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## Key indicators

Single-crystal X-ray study  
 $T = 292$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.041  
 $wR$  factor = 0.100  
Data-to-parameter ratio = 15.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.(Benzene-1,2-dicarboxylato)bis[4-(1*H*-1,3,7,8-  
tetraazacyclopenta[*l*]phenanthren-2-yl)phenol]-  
manganese(II)

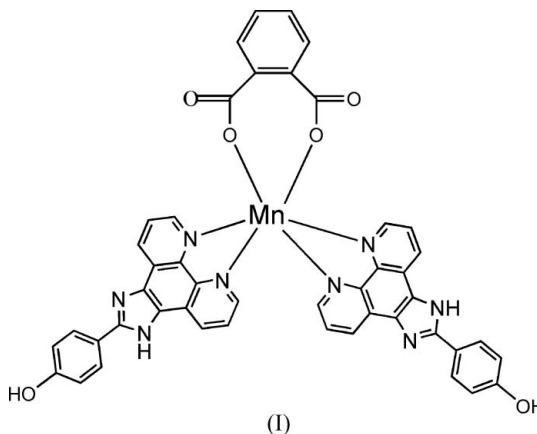
In the title compound,  $[\text{Mn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{19}\text{H}_{12}\text{N}_4\text{O})_2]$ , the  $\text{Mn}^{\text{II}}$  atom is six-coordinated by four N atoms from two bidentate 4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)phenol (*L*) ligands and two carboxylate O atoms from a bidentate benzene-1,2-dicarboxylate (BDC) ligand, resulting in a distorted *cis*- $\text{MnO}_2\text{N}_4$  octahedron. The complete molecule is generated by twofold symmetry, with the Mn atom lying on a twofold rotation axis. Aromatic  $\pi$ - $\pi$  stacking interactions between *L* ligands, and N—H $\cdots$ O and O—H $\cdots$ O hydrogen bonds complete the structure.

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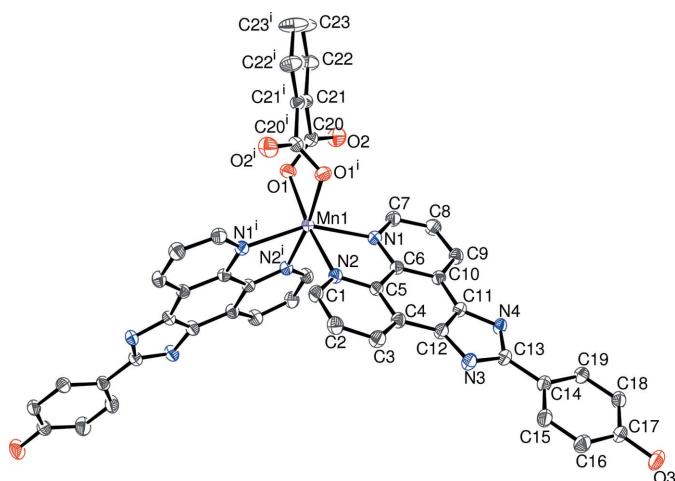
Accepted 5 September 2006

## Comment

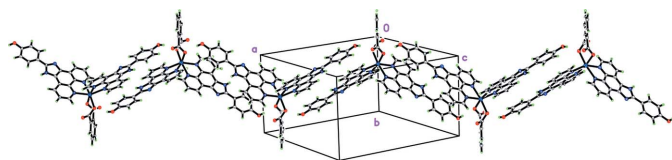
1,10-Phenanthroline (phen) has been widely used as a ligand in the construction of metal-organic frameworks, while an important derivative of phen, 4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)phenol (*L*) has recently been used to synthesize related metal-organic networks (Che *et al.*, 2006). As a continuation of this work, we have prepared the title compound,  $[\text{Mn}(\text{BDC})(\text{L})_2]$  (BDC<sup>2-</sup> is benzene-1,2-dicarboxylate), (I), from a combination of  $\text{Mn}^{2+}$ ,  $\text{H}_2\text{BDC}$  and *L* as a secondary chelating ligand.



In (I), each  $\text{Mn}^{\text{II}}$  atom is six-coordinated by four N atoms from two bidentate *L* ligands and two carboxylate O atoms from the same BDC ligand in a distorted *cis*- $\text{MnO}_2\text{N}_4$  octahedral coordination geometry (Fig. 1). The complete molecule is generated by twofold symmetry with the Mn atom lying on the rotation axis, which also bisects the C23—C23<sup>1</sup> bond [symmetry code: (i)  $1 - x, y, \frac{3}{2} - z$ ] of the BDC species. The Mn—O and mean Mn—N distances in (I) (Table 1) are comparable to those observed for  $[\text{Mn}(1,4\text{-BDC})(\text{L})_2]$  (Che, 2006). The carboxylate C20—O1 and C20—O2 bond lengths are very different, suggesting localization of bonding in the carboxylate groups.



**Figure 1**  
The molecular structure of (I) with displacement ellipsoids drawn at the 40% probability level and H atoms omitted for clarity. [Symmetry code: (i)  $1 - x, y, \frac{3}{2} - z$ .]



**Figure 2**  
View of the supramolecular chain structure of (I) arising from  $\pi$ - $\pi$  stacking.

Neighbouring  $[\text{Mn}(\text{BDC})(L)_2]$  molecules are connected through  $\pi$ - $\pi$  interactions between  $L$  ligands with a stacking distance of 3.49 Å, resulting in a chain-like supramolecular structure (Fig. 2). Finally,  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2) complete the structure of (I).

## Experimental

The  $L$  ligand was synthesized according to the method of Steck & Day (1943). An ethanol solution (14 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 1,2- $\text{H}_2\text{BDC}$  (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 one week, yielding yellow crystals of (I) (42% yield, based on Mn).

### Crystal data

$[\text{Mn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{19}\text{H}_{12}\text{N}_4\text{O})_2]$	$Z = 4$
$M_r = 843.70$	$D_x = 1.496 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 19.024 (4) \text{ \AA}$	$\mu = 0.42 \text{ mm}^{-1}$
$b = 11.375 (2) \text{ \AA}$	$T = 292 (2) \text{ K}$
$c = 17.513 (4) \text{ \AA}$	Block, yellow
$\beta = 98.77 (3)^\circ$	$0.27 \times 0.21 \times 0.17 \text{ mm}$
$V = 3745.5 (14) \text{ \AA}^3$	

### Data collection

Rigaku R-Axis RAPID  
diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)  
 $T_{\min} = 0.895$ ,  $T_{\max} = 0.930$

18033 measured reflections  
4281 independent reflections  
3392 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.042$   
 $\theta_{\max} = 27.5^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.100$   
 $S = 1.03$   
4281 reflections  
276 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 3.3682P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.71 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.25 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

C20—O1	1.282 (2)	Mn1—N1	2.2647 (15)
C20—O2	1.228 (2)	Mn1—N2	2.3001 (16)
Mn1—O1	2.1702 (14)		
O1 <sup>i</sup> —Mn1—O1	79.01 (7)	N1—Mn1—N2	72.84 (6)

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

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O3—H3 $\cdots$ O1 <sup>ii</sup>	0.82	1.98	2.741 (2)	155
N4—H4 $\cdots$ O2 <sup>iii</sup>	0.86	1.85	2.713 (2)	175

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

All H atoms were positioned geometrically ( $\text{C}-\text{H} = 0.93 \text{ \AA}$ ,  $\text{N}-\text{H} = 0.86 \text{ \AA}$ ,  $\text{O}-\text{H} = 0.82 \text{ \AA}$ ) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$  or  $1.5U_{\text{eq}}(\text{O})$ .

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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