Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

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

Guang-Bo Che

Department of Chemistry, Jilin Normal University, Siping 136000, People's Republic of China

Correspondence e-mail:
guangbochejl@yahoo.com

Received 4 May 2006
Accepted 5 May 2006

In the title compound, $[Mn(C_8H_4O_4)(C_{19}H_{12}N_4)_2]$, the Mn^{II} atom (site symmetry $\overline{1}$) is six-coordinated by two bidentate phenanthrene and two monodentate benzene-1,4-dicarboxylate ligands, resulting in a distorted *trans*-MnO_2N_4 octahedral coordination geometry. The Mn^{II} atoms are bridged by the centrosymmetric benzene-1,4-dicarboxylate ligands to form an extended single-chain structure. In addition, neighbouring single chains interact through π–π interactions, generating a two-dimensional network.

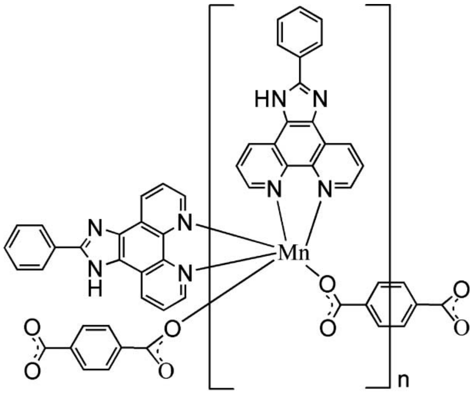
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
R factor = 0.054
wR factor = 0.142
Data-to-parameter ratio = 15.0

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

Comment

Coordination polymers with a variety of supramolecular structures have been studied extensively 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 aromatic π–π interactions (Chen & Liu, 2002). An important derivative of phen, 2-phenyl-1H-1,3,7,8-tetraazacyclopenta[l]phenanthrene (L) was used to synthesize various Ru^{II} complexes in order to recognise the secondary structure of DNA (Wu *et al.*, 1997). However, coordination polymers based on the ligand L have rarely been documented. We selected benzene-1,4-dicarboxylic acid (1,4-H_2BDC) as a linker and L as a secondary ligand, generating a new coordination polymer, [Mn(1,4-BDC)$(L)_2$], (I), which is reported here.



(I)

In compound (I), the Mn^{II} atom (site symmetry $\overline{1}$) is coordinated by four N atoms from two L ligands and two O atoms from two 1,4-BDC ligands in a distorted octahedral coordination (Fig. 1). The single unique 1,4-BDC species is generated from the atoms of the asymmetric unit by inversion. The dihedral angle between the C20/O1/O2 group and the benzene ring is 32.5 (2)°. The Mn—O and average Mn—N

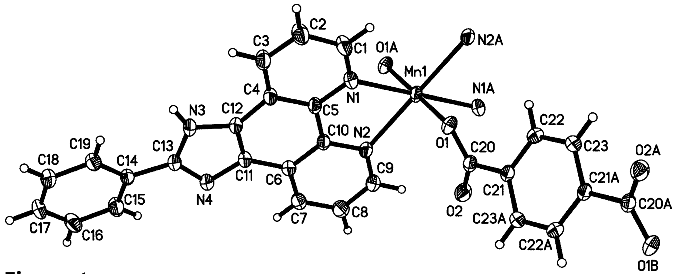


Figure 1
The asymmetric unit of (I), together with further atoms to complete the Mn1 coordination and the 1,4-BDC ligand. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). Atoms O1A/N1A/N2A are generated by the symmetry code ($-x$, $-y$, $-z$) and C20A/C21A/C22A/C23A/O1A/O2A by ($1 - x$, $1 - y$, $-z$).

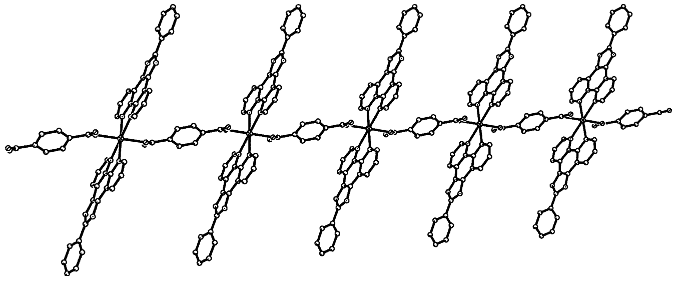


Figure 2
View of the single-chain structure of (I). H atoms have been omitted.

