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catena-Poly[[[bis(1,10-phenanthroline)-cadmium(II)]-μ-naphthalene-2,6-dicarboxylato] monohydrate]

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Key indicators

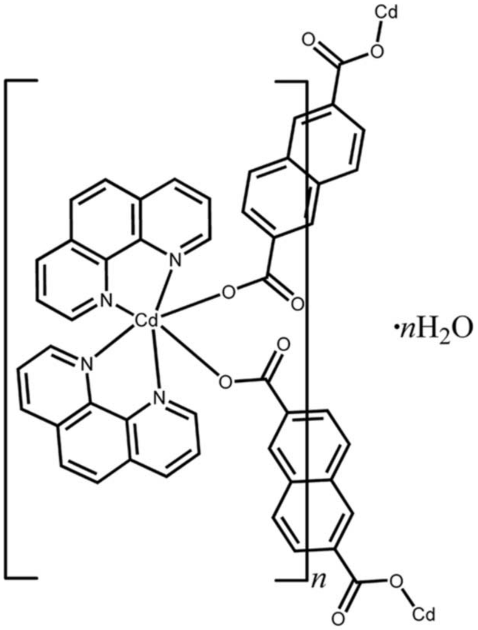
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.027
wR factor = 0.069
Data-to-parameter ratio = 15.6

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

The title cadmium coordination polymer, $\{[Cd(C_{12}H_6O_4)(C_{12}H_8N_2)_2]\cdot H_2O\}_n$, has been synthesized and characterized by single-crystal X-ray diffraction. Each Cd^{II} cation is coordinated by two carboxylate O atoms belonging to two NDC anions (NDC is naphthalene-2,6-dicarboxylate) and four N atoms from two phen ligands (phen is 1,10-phenanthroline). Each NDC anion bridges two Cd^{II} cations through the two terminal carboxylate groups in a monodentate fashion to form a zigzag polymeric chain and there are π–π interactions between adjacent chains. The title coordination polymer exhibits an extended three-dimensional network feature based on interchain hydrogen bonding and and π–π stacking interactions.

Comment

Recently, great interest has been focused on the design and synthesis of coordination polymers because of their intriguing network topologies and promising applications (Moulton & Zaworotko, 2001; Rao *et al.*, 2004; Yaghi *et al.*, 1998). Among the frameworks reported so far, polycarboxylate ligands such as terephthalate, 1,3,5-benzenetricarboxylate and 1,2,4,5-benzenetetracarboxylate have been proven to be particularly effective for the construction of one-, two- and three-dimensional coordination polymers (Chui *et al.*, 1999; Lo *et al.*, 2000).



(I)

The naphthalene-2,6-dicarboxylate anion (NDC) is a versatile ligand for the construction of coordination polymers, because

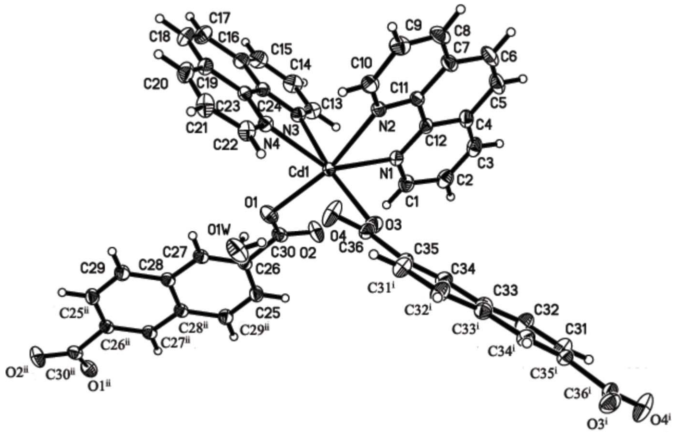


Figure 1
Part of the polymeric structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii. [Symmetry codes: (i) $2 - x, 1 - y, 1 - z$; (ii) $1 - x, -y, 1 - z$.]

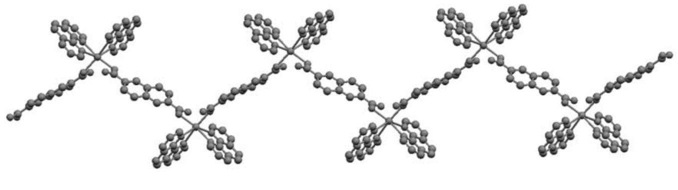


Figure 2
Ball-and-stick view of the one-dimensional zigzag chain arrangement in (I). H atoms and water molecules have been omitted for clarity.

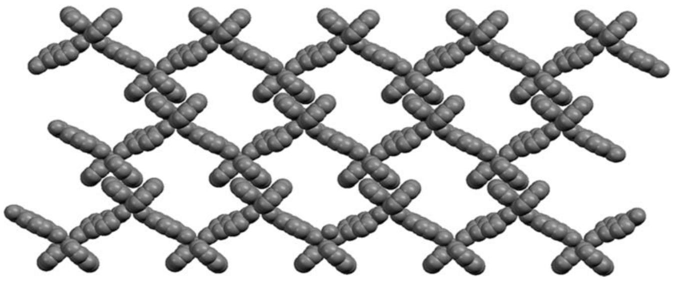


Figure 3
Space-filling view of the arrangement in (I). H atoms and water molecules have been omitted for clarity.

it is a rigid linear ligand with two carboxylate groups on opposite sides, so that it is a building block that can link other building blocks in the polymer, and also because the bulky nature and extended π-conjugate system of the naphthalene rings in NDC facilitate the formation of large cavities in networks and may endow the networks with emission properties (He *et al.*, 2005). We present here the hydrothermal synthesis and crystal structure of a one-dimensional cadmium(II)-based metal–organic framework solid, $[Cd(NDC)(phen)_2 \cdot (H_2O)]_n$, (I).

