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catena-Poly[[[4-(1*H*-1,3,7,8-tetraazacyclopenta-[*l*]phenanthren-2-yl)phenol]manganese(II)]-μ-benzene-1,4-dicarboxylato]

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Key indicators

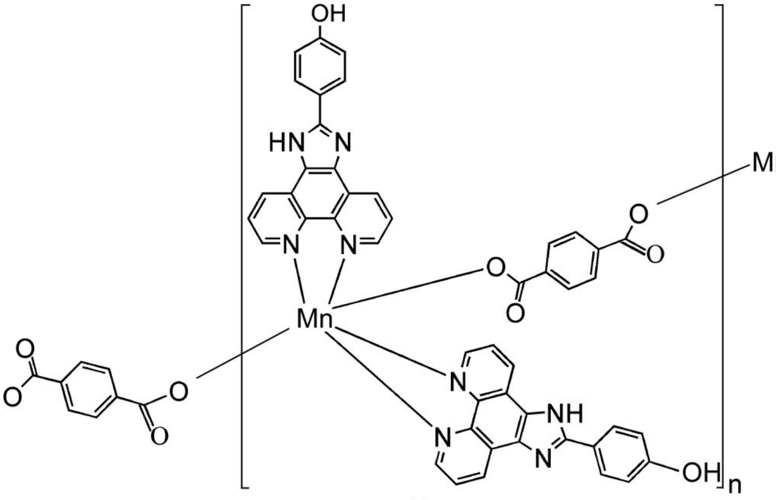
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.126
Data-to-parameter ratio = 14.8

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

In the title compound, $[Mn(C_8H_4O_4)(C_{19}H_{12}N_4O)_2]_n$ or $[Mn(1,4\text{-BDC})(L)_2]_n$, where 1,4-BDC is the benzene-1,4-dicarboxylate dianion and L is 4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)phenol, the Mn^{II} atom is six-coordinated by two bidentate L and two monodentate 1,4-BDC ligands, resulting in a distorted *trans*-MnO_2N_4 octahedral geometry. The Mn^{II} atoms are bridged by the 1,4-BDC ligands, forming a single-chain polymer structure. In addition, neighboring single chains interact through π–π interactions, generating a two-dimensional network. Mn has site symmetry $\overline{1}$; the complete 1,4-BDC unit is also built up by inversion symmetry.

Comment

Coordination polymers with a variety of supramolecular structures are attracting increasing interest because of their novel topologies and potential applications as functional materials (Eddaoudi *et al.*, 2001). The 1,10-phenanthroline (phen) ligand has been widely used to build novel supramolecular architectures through its aromatic π–π interactions (Chen & Liu, 2002). As one important derivative of phen, 4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)-phenol (L), was recently shown to form a coordination polymer with a distinctive supramolecular architecture (Che *et al.*, 2006). We selected benzene-1,4-dicarboxylic acid (1,4-H_2BDC) to act as a metal–metal linker in its deprotonated form and L as a secondary ligand, generating the title compound, [Mn(1,4-BDC)$(L)_2$], (I), a new coordination polymer, which is reported here.



(I)

In compound (I), the Mn^{II} atom is coordinated by four N atoms from two bidentate L ligands and two O atoms from

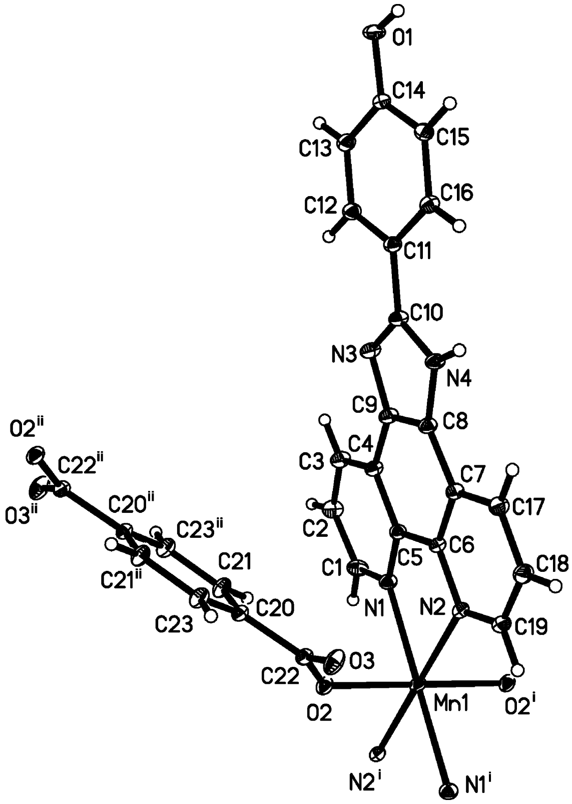


Figure 1
The asymmetric unit of compound (I), together with symmetry-equivalent atoms to complete the Mn coordination and the 1,4-BDC ligand, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry codes: (i) $-x$, $-y$, $1 - z$; (ii) $-x$, $-y$, $-z$.]

