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

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Key indicators

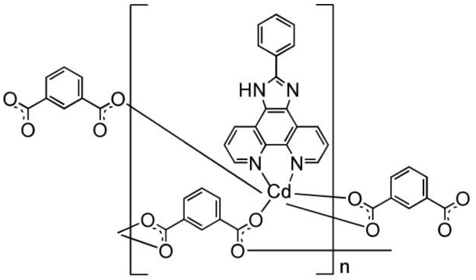
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.007 Å
R factor = 0.044
wR factor = 0.096
Data-to-parameter ratio = 15.3

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

In the title compound, [Cd(*m*-BDC)(*L*)], where *m*-BDC is the benzene-1,3-dicarboxylate dianion ($C_8H_4O_4^{2-}$) and *L* is 2-phenyl-1*H*-1,3,7,8,-tetraazacyclopenta[*l*]phenanthrene ($C_{19}H_{12}N_4$), the Cd^{II} atom is six-coordinated by one bidenatate *L*, one bidentate *m*-BDC and two monodentate *m*-BDC ligands, resulting in a very distorted *cis*-CdN_2O_4 octahedral coordination geometry. The Cd^{II} atoms are bridged by the *m*-BDC ligands to form an unusual double-chain structure. In addition, neighboring double chains interact through π–π interactions, resulting in a two-dimensional network.

Comment

Coordination polymers based on metals and organic ligands have been extensively studied in recent years owing to their novel topologies and potential applications as functional materials (Eddaoudi *et al.*, 2001). As part of this effort, many coordination polymers containing 1,10-phenanthroline have been reported. One report of the related ligand 2-phenyl-1*H*-1,3,7,8,-tetraazacyclopenta[*l*]phenanthrene ($C_{19}H_{12}N_4$, *L*) forming a coordination polymer has appeared (Chen & Liu, 2002). We selected *m*-benzenedicarboxylic acid ($C_8H_6O_4$, *m*-H_2BDC) as a linker and *L* as a secondary ligand, resulting in a new coordination polymer, [Cd(*m*-BDC)(*L*)], (I).



(I)

In compound (I), the Cd^{II} atom is surrounded by two N atoms from one *L* ligand and four O atoms from three different *m*-BDC ligands – one bidentate and two monodentate (Fig. 1). The mean Cd—O and Cd—N bond lengths are 2.314 (3) and 2.361 (4) Å, respectively. The CdN_2O_4 polyhedron can be regarded as a very distorted octahedron. In particular, the O1—Cd1—O2 bond angle is highly compressed (Table 1). The C—O bond lengths of the *m*-BDC species suggest that the negative charges of the C20/O1/O2 and C21/O3/O4 carboxylate groups are largely delocalized.

The Cd^{II} atoms are bridged by the *m*-BDC ligands to form an unusual double-chain structure (Fig. 2). A two-dimensional supramolecular network is then formed through π–π stacking

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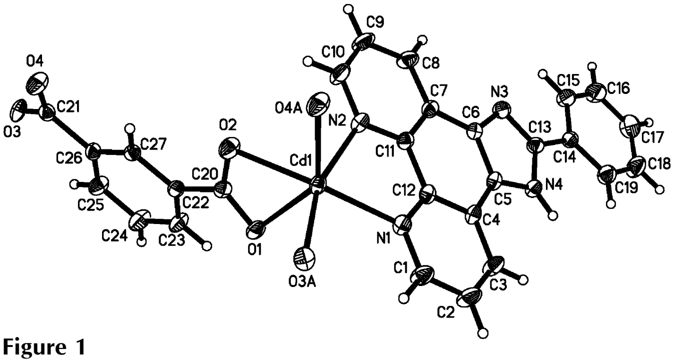

Figure 1
The asymmetric unit of (I) and additional atoms to complete the Cd coordination, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). Atoms O3*A* and O4*A* are generated by the symmetry operations (x, $-1 - y$, $\frac{1}{2} + z$) and ($-x$, $-1 - y$, $1 - z$), respectively.

