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

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Key indicators

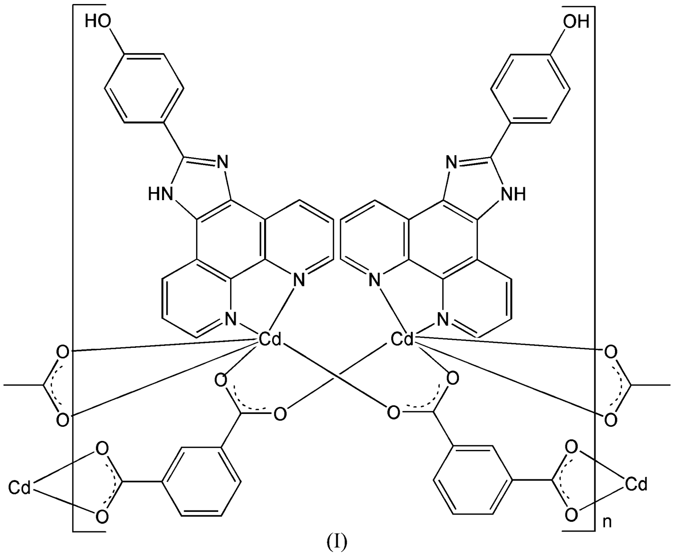
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.030
wR factor = 0.073
Data-to-parameter ratio = 12.7

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

In the title compound, $[Cd_2(C_8H_4O_4)_2(C_{19}H_{12}N_4O)_2]_n$, each Cd atom is six-coordinated by two N atoms from the substituted phenanthroline ligand and four O atoms from three different benzene-1,3-dicarboxylate (*m*-BDC) ligands. Pairs of Cd atoms with two carboxylate bridges form a dimeric unit with twofold rotation symmetry, and these dimeric units are further bridged by *m*-BDC ligands to form a double-chain structure. Furthermore, neighbouring double-chain polymers are interdigitated, leading to a two-dimensional supramolecular structure.

Comment

Metal–organic coordination polymers have attracted increasing interest over the past decade, not only because of their intriguing structural diversity but also because of their tremendous potential applications in catalysis, molecular adsorption, magnetism, nonlinear optics and molecular sensing (Hagrman *et al.*, 1999; Eddaoudi *et al.*, 2001). The most efficient approach to preparing coordination polymers is *via* direct chemical combination of functional inorganic and organic components (Ma *et al.*, 2003). 1,10-Phenanthroline (phen) and its derivatives, as one type of common organic ligand, have 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*) (Steck & Day, 1943), a derivative of phen possessing a large aromatic system, has received considerably less attention in the chemistry of coordination polymers. We present here the structure of a new compound, $[Cd_2(L)_2(m\text{-BDC})_2]_n$, (I).



(I)

doi:10.1107/S1600536806018654

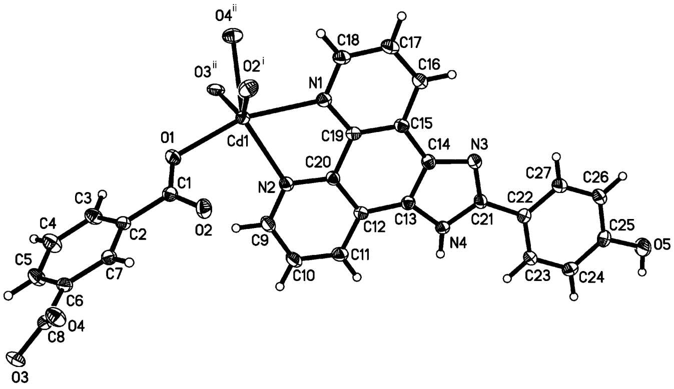


Figure 1

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

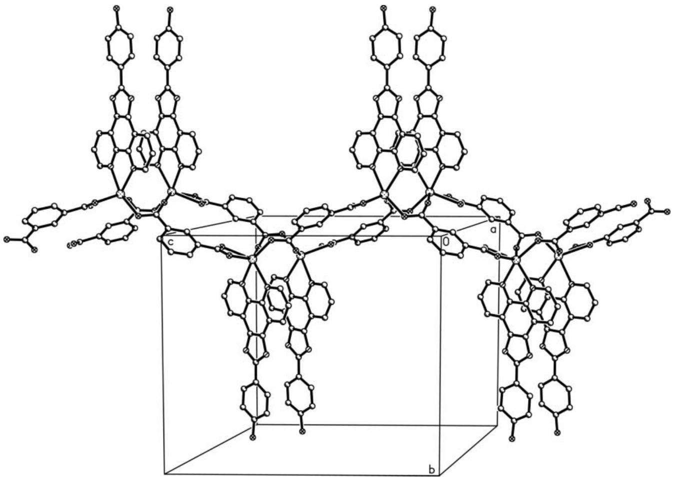


Figure 2

View of the double-chain structure in (I). H atoms have been omitted.

