Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

A new Mn^{II} coordination polymer with a double-chain structure

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Received 3 May 2006
Accepted 25 May 2006

Key indicators

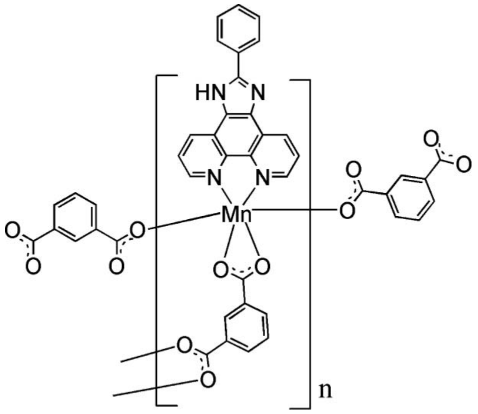
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.118
Data-to-parameter ratio = 15.2

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

In the title compound, poly[[(2-phenyl-1*H*-1,3,7,8,-tetraazacyclopenta[*l*]phenanthrene)manganese(II)]-μ-benzene-1,3-dicarboxylato], $[Mn(C_8H_4O_4)(C_{19}H_{12}N_4)]_n$, the Mn^{II} atom is hexacoordinated by two N atoms from the phenanthrene ligand, and four O atoms from three different benzene-1,3-dicarboxylate (*m*-BDC) ligands. The Mn^{II} atoms are bridged by the *m*-BDC ligands, forming a double-chain structure. Moreover, neighbouring double chains are in contact through π–π interactions, generating a two-dimensional supramolecular structure.

Comment

In recent years, metal coordination polymers have received much attention for their intriguing structural features and potential applications (Eddaoudi *et al.*, 2002; Ma *et al.*, 2001, 2003). In general, two different types of interactions (covalent bonds and non-covalent intermolecular forces) can be used to construct varied supramolecular architectures. On this basis, a number of compounds 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) is an important ligand, having often been used to build novel supramolecular architectures due to its excellent coordinating ability and large conjugated system that can easily form π–π interactions (Chen & Liu, 2002). However, coordination polymers based on 2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene (*L*) derived from phen have not been investigated. We report here the crystal structure of [Mn(*m*-BDC)(*L*)] (*m*-BDC is benzene-1,3-dicarboxylate), (I), based on this ligand.



(I)

Selected bond lengths and angles for (I) are given in Table 1. In (I), the Mn^{II} centre is coordinated by four O atoms

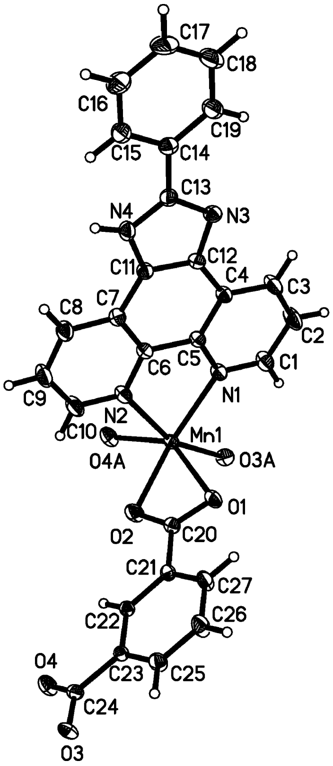


Figure 1

The asymmetric structure together with additional atoms to complete the Mn coordination, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (A) x, $1-y$, $\frac{1}{2}-z$ for O3A; $2-x$, $1-y$, $1-z$ for O4A.]

