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A cadmium coordination polymer containing helical chains: *catena*-poly[[(dipyrido[3,2-*a*:2′-*c*]-phenazine)cadmium]-μ-benzene-1,3-dicarboxylato]

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The title compound, $[Cd(C_8H_4O_4)(C_{18}H_{10}N_4)]_n$, was synthesized under mild hydrothermal conditions. The Cd center is coordinated by four O atoms from three different benzene-1,3-dicarboxylate ligands and two N atoms from the dipyrido[3,2-*a*:2′,3′-*c*]phenazine ligand in a distorted octahedral geometry. The polymeric chain extends along the *c* axis, forming a one-dimensional helical structure.

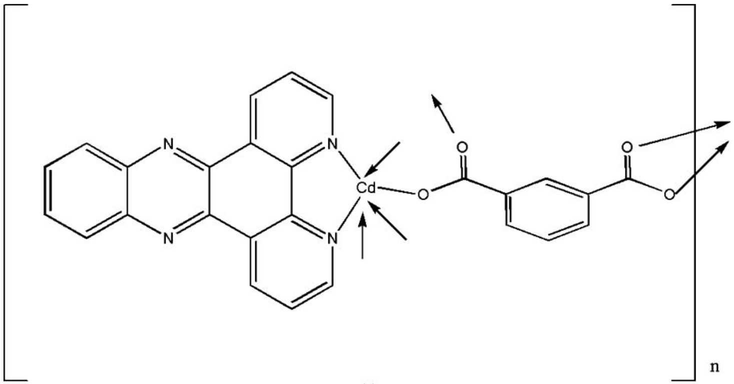
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.030
wR factor = 0.075
Data-to-parameter ratio = 12.9

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

Comment

Rapid developments in supramolecular chemistry and metal–organic polymeric network research have produced many new complexes with unique structures (see, for example, Lu *et al.*, 2003; Cheng *et al.*, 2004). Metal–organic network structures depend on the judicious selection of metal centers and organic ligands that can afford covalent bonds, hydrogen bonding linkages, or π–π interactions for the construction of new supramolecular or polymeric complexes. To date, one of the main rational synthetic strategies has been the use of spacer ligands whereby network structures can be controlled and modified by changing the chemical structure of the organic ligand. Phenanthroline derivatives are convenient linkers for constructing metal–organic frameworks, and a wide range of coordination polymers has been generated using them. 1,3-Benzenedicarboxylic acid, which can serve as a bifunctional ligand, has also been utilized effectively to build coordination networks (Zhang *et al.*, 2001; Sun *et al.*, 2001; Abourahma *et al.*, 2002). We anticipated that the mixed bdc/dppz ligand system could be used to generate some coordination polymers with various structures.



(I)

Single-crystal X-ray diffraction analysis reveals that the title compound, (I), has a one-dimensional framework which is constructed from the basic unit [[(dipyrido[3,2-*a*:2′,3′-*c*]-phenazine)cadmium]-μ-benzene-1,3-dicarboxylato], as illustrated in Fig. 1. The asymmetric unit contains one Cd atom,

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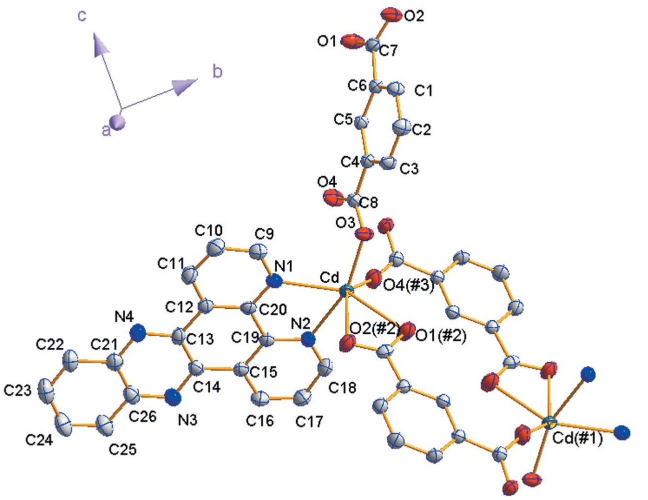

Figure 1
The local coordination enviroment of cadmium(II), with 30% probability displacement ellipsoids. H atoms have been omitted for clarity. [Symmetry codes: (#1) $-x, 1 - y, -z$; (#2) $x, 1 - y, -\frac{1}{2} + z$; (#3) $-x, y, \frac{1}{2} - z$.]

