

Poly[bis[[4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)phenol- $\kappa^2 N^7, N^8$]manganese(II)]-di- μ_3 -benzene-1,3-dicarboxylato- $\kappa^4 O:O':O'', O'''$]

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Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(C-C) = 0.006$ Å
 R factor = 0.063
 wR factor = 0.144
Data-to-parameter ratio = 14.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

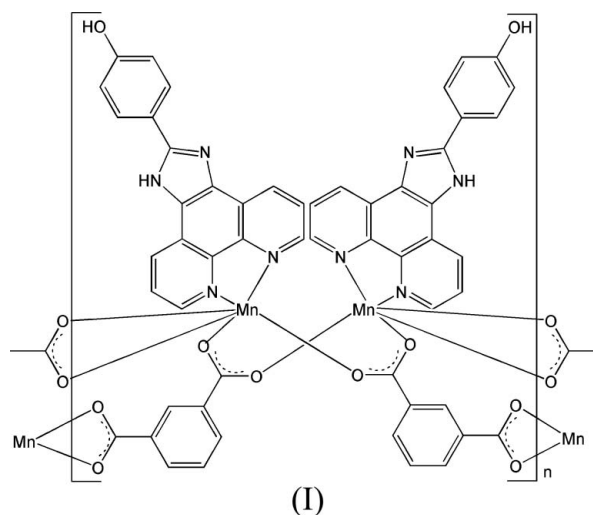
In the title complex, $[Mn_2(C_8H_4O_4)_2(C_{19}H_{12}N_4O)_2]_n$, the Mn^{II} atom is six-coordinated by two N atoms from the substituted phenanthroline ligand and four O atoms from three different benzene-1,3-dicarboxylate (1,3-BDC) ligands. Adjacent Mn^{II} atoms are bridged by the 1,3-BDC ligands to form a double-chain structure which, in turn, is linked to neighboring double chains *via* π - π contacts to form a two-dimensional supramolecular structure.

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Comment

Research into metal-organic coordination polymers has attracted increasing attention over the past decade, not only because of their intriguing structural diversity but also because of their tremendous potential applications (Eddaoudi *et al.*, 2001). In general, two different types of interactions, *viz.* covalent bonds and non-covalent intermolecular forces, can be used to construct varied supramolecular architectures. As such, a number of metal-organic coordination polymers have been prepared from one-dimensional covalently bonded chains, yielding extended two-dimensional or three-dimensional supramolecular architectures through π - π interactions or hydrogen bonds. 1,10-Phenanthroline (phen), as a common organic ligand, has been widely used in the construction of metal-organic coordination polymers (Chen & Liu, 2002). However, 4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)phenol (*L*) (Che *et al.*, 2006), a derivative of phen, possessing a large aromatic system, has been used less in the construction of coordination polymers. The structure of a new complex $[Mn_2(L)_2(1,3-BDC)_2]_n$, (I), where 1,3-BDC is benzene-1,3-dicarboxylate, is presented here.



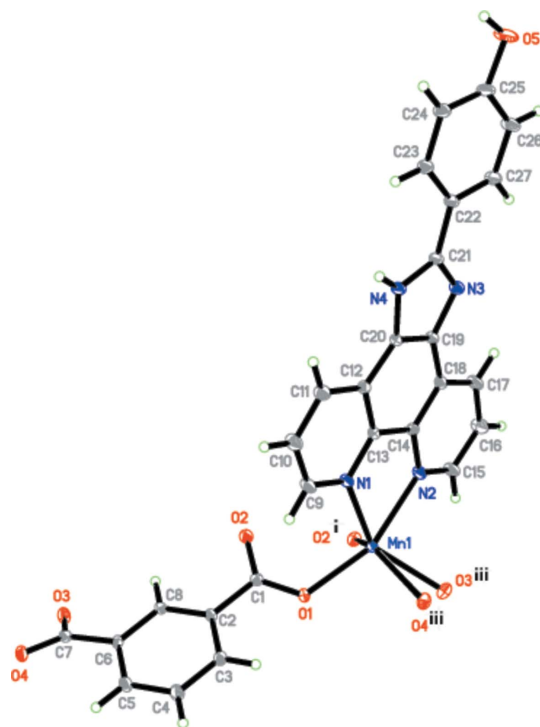


Figure 1
The asymmetric unit of (I), together with additional atoms to complete the coordination of Mn1, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $1 - x, y, \frac{3}{2} - z$; (iii) $x, -y, z - \frac{1}{2}$.]

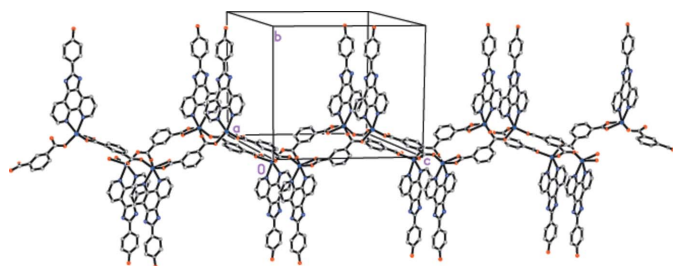


Figure 2
View of the double-chain structure of (I). H atoms have been omitted for clarity.