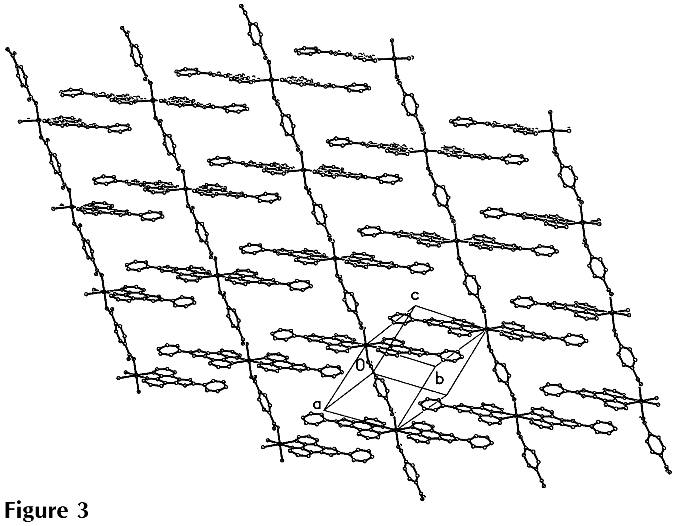


Figure 3
View of the two-dimensional supramolecular structure of (I) formed through π–π interactions. H atoms have been omitted.

[2.310 (2)Å] distances in (I) (Table 1) are comparable to those observed in $[Mn(bqdc)(phen)(H_2O)_2]_n$ (bqdc = 2,2′-biquinoline-4,4′-dicarboxylate) (Ye *et al.*, 2006). Neighbouring Mn^{II} atoms are bridged by 1,4-BDC ligands, forming a single-chain structure with an $Mn\cdots Mn^{i}$ [symmetry code: (i) $1 - x$, $1 - y$, $-z$] separation of 11. 16 (2) Å (Fig. 2). The C—O bond lengths (Table 1) indicate delocalization of the negative charge of the carboxylate group.

It is noteworthy that neighbouring single chains are connected through π–π interactions between *L* ligands with a π–π stacking distance of 3.58Å, resulting in a two-dimensional supramolecular structure (Fig. 3). It is clear that these aromatic–aromatic interactions help to stabilize the supramolecular structure of (I) (Noveron *et al.*, 2002), as does an interchain N—H$\cdots$O hydrogen bond (Table 2).

Experimental

Ligand *L* was synthesized by the literature method (Steck & Day, 1943). An ethanolic solution (10 ml) of *L* (0.5 mmol) was added slowly to an aqueous solution (10 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 several weeks, yielding yellow crystals of (I) (63% yield based on Mn).

Crystal data

$[Mn(C_8H_4O_4)(C_{19}H_{12}N_4)_2]$
$M_r = 811.72$
Triclinic, $P\bar{1}$
$a = 9.6550$ (19) Å
$b = 10.451$ (2) Å
$c = 10.626$ (2) Å
$\alpha = 90.48$ (3)°
$\beta = 114.87$ (3)°
$\gamma = 111.63$ (3)°
$V = 887.1$ (5) Å^3
$Z = 1$
$D_x = 1.519$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.43$ mm^{-1}
$T = 292$ (2) K
Block, yellow
0.30 × 0.27 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.872$, $T_{max} = 0.918$
8728 measured reflections
4009 independent reflections
2443 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.143$
$S = 1.05$
4009 reflections
268 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 0.1905P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.106 (2)	C20—O2	1.246 (4)
Mn1—N1	2.300 (2)	C20—O1	1.261 (4)
Mn1—N2	2.321 (3)		
N1—Mn1—N2	72.02 (9)		

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
N3—H3*A*$\cdots$O2^{ii}	0.86	1.94	2.769 (4)	163

Symmetry code: (ii) x, $y - 1$, z.

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

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 author thanks Jilin Normal University for supporting this work.

References

Chen, X.-M. & Liu, G.-F. (2002). *Chem. Eur. J.* **8**, 4811–4817.

Eddaoudi, M., Moler, D. B., Li, H., Chen, B., Reineke, T. M., O'Keeffe, M. & Yaghi, O. M. (2001). *Acc. Chem. Res.* **34**, 319–330.

Higashi, A. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.

Noveron, J. C., Lah, M. S., Sesto, R. E. D., Arif, A. M., Miller, J. S. & Stang, P. J. (2002). *J. Am. Chem. Soc.* **124**, 6613–6625.

Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.

Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Góttingen, Germany.

Steck, E. A. & Day, A. R. (1943). *J. Am. Chem. Soc.* **65**, 452–456.

Wu, J.-Z., Li, L., Zeng, T.-X., Ji, L.-N., Zhou, J.-Y., Luo, T. & Li, R.-H. (1997). *Polyhedron*, **16**, 103–107.

Ye, J.-W., Zhang, P., Ye, K.-Q., Zhang, H.-Y., Jiang, S.-M., Ye, L., Yang, G.-D. & Wang, Y. (2006). *J. Solid State Chem.* **179**, 438–449.