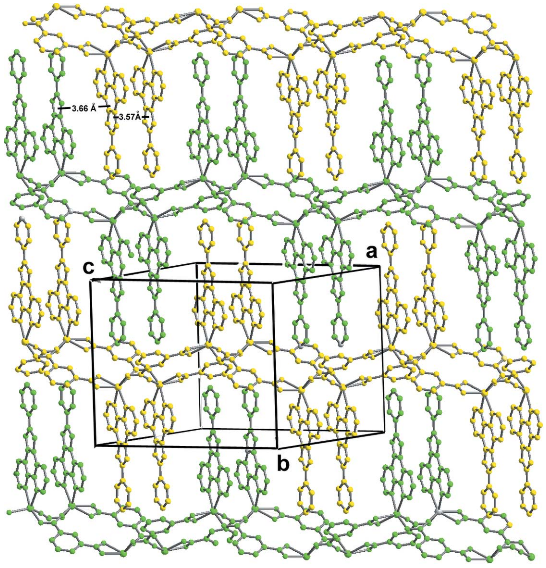


Figure 2

View of the two-dimensional supramolecular structure of (I), showing the double chains connected through π–π interactions. H atoms have been omitted.

from three *m*-BDC ligands and two N atoms from one *L* ligand in a slightly distorted octahedral coordination geometry (Fig. 1). The average Mn—O and Mn—N distances [2.2039 (12) and 2.295 (2) Å, respectively] are comparable to those observed for $[Mn(bqdc)(phen)(H_2O)_2]_n$ (bqdc = 2,2′-biquinoline-4,4′-dicarboxylate) (Ye *et al.*, 2006). Neighbouring Mn^{II} atoms are bridged by *m*-BDC ligands, forming a one-dimensional double-chain structure (Fig. 2).

Neighbouring double chains are connected by π–π interactions, generating a two-dimensional supramolecular structure (Fig. 2). The π–π stacking distance is about 3.57 Å between *L* ligands in the same double chain, while it is about 3.66 Å between adjacent double chains. It is obvious that aromatic interactions help to improve the stability of many current architectures (Noveron *et al.*, 2002).

Experimental

The ligand *L* was synthesized according to a literature method (Steck & Day, 1943). Complex (I) was prepared by adding an ethanol solution (10 ml) of *L* (0.5 mmol) slowly to an aqueous solution (10 ml) of $MnCl_2{\cdot}2H_2O$ (0.5 mmol) and *m*-H_2BDC (1 mmol) while stirring at 353 K. The resulting solution was filtered and the filtrate was left to stand in air at room temperature for several weeks, yielding pale-yellow crystals of (I) (70% yield based on Mn).

Crystal data

$[Mn(C_8H_4O_4)(C_{19}H_{12}N_4)]$
$M_r = 515.38$
Monoclinic, $C2/c$
$a = 15.390$ (5) Å
$b = 15.935$ (5) Å
$c = 18.839$ (5) Å
$\beta = 109.328$ (5)°
$V = 4360$ (2) Å^3
$Z = 8$
$D_x = 1.570$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.65$ mm^{-1}
$T = 292$ (2) K
Block, light yellow
0.33 × 0.28 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.804$, $T_{max} = 0.877$
18605 measured reflections
4944 independent reflections
3595 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.118$
$S = 1.03$
4944 reflections
325 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 2.055P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.02$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

N1—Mn1	2.312 (2)	O2—Mn1	2.2430 (18)
N2—Mn1	2.277 (2)	O3—Mn1^{i}	2.1211 (17)
O1—Mn1	2.347 (2)	O4—Mn1^{ii}	2.1046 (19)
O4^{ii}—Mn1—O3^{iii}	98.59 (7)	O2—Mn1—N1	141.86 (7)
O4^{ii}—Mn1—O2	85.22 (7)	N2—Mn1—N1	71.50 (7)
O3^{iii}—Mn1—O2	112.13 (8)	O4^{ii}—Mn1—O1	141.21 (7)
O4^{ii}—Mn1—N2	84.82 (8)	O3^{iii}—Mn1—O1	89.82 (7)
O3^{iii}—Mn1—N2	158.76 (7)	O2—Mn1—O1	56.80 (6)
O2—Mn1—N2	89.00 (8)	N2—Mn1—O1	100.67 (7)
O4^{ii}—Mn1—N1	123.62 (8)	N1—Mn1—O1	94.06 (7)
O3^{iii}—Mn1—N1	89.51 (7)		

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

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\rm iso}$(H)= 1.2$U_{\rm eq}$(C). The highest residual electron-density peak is located 1.04 Å from atom H2.

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: *SHELXTL-Plus*.

The authors thank Jilin Normal University for supporting this work.

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