In the crystal structure of (I), the asymmetric unit consists of one crystallogaphically independent Cd^{II} cation, one NDC anion, two phen ligands and one solvent water molecule. Each Cd^{II} cation is six-coordinated by two O atoms from two carboxylate groups of two NDC anions and four N atoms from two chelating phen ligands, with Cd—O distances of 2.2648 (13)–2.2649 (12) Å and Cd—N distances in the range 2.3829 (14)–2.4526 (13) Å. These values are in good agreement with those found in another extended structure (Liu *et al.*, 2004). The O—Cd—O bond angle is 97.07 (5)°, and the N—Cd—O and N—Cd—N angles range from 79.70 (5) to 165.16 (4)° and from 68.24 (4) to 140.00 (4)°, respectively, *i.e.* the coordination environment of the Cd^{II} cation can be described as distorted octahedral (Fig. 1).

In complex (I), two carboxylate groups of each NDC anion exhibit bis-monodentate coordination modes, *i.e.* the NDC anion acts as a μ_2-bridging ligand to connect to two Cd^{II} centres, and each Cd^{II} centre connects to two NDC anions to form a zigzag arrangement with a Cd···Cd distance of 13.520 (4) Å (Fig. 2). The phen ligands are alternately attached to both sides of the chain. π–π stacking interactions exist between phen ligands of adjacent chains, with plane-to-plane distances in the range 3.515 (5)–3.763 (5) Å (Fig. 3).

There are two types of weak hydrogen-bonding interactions between adjacent chains. One type of hydrogen bond involves the uncoordinated carboxylate O atoms of the NDC anions and the C—H groups of the phen ligands of adjacent chains. The other type is C—H···O hydrogen bonds between the coordinated carboxylate O atoms and C—H groups of phen ligands of adjacent chains. In addition, water molecules located in the crystal structure form O—H···O and C—H···O hydrogen-bonding interactions involving the carboxylate O atoms and water molecules, and the C—H groups of phen and water molecules (Table 2). Finally, the chains are linked together by hydrogen-bonding and π–π stacking interactions to form a three-dimensional supramolecular network.

Experimental

Compound (I) was prepared hydrothermally from a mixture of $CdSO_4 \cdot 8H_2O$ (0.385 g), H_2NDC (0.108 g) and phen (0.198 g) in H_2O (10 ml), which was stirred for 30 min and heated at 433 K for 72 h in a Teflon-lined stainless steel autoclave (25 ml) under autogenous pressure. After cooling to room temperature, colourless block-shaped crystals of (I) were obtained and these were washed with water and dried in air.

Crystal data

$[Cd(C_{12}H_6O_4)(C_{12}H_8N_2)_2] \cdot H_2O$
$M_r = 704.99$
Monoclinic, $P2_1/n$
$a = 12.413$ (4) Å
$b = 18.573$ (5) Å
$c = 12.555$ (4) Å
$\beta = 93.970$ (14)°
$V = 2887.5$ (15) Å^3
$Z = 4$
$D_x = 1.622$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.81$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.44 × 0.33 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.718$, $T_{max} = 0.841$
27995 measured reflections
6582 independent reflections
5812 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 27.5°$

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.069$
$S = 1.16$
6582 reflections
423 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 1.3871P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.82$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.2648 (13)	Cd1—N4	2.4316 (13)
Cd1—O3	2.2649 (12)	Cd1—N2	2.4367 (13)
Cd1—N1	2.3829 (14)	Cd1—N3	2.4526 (13)
O1—Cd1—O3	97.07 (5)	N1—Cd1—N2	69.08 (5)
O1—Cd1—N1	128.21 (5)	N4—Cd1—N2	83.29 (5)
O3—Cd1—N1	82.61 (4)	O1—Cd1—N3	87.28 (4)
O1—Cd1—N4	79.70 (5)	O3—Cd1—N3	165.16 (4)
O3—Cd1—N4	126.45 (4)	N1—Cd1—N3	83.56 (4)
N1—Cd1—N4	140.00 (4)	N4—Cd1—N3	68.24 (4)
O1—Cd1—N2	162.22 (4)	N2—Cd1—N3	91.25 (4)
O3—Cd1—N2	88.84 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O2^{iv}	0.93	2.65	3.298 (2)	128
C6—H6···O1W^{v}	0.93	2.51	3.240 (3)	135
C8—H8···O3^{iii}	0.93	2.65	3.463 (2)	147
C1—H1···O2	0.93	2.34	3.113 (2)	140
C22—H22···O4	0.93	2.54	3.339 (2)	144
O1W—H1WB···O1	0.83 (3)	2.00 (3)	2.818 (2)	169 (3)
O1W—H1WA···O4	0.81 (2)	2.15 (2)	2.946 (2)	166 (2)

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

Water H atoms were found in a difference Fourier synthesis and their coordinates were refined freely, with O—H distances of 0.81 (2) and 0.83 (3) Å. All other H atoms were treated as riding, with C—H distances of 0.93 Å. A common displacement parameter was used for all H atoms.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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