In complex (I) (Fig. 1 and Table 1), each Mn^{II} atom is six-coordinated by two N atoms derived from an *L* ligand and four O atoms from three different 1,3-BDC ligands. Neighboring Mn^{II} atoms are bridged by 1,3-BDC ligands, forming a one-dimensional double-chain structure as shown in Fig. 2. Neighboring double chains are connected by π - π interactions, generating a two-dimensional supramolecular structure as illustrated in Fig. 3. The π - π stacking distance is approximately 3.51 Å between *L* ligands within a double chain, while this distance is approximately 3.64 Å between adjacent double chains. Finally, interchain $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2) complete the crystal structure of (I).

Experimental

The *L* ligand was synthesized according to the literature (Steck & Day, 1943). A methanol solution (10 ml) of *L* (0.5 mmol) was added

slowly to an aqueous solution (10 ml) of $\text{MnCl}_2\cdot 2\text{H}_2\text{O}$ (0.5 mmol) and 1,3- H_2BDC (1 mmol) with stirring at 353 K. The resulting solution was filtered, the filtrate was allowed to stand in air at room temperature for several days, and pale-yellow crystals of (I) were obtained (yield 43% based on Mn).

Crystal data

$[\text{Mn}_2(\text{C}_8\text{H}_4\text{O}_4)_2(\text{C}_{19}\text{H}_{12}\text{N}_4\text{O})_2]$
 $M_r = 531.38$
 Monoclinic, $C2/c$
 $a = 15.318$ (3) Å
 $b = 16.453$ (3) Å
 $c = 18.660$ (4) Å
 $\beta = 109.78$ (3)°
 $V = 4425.4$ (17) Å³

$Z = 8$
 $D_x = 1.595$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.65$ mm⁻¹
 $T = 292$ (2) K
 Block, pale yellow
 $0.31 \times 0.28 \times 0.22$ mm

Data collection

Rigaku R-Axis RAPID
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.811, T_{\text{max}} = 0.863$

21264 measured reflections
 5038 independent reflections
 2882 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.113$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.063$
 $wR(F^2) = 0.144$
 $S = 1.04$
 5038 reflections
 337 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 3.4614P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.62$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.44$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Mn1—O1	2.155 (2)	O2—Mn1 ⁱ	2.106 (3)
Mn1—N1	2.313 (3)	O3—Mn1 ⁱⁱ	2.275 (3)
Mn1—N2	2.263 (3)	O4—Mn1 ⁱⁱ	2.303 (3)
O2 ⁱ —Mn1—O1	95.80 (11)	N2—Mn1—O4 ⁱⁱⁱ	106.67 (11)
O2 ⁱ —Mn1—N2	83.35 (12)	O3 ⁱⁱⁱ —Mn1—O4 ⁱⁱⁱ	57.02 (10)
O1—Mn1—N2	158.72 (11)	O2 ⁱ —Mn1—N1	122.07 (12)
O2 ⁱ —Mn1—O3 ⁱⁱⁱ	85.44 (11)	O1—Mn1—N1	91.44 (10)
O1—Mn1—O3 ⁱⁱⁱ	115.44 (11)	N2—Mn1—N1	71.49 (11)
N2—Mn1—O3 ⁱⁱⁱ	85.74 (11)	O3 ⁱⁱⁱ —Mn1—N1	140.35 (11)
O2 ⁱ —Mn1—O4 ⁱⁱⁱ	139.26 (10)	O4 ⁱⁱⁱ —Mn1—N1	98.29 (11)
O1—Mn1—O4 ⁱⁱⁱ	87.89 (10)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O5—H5A ^v ···O1 ^{iv}	0.86 (4)	1.95 (4)	2.705 (4)	145 (4)
N4—H4A ^v ···O4 ^v	0.86	2.03	2.839 (4)	156

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

The C- and N-bound H atoms were included in the riding model approximation with $\text{C}-\text{H} = 0.93$ Å and $\text{N}-\text{H} = 0.86$ Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$. The position of the H atom of the OH group was refined freely, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

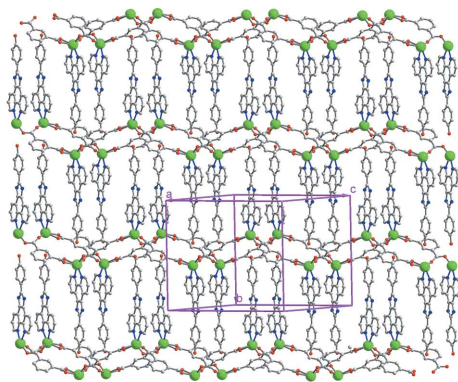


Figure 3
View of the two-dimensional supramolecular structure of (I) generated by π - π interactions. H atoms have been omitted for clarity.

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 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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