Selected bond lengths and angles for (I) are given in Table 1. In (I), each Cd atom is six-coordinated by two N atoms from an *L* ligand and four O atoms from three different *m*-BDC ligands (Fig. 1). Two adjacent Cd atoms are bridged by two *m*-BDC ligands through the bidentate carboxylate groups to form a dimeric unit with twofold rotation symmetry. There are π–π interactions between the phenanthroline units of the *L* ligands in the dimeric unit, with the shortest atom-to-atom distance being 3.578 (4) Å. The dimeric units are further connected by the *m*-BDC ligands through the chelating carboxylate groups to generate an interesting double-chain structure (Fig. 2). Neighbouring double-chain polymers are interdigitated, leading to a two-dimensional supramolecular structure (Fig. 3).

Experimental

Ligand *L* was synthesized according to a literature method (Steck & Day, 1943). A methanol solution (10 ml) of *L* (0.5 mmol) was added slowly to an aqueous solution (10 ml) of $CdCl_2 \cdot 2H_2O$ (0.5 mmol) and *m*-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 66% based on Cd).

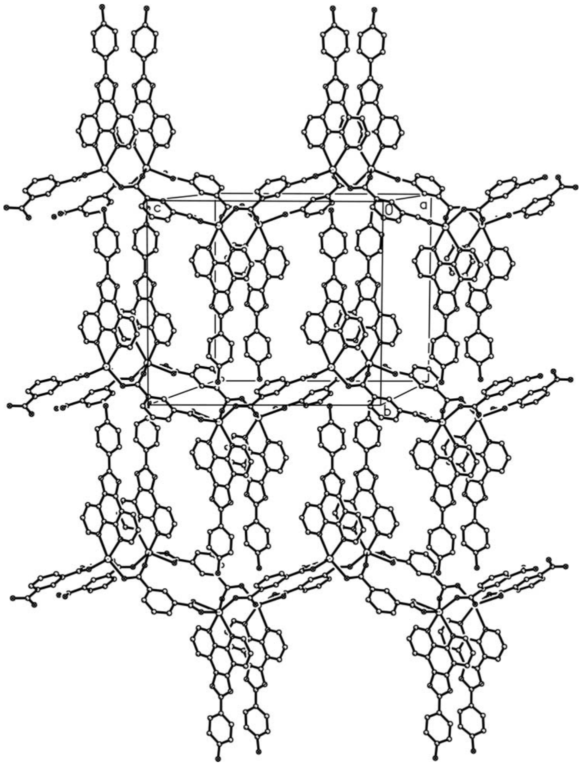


Figure 3

View of the two-dimensional supramolecular structure in (I). H atoms have been omitted.

Crystal data

$[Cd_2(C_8H_4O_4)_2(C_{19}H_{12}N_4O)_2]$
$M_r = 1177.70$
Monoclinic, $C2/c$
$a = 15.1504\ (12)$ Å
$b = 16.5593\ (13)$ Å
$c = 18.9423\ (15)$ Å
$\beta = 110.274\ (1)^\circ$
$V = 4457.8\ (6)$ Å^3
$Z = 4$
$D_x = 1.755$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.03$ mm^{-1}
$T = 292\ (2)$ K
Block, yellow
0.26 × 0.18 × 0.12 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SAINT*; Bruker, 1998)
$T_{\min} = 0.805$, $T_{\max} = 0.882$
11050 measured reflections
4256 independent reflections
3658 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 25.7^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.073$
$S = 1.05$
4256 reflections
334 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 2.4711P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.57$ e Å^{-3}
$\Delta\rho_{\min} = -0.27$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Cd1	2.341 (2)	O2—Cd1^{i}	2.2600 (19)
N2—Cd1	2.368 (2)	O3—Cd1^{ii}	2.3605 (19)
O1—Cd1	2.2520 (18)	O4—Cd1^{ii}	2.4049 (19)
O1—Cd1—O2^{i}	97.95 (8)	N1—Cd1—N2	70.17 (8)
O1—Cd1—N1	161.88 (7)	O3^{iii}—Cd1—N2	101.59 (7)
O2^{i}—Cd1—N1	81.61 (8)	O1—Cd1—O4^{iii}	113.30 (7)
O1—Cd1—O3^{iii}	88.06 (7)	O2^{i}—Cd1—O4^{iii}	83.66 (7)
O2^{i}—Cd1—O3^{iii}	136.35 (7)	N1—Cd1—O4^{iii}	84.72 (7)
N1—Cd1—O3^{iii}	104.84 (7)	O3^{iii}—Cd1—O4^{iii}	54.86 (6)
O1—Cd1—N2	95.09 (7)	N2—Cd1—O4^{iii}	140.29 (7)
O2^{i}—Cd1—N2	120.65 (7)		

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

All H atoms were positioned geometrically and refined as riding atoms, with C—H distances of 0.93 Å, an N—H distance of 0.86 Å, an O—H distance of 0.82 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,N) and 1.5$U_{\rm eq}$(O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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References

Bruker (1998). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

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.

Hagrman, P. J., Hagrman, D. & Zubieta, J. (1999). *Angew. Chem. Int. Ed.* **38**, 2638–2684.

Ma, J.-F., Yang, J., Zheng, G.-L., Li, L. & Liu, J.-F. (2003). *Inorg. Chem.* **42**, 7531–7534.

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

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