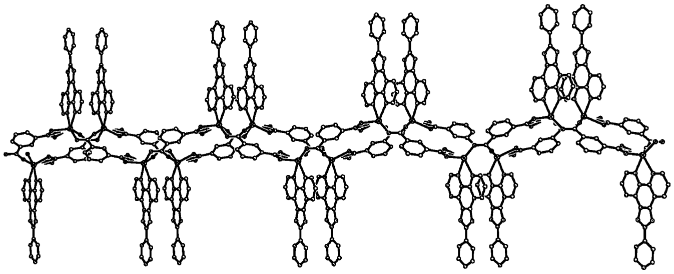

Figure 2
A view of the double-chain structure of (I). H atoms have been omitted.

interactions between adjacent *L* ligands (Fig. 3). The π–π stacking distances range between 3.56 and 3.63 Å. Clearly, these aromatic–aromatic interactions help stabilize the present structure in a similar way to previously reported structures (Noveron *et al.*, 2002).

Experimental

The ligand *L* was synthesized according to the 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 and the filtrate was allowed to stand in air at room temperature for two weeks, yielding pale-yellow crystals of (I) (79% yield based on Cd).

Crystal data

$[Cd(C_8H_4O_4)(C_{19}H_{12}N_4)]$
$M_r = 572.84$
Monoclinic, $C2/c$
$a = 15.254$ (3) Å
$b = 16.018$ (3) Å
$c = 19.069$ (4) Å
$\beta = 109.56$ (3)°
$V = 4390.4$ (17) Å^3
$Z = 8$
$D_x = 1.733$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.04$ mm^{-1}
$T = 292$ (2) K
Block, pale-yellow
0.35 × 0.29 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.687$, $T_{max} = 0.785$
20840 measured reflections
4968 independent reflections
3217 reflections with $I > 2\sigma(I)$
$R_{int} = 0.085$
$\theta_{max} = 27.5°$

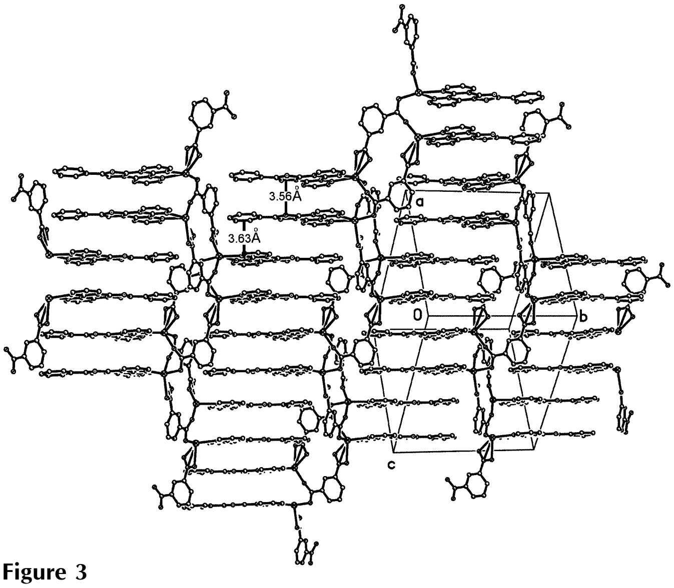

Figure 3
A view of the two-dimensional superamolecular structure of (I), formed through π–π interactions. H atoms have been omitted.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.096$
$S = 1.01$
4968 reflections
325 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.12$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.372 (4)	Cd1—O4^{ii}	2.260 (3)
Cd1—N2	2.349 (4)	C20—O1	1.262 (5)
Cd1—O1	2.397 (3)	C20—O2	1.253 (5)
Cd1—O2	2.377 (3)	C21—O3	1.262 (5)
Cd1—O3^{i}	2.222 (3)	C21—O4	1.247 (5)
N2—Cd1—N1	70.29 (12)	O2—Cd1—O1	54.77 (10)

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

All H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}$(carrier). The highest residual density peak is located 0.99 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*.

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