate

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In the title compound, $[Mn(C_7H_3NO_4)(C_{12}H_8N_2)(H_2O)_2]\cdot H_2O$, the Mn^{II} atom is surrounded by one 1,10-phenanthroline (phen) ligand, one pyridine-2,5-dicarboxylate (pydc) dianion and two water molecules in a distorted octahedral MnN_3O_3 coordination. Hydrogen bonding between neighbouring molecules leads to a two-dimensional network.

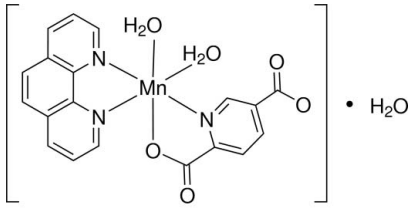
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.093
Data-to-parameter ratio = 15.4

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

Comment

The pyridine-2,5-dicarboxylate anion (pydc) displays different coordination modes, owing to the presence of two carboxylate groups in the 2- and 5-positions and an N atom in the 1-position (Zhang *et al.*, 2005; Mohamed & Thomas, 1994; Zhao *et al.*, 2005). We have prepared and structurally characterized the title complex, (I).



(I)

Complex (I) is the second example of an Mn–pydc–phen complex, (II) (Zhang *et al.*, 2005) but the crystal structure is different from that reported previously. The Mn^{II} atom is coordinated by one 1,10-phenanthroline (phen), one pydc and two water molecules with a distorted octahedral geometry (Fig. 1). Both the pydc and phen ligands chelate in a bidentate fashion to the Mn atom; two coordinated water molecules occupy *cis*-positions of the octahedron. The two five-

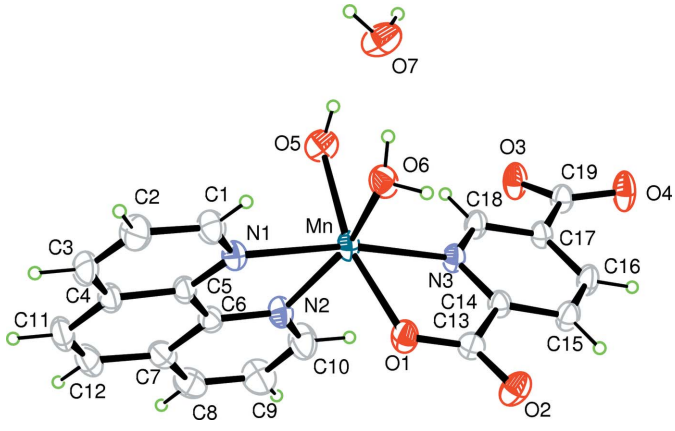


Figure 1
The molecular structure of (I), shown with 40% probability displacement ellipsoids.

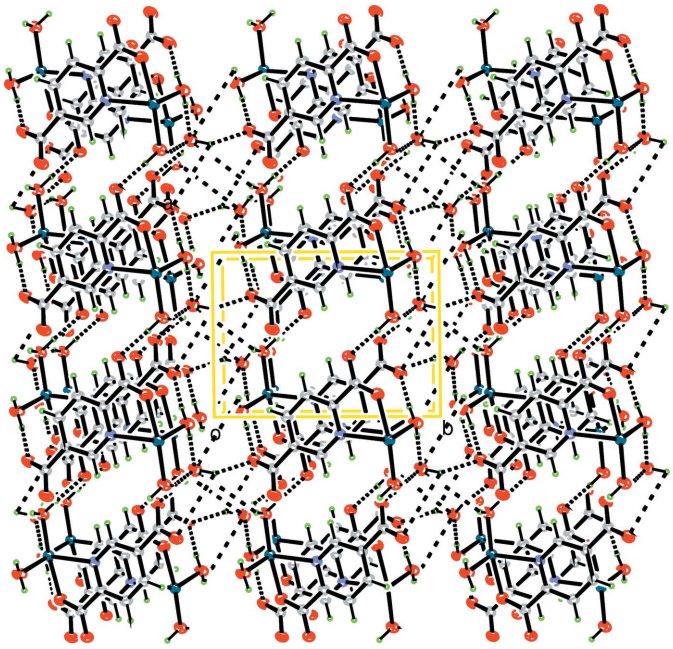
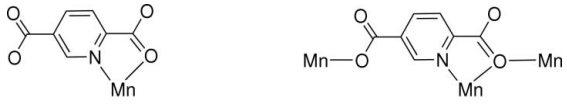