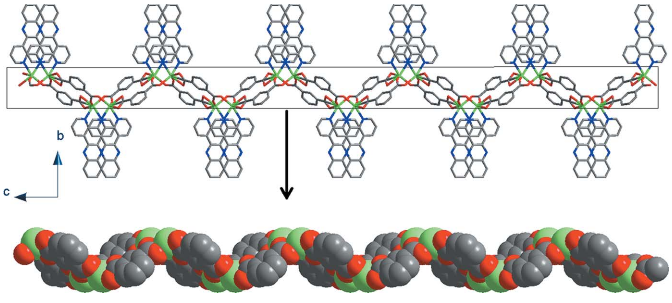

Figure 2
The one-dimensional chain in the title compound.

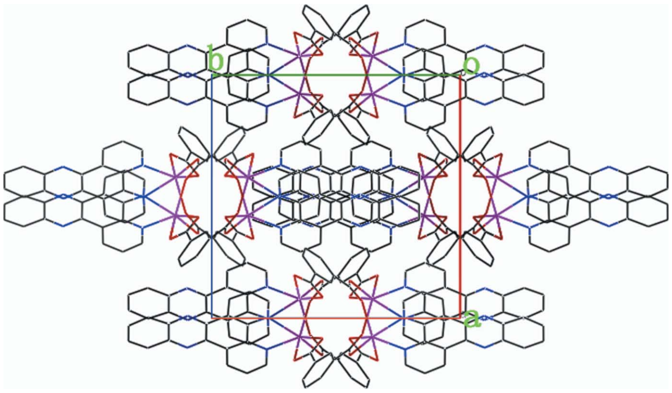

Figure 3
The three-dimensional supramolecular arrangement, viewed along the c axis. H atoms have been omitted.

one dipyrido[3,2-*a*:2′,3′-*c*]phenazine (dppz) molecule and one benzene-1,3-dicarboxylate (bdc) dianion.

All the Cd atoms are equivalent and each cadmium center is six-coordinate with a distorted octahedral geometry. The Cd center is coordinated by four O atoms from three different bdc ligands, with an average Cd—O distance of 2.297 (2) Å, and the other two sites are occupied by two N atoms from the dppz ligand with an average Cd—N distance of 2.390 (2) Å. The parallel dppz ligands coordinate neighboring Cd atoms and partake in π–π stacking interactions in which the shortest perpendicular distance between the C atom and aromatic ring is 3.490 Å. Two atoms, O3 and O4, belonging to one bdc ligand bridge two Cd atoms, whereas the other carboxylate O atoms (O1 and O2) coordinate to only one Cd atom. The carboxylate bridge forms an eight-membered ring with a Cd$\cdots$Cd distance of 4.062 (4) Å. Interestingly, this arrangement extends along the c axis, forming a helical chain encased by dppz molecules (Fig. 2). In addition, between neighboring chains, there are π–π stacking interactions between the dppz molecules (shortest C–ring perpendicular distance 3.390 Å) and thus infinite helical chains of the title compound form a three-dimensional supramolecular framework, as shown in Fig. 3.

Experimental

All chemicals were obtained from commercial sources and were used as received. To a solution of $CdCl_2 \cdot 2.5H_2O$ (0.3 mmol) in 30 ml distilled water, dppz (0.1 mmol) and H_2bdc (0.3 mmol) were added and the mixture was stirred thoroughly for 1 h at ambient temperature. The pH value was adjusted to about 7.5 with NaOH aqueous solution. The suspension was placed inside a stainless steel Teflon-lined reaction vessel (4 0 ml). The reaction was performed under autogeneous pressure and static conditions in an oven at 443 K for 4.5 d. The vessel was then cooled slowly inside the oven to 298 K at a rate of 5 K h^{-1} before opening. The crystalline product was collected, manually separated and preserved in a portion of the reaction vessel solution.

Crystal data

$[Cd(C_8H_4O_4)(C_{18}H_{10}N_4)]$
$M_r = 558.82$
Monoclinic, $C2/c$
$a = 15.467$ (4) Å
$b = 14.971$ (4) Å
$c = 18.847$ (4) Å
$\beta = 109.064$ (5)°
$V = 4124.9$ (18) Å^3

$Z = 8$
$D_x = 1.800$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.11$ mm^{-1}
$T = 293$ (2) K
Block, dark brown
0.43 × 0.40 × 0.28 mm

Data collection

Bruker APEX CCD diffractometer
ω and φ scans
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
$T_{min} = 0.628$, $T_{max} = 0.734$

11009 measured reflections
4062 independent reflections
3407 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.075$
$S = 1.03$
4062 reflections
316 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 2.2127P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

H atoms were placed in calculated positions (C—H = 0.93 Å) nd allowed to ride on aromatic C atoms during subsequent refinements, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

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