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Key indicators

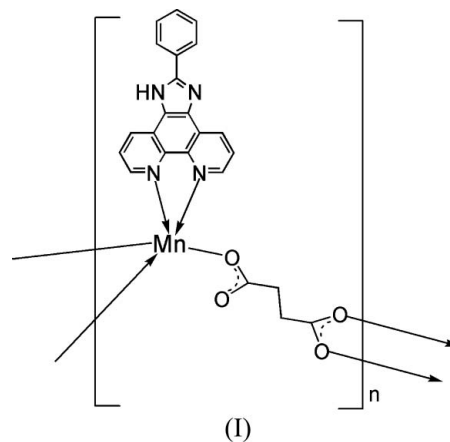
Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.045
 wR factor = 0.108
Data-to-parameter ratio = 18.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[[2-phenyl-1*H*-1,3,7,8-tetraaza-
cyclopenta[*l*]phenanthrene)manganese(II)]-
 μ -succinato]**

In the title compound, $[\text{Mn}(\text{C}_4\text{H}_4\text{O}_4)(\text{C}_{19}\text{H}_{12}\text{N}_4)]_n$ or $[\text{Mn}(\text{suc})(L)]_n$, where *suc* is the succinate dianion and *L* is 2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene, each Mn^{II} atom is five-coordinated by two N atoms from one bidentate *L* ligand and three O atoms from three *suc* anions in a distorted square-based pyramidal geometry, with the N atoms in the basal plane. The Mn^{II} atoms are bridged by the *suc* ligands, generating a one-dimensional chain structure. Neighboring chains interact through π - π contacts, leading to a two-dimensional supramolecular structure. $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds complete the structure.

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Comment

Metal-organic coordination polymers utilizing simple hetero-aromatic *N*-donor chelating ligands such as 1,10-phenanthroline (*phen*) and more complex derivatives such as 2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene (*L*) are the subjects of increasing interest (Che, 2006; Che & Liu, 2006). We have now combined manganese(II) cations with the succinate (*suc*) dianion as a linker and *L* as a secondary ligand, forming a new coordination polymer, $[\text{Mn}(\text{suc})(L)]_n$, (I), which is reported here.



Selected bond lengths and angles for (I) are given in Table 1. In compound (I), the Mn^{II} atom is five-coordinated by three O atoms from three different *suc* ligands, and two N atoms from one *L* molecule in a distorted square-based pyramidal geometry, in which atoms N1, N2, O3ⁱ and O4ⁱⁱ form the basal plane [symmetry codes: (i) $2 - x, 1 - y, 1 - z$; (ii) $2 - x, y, 1 - z$], and O1 occupies the apical position (Fig. 1). Neighbouring Mn^{II} atoms are bridged by the *suc* ligands, forming a chain structure (Fig. 2). The carboxylate C—O bond distances of the *suc* species suggest that their bonding is more or less delocalized.

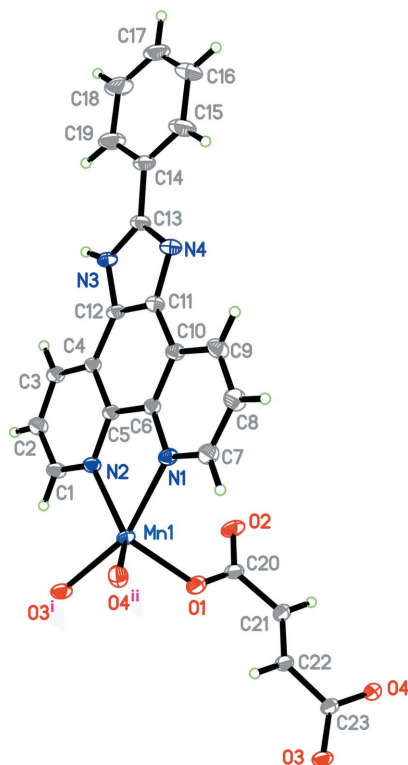


Figure 1

The asymmetric unit of (I), expanded to show the Mn coordination environment. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry codes: (i) $2 - x, 1 - y, 1 - z$; (ii) $2 - x, y, 1 - z$.]

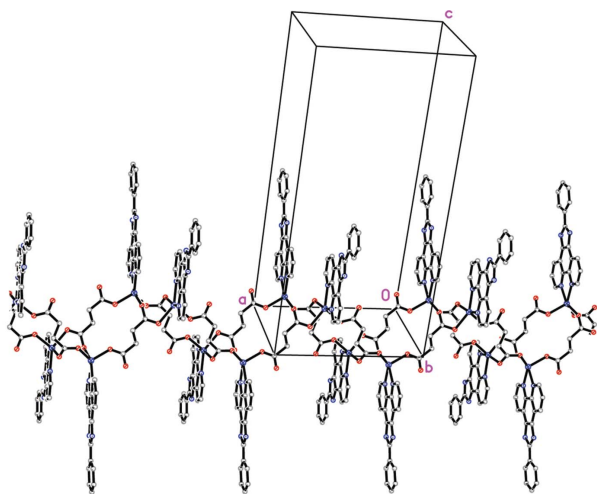


Figure 2

View of the one-dimensional chain structure of (I). H atoms have been omitted for clarity.