Figure 2
View of the O—H···O hydrogen-bonded (dashed lines) two-dimensional network. Phen rings not involved in hydrogen bonding have been omitted.

membered rings display an envelope conformation, with the Mn^{II} atom in the flap position and deviating from the mean planes formed by the other four atoms by 0.0752 (6) and 0.0296 (6) Å. The Mn—N bond lengths are almost equal to those of the aforementioned Mn^{II} complex, while the Mn—O bond lengths are slightly shorter (Zhang *et al.*, 2005; Mohamed & Thomas, 1994). The pyridine ring plane of pydc and the phen plane are nearly perpendicular to each other, the dihedral angle being 71.76 (5)°. In the analogous Mn^{II} complex, (II), which has the same ligands as in (I), pydc acts as a chelating–bridging ligand (Zhang *et al.*, 2005). The two coordination modes are depicted in the scheme below.



H and O atoms of water molecules and uncoordinated O atoms of pydc are all involved in intermolecular O—H···O hydrogen bonding, resulting in a two-dimensional network (Table 2 and Fig. 2). The crystal structure appears to be tightly consolidated by extensive hydrogen bonds.

Experimental

A solution of $MnCl_2·H_2O$ (0.0396 g, 0.2 mmol) and pyridine-2,5-dicarboxylate (0.0334 g, 0.2 mmol) dissolved in water (20 ml) was added to an ethanol solution (5 ml) of 1,10-phenanthroline (0.0396 g, 0.2 mmol). The pale-yellow solution was left to stand to allow the solvent to evaporate. Yellow needle-shaped crystals of (I) were obtained after three weeks.

Crystal data

$[Mn(C_7H_3NO_4)(C_{12}H_8N_2)(H_2O)_2]·H_2O$
M_r = 454.30
Triclinic, $P\overline{1}$
a = 7.4549 (3) Å
b = 10.2413 (4) Å
c = 12.4397 (9) Å
α = 90.141 (4)°
β = 92.127 (3)°
γ = 90.4630 (10)°
V = 949.06 (9) Å^3
Z = 2
D_x = 1.590 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3497 reflections
θ = 2.6–27.4°
μ = 0.75 mm^{-1}
T = 295 (1) K
Needle, yellow
0.28 × 0.13 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.786, T_{max} = 0.928
8776 measured reflections
4176 independent reflections
3652 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.5°
$h = -9 \rightarrow 8$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.093
S = 1.06
4176 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.3299P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn—O1	2.1242 (13)	Mn—N2	2.2716 (16)
Mn—O5	2.1420 (14)	Mn—N1	2.2727 (15)
Mn—O6	2.1636 (13)	Mn—N3	2.3167 (14)
O1—Mn—O5	164.75 (5)	O6—Mn—N1	88.45 (5)
O1—Mn—O6	86.35 (5)	N2—Mn—N1	73.08 (5)
O5—Mn—O6	87.36 (5)	O1—Mn—N3	74.36 (5)
O1—Mn—N2	95.97 (6)	O5—Mn—N3	93.52 (5)
O5—Mn—N2	94.40 (6)	O6—Mn—N3	102.56 (5)
O6—Mn—N2	161.48 (5)	N2—Mn—N3	95.74 (5)
O1—Mn—N1	101.58 (5)	N1—Mn—N3	167.85 (5)
O5—Mn—N1	92.12 (6)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H71···O3^{i}	0.84	1.90	2.721 (2)	169
O7—H72···O4^{ii}	0.92	1.94	2.760 (2)	147
O6—H61···O4^{iii}	0.88	1.82	2.6953 (19)	176
O6—H62···O7	0.83	1.88	2.692 (2)	168
O5—H52···O7	0.84	2.07	2.861 (2)	155
O5—H51···O2^{iv}	0.88	1.75	2.6302 (19)	178

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

The H atoms of the phen and pyridine-2,5-dicarboxylate were placed in calculated positions, with C—H = 0.93 Å, and were included in the final cycles of refinement in riding mode, with U_{iso}(H) = 1.2U_{eq}(C). The H atoms of the water molecules were located in difference Fourier maps and treated as riding in their as-found relative positions, with U_{iso}(H) = 1.2U_{eq}(O).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/

MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); 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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