two 1,4-BDC ligands in a distorted *cis*-MnO_2N_4 octahedral geometry (Fig. 1). Mn1 has site symmetry $\overline{1}$ and the complete 1,4-BDC dianion is also generated by inversion. The Mn—O and mean Mn—N distances [2.296 (2) Å] in (I) (Table 1) are comparable to those observed for [Mn(1,4-BDC)(L')$_2$] [L' is (2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]-phenanthrene] (Che, 2006). Neighbouring Mn^{II} atoms are bridged by 1,4-BDC ligands, forming a single-chain structure (Fig. 2). The C—O bond lengths (Table 1) indicate that the carboxylate bonding is essentially localized.

Neighbouring single chains in (I) are connected through π–π interactions between L ligands with a π–π stacking distance of 3.53 Å, resulting in a two-dimensional supramolecular structure (Fig. 3) (Noveron *et al.*, 2002). Finally, interchain N—H$\cdots$O and O—H$\cdots$O hydrogen bonds (Table 2) complete the structure of (I).

Experimental

Ligand L was synthesized according to the literature method of Steck & Day (1943). An ethanolic solution (8 ml) of L (0.5 mmol) was added slowly to an aqueous solution (6 ml) of $MnCl_2\cdot 2H_2O$ (0.5 mmol) and 1,4-H_2BDC (1 mmol) with stirring at refluxing temperature. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature for two weeks, yielding yellow crystals of (I) (49% yield based on Mn).

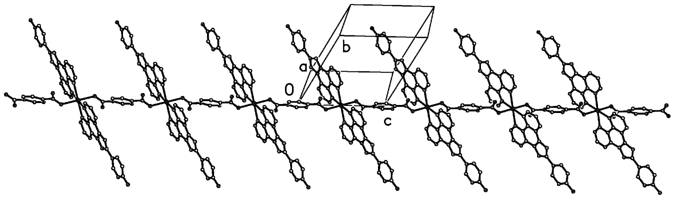


Figure 2
View of the single-chain structure of (I). H atoms have been omitted.

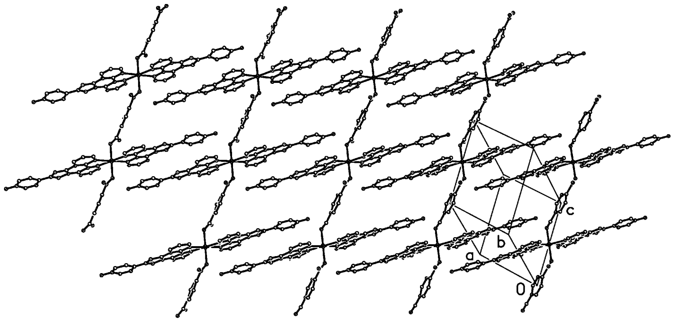


Figure 3
View of the two-dimensional supramolecular structure of (I) formed through π–π interactions. H atoms have been omitted.

Crystal data

$[Mn(C_8H_4O_4)(C_{19}H_{12}N_4O)_2]$
$M_r = 843.70$
Triclinic, $P\overline{1}$
$a = 9.1936$ (18) Å
$b = 10.515$ (2) Å
$c = 11.056$ (2) Å
$\alpha = 61.77$ (3)°
$\beta = 78.55$ (3)°
$\gamma = 75.90$ (3)°
$V = 909.0$ (4) Å^3
$Z = 1$
$D_x = 1.541$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.43$ mm^{-1}
$T = 292$ (2) K
Block, yellow
0.32 × 0.30 × 0.27 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.865$, $T_{max} = 0.891$
8954 measured reflections
4106 independent reflections
3064 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.126$
$S = 1.10$
4106 reflections
277 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.1901P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.51$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C22—O3	1.224 (3)	Mn1—N1	2.283 (2)
C22—O2	1.283 (3)	Mn1—N2	2.309 (2)
Mn1—O2	2.1635 (16)		
N1—Mn1—N2	73.22 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O3^{i}	0.86	1.92	2.775 (3)	173
O1—H1A···O2^{ii}	0.82	1.93	2.654 (2)	147

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

All H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 Å) and refined as riding, with $U_{\rm iso}$(H)= 1.2$U_{\rm eq}$(carrier). The highest residual density peak is located 0.90 Å from atom H18.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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