Neighboring chains in (I) are connected through π - π interactions between *L* ligands with a stacking distance of 3.63 Å, resulting in a two-dimensional supramolecular structure (Fig. 3). Finally, an N—H...O hydrogen bond between atom N3 of *L* and a symmetry-equivalent of the suc carboxylate O2 atom (the only one not bonded to Mn) completes the structure (Table 2).

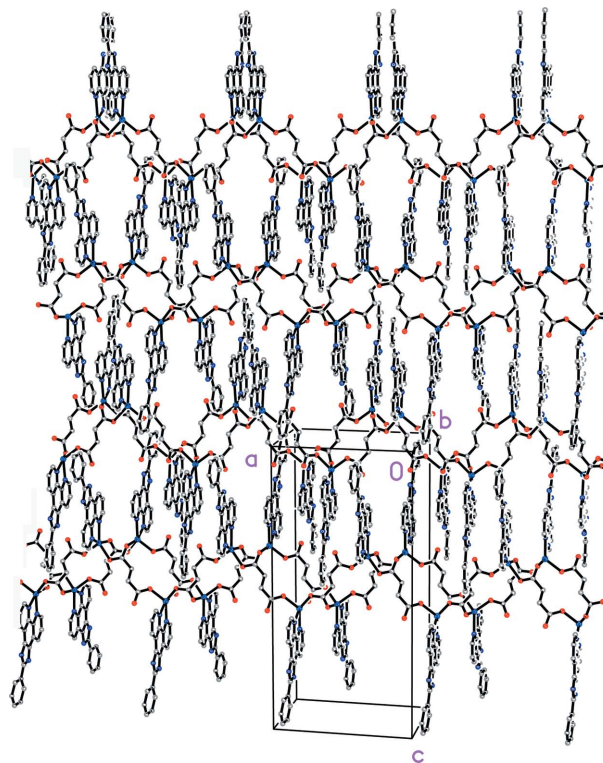


Figure 3

View of the two-dimensional supramolecular structure of (I) built up via π - π interactions. H atoms have been omitted.

Experimental

The *L* ligand was synthesized according to a literature method (Steck & Day, 1943). A methanol solution (10 ml) of *L* (0.5 mmol, 148 mg) was added slowly to an aqueous solution (10 ml) of $\text{MnCl}_2 \cdot 6\text{H}_2\text{O}$ (0.5 mmol, 116 mg) and H_2suc (0.5 mmol, 59 mg) with stirring. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature for several days, yielding colorless crystals of (I) (33% yield based on Mn).

Crystal data

$[\text{Mn}(\text{C}_4\text{H}_4\text{O}_4)(\text{C}_{19}\text{H}_{12}\text{N}_4)]$
 $M_r = 465.32$
 Orthorhombic, *Pcca*
 $a = 13.920$ (3) Å
 $b = 9.879$ (2) Å
 $c = 28.548$ (6) Å
 $V = 3925.9$ (14) Å³

$Z = 8$
 $D_x = 1.575$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.71$ mm⁻¹
 $T = 292$ (2) K
 Block, colorless
 $0.24 \times 0.21 \times 0.19$ mm

Data collection

Rigaku R-Axis RAPID
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.830, T_{\max} = 0.880$

36189 measured reflections
 4487 independent reflections
 2470 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.103$
 $\theta_{\max} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.108$
 $S = 0.94$
 4487 reflections
 245 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0524P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.44$ e Å⁻³
 $\Delta\rho_{\min} = -0.23$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

C20—O2	1.230 (3)	Mn1—O4 ⁱ	2.1289 (19)
C20—O1	1.259 (3)	Mn1—O3 ⁱⁱ	2.130 (2)
C23—O4	1.242 (3)	Mn1—N1	2.220 (2)
C23—O3	1.271 (3)	Mn1—N2	2.231 (2)
Mn1—O1	2.0292 (18)		
O1—Mn1—O4 ⁱ	92.83 (8)	O3 ⁱⁱ —Mn1—N1	159.20 (7)
O1—Mn1—O3 ⁱⁱ	99.30 (8)	O1—Mn1—N2	126.02 (8)
O4 ⁱ —Mn1—O3 ⁱⁱ	93.79 (8)	O4 ⁱ —Mn1—N2	140.02 (8)
O1—Mn1—N1	100.49 (8)	O3 ⁱⁱ —Mn1—N2	89.20 (7)
O4 ⁱ —Mn1—N1	91.56 (8)	N1—Mn1—N2	73.99 (8)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N3—H3A \cdots O2 ⁱⁱⁱ	0.86	1.92	2.760 (3)	166

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

All H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

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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