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catena-Poly[[(1,10-phenanthroline-κ^2N,N')-cadmium(II)]-μ-imidazole-4,5-dicarboxylato-$\kappa^4N,O:N,O'$]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.020
wR factor = 0.052
Data-to-parameter ratio = 14.6

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

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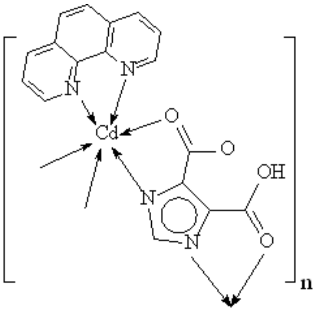
In the title one-dimensional coordination polymer, [Cd(HIDC)(1,10-phen)]$_n$ (where HIDC^{2-} is the imidazole-4,5-dicarboxylate dianion, $C_5H_2N_2O_4^{2-}$, and 1,10-phen is 1,10-phenanthroline, $C_{12}H_8N_2$), the Cd^{II} atom has a distorted octahedral coordination geometry, defined by two N donors from a chelating 1,10-phen molecule, two N-atom donors and two O-atom donors from two individual HIDC^{2-} groups. Adjacent Cd^{II} ions are bridged by HIDC^{2-} groups, resulting in a one-dimensional chain structure. The Cd$\cdots$Cd separation within the polymer is 6.661 (2) Å. The chains are linked into a two-dimensional supramolecular network *via* π–π stacking interactions.

Comment

The rational design and construction of supramolecular architectures have received extensive attention during recent decades. The choice of suitable ligands is an important factor that greatly influences the structure and stabilization of the coordination architecture formed (Tao *et al.*, 2000; Choi & Jeon, 2003). *N*-Heterocyclic carboxylic acids, such as 1*H*-imidazole-4,5-dicarboxylic acid (H_3IDC), have great potential for coordinative interaction and hydrogen bonding. This acid can be successively deprotonated to generate H_2IDC$^-$, HIDC^{2-}, IDC^{3-}, and hence may result in a large diversity of supramolecular architectures. To our knowledge, some related Mn^{II}, Cu^{II}, Zn^{II}, Co^{II}, Cd^{II}, Ru^{II} and VO^{IV} complexes have been reported, with various structures, such as mononuclear (Zhang *et al.*, 2004; Xiao *et al.*, 2004; Ma *et al.*, 2003; Sengupta *et al.*, 2001; Sanna *et al.*, 1998) and dinuclear (Rajendiran *et al.*, 2003). However, coordinations polymer based on the H_3IDC ligand remain largely unexplored (Wang *et al.*, 2004). In the case of the mononuclear complex [Cd(H_2IDC)(H_2O)$_2$], the Cd^{II} atom shows an octahedral configuration with the H_2IDC$^-$ ligand.



(I)

We report here a new one-dimensional chain cadmium(II) coordination polymer, [Cd(HIDC)(1,10-phen)]$_n$ (1,10-phen is

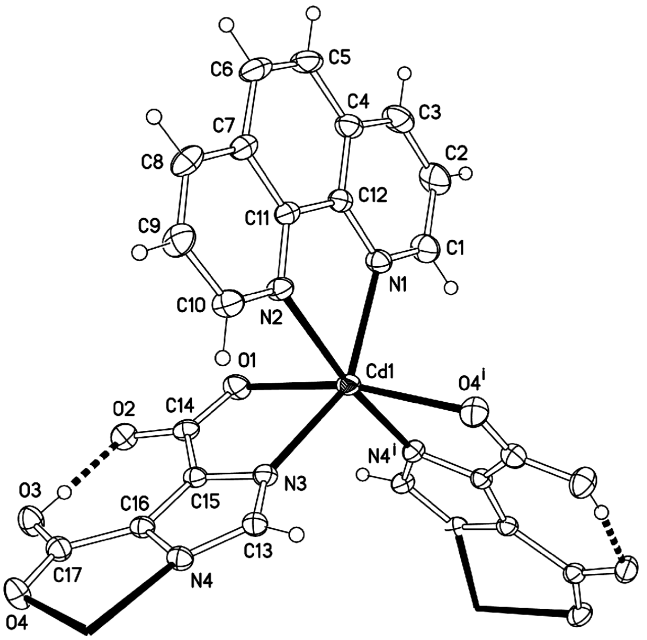


Figure 1

*ORTEP*II plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines (symmetry codes as in Table 1).

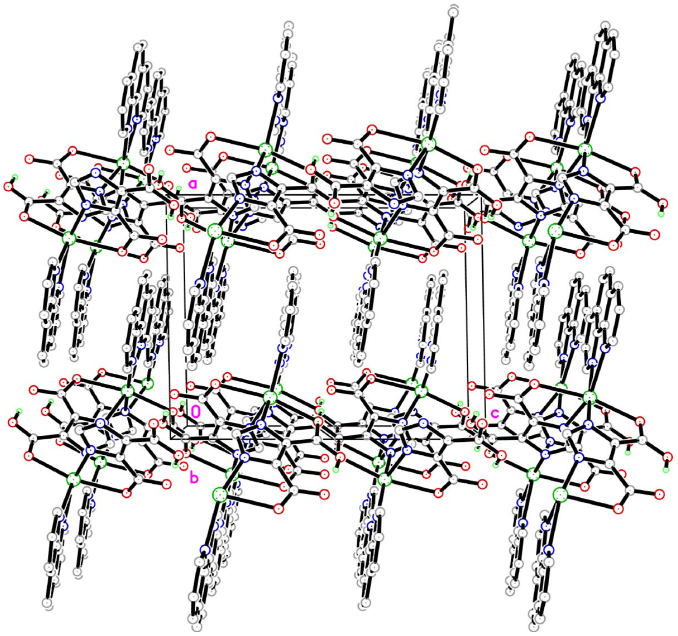


Figure 2

Packing diagram of the title complex. H atoms on C atoms have been omitted. Key: green Cd, blue N, red O, gray C.

1,10-phenanthroline), (I), obtained by the hydrothermal reaction of cadmium dinitrate tetrahydrate, 1*H*-imidazole-4,5-dicarboxylic acid and 1,10-phenanthroline.

As illustrated in Fig. 1, the carboxylic acid ligand bears a formal charge of −2, deprotonated at the imidazole N4 and carboxyl O2 atoms. Uncoordinated carboxylate atoms O3 and O2 form an intramolecular hydrogen bond (Table 2). The Cd^{II} ion is six-coordinated by two N-atom donors from a terminal 1,10-phen molecule, two N-atom donors and two O-atom donors from two bidentate $HIDC^{2-}$ groups (Table 1). The local coordination geometry around the Cd^{II} ion can best be described as distorted octahedral with a CdO_2N_4 chromophore. Its equatorial plane is defined by atoms N1, N2, N3 and $N4^i$ [symmetry code: (i) $-x, y-\frac{1}{2}, \frac{3}{2}-z$] [r.m.s. deviation = 0.11 (3) Å; deviation of Cd atom from this plane is 0.16 (4) Å]. The axial positions are occupied by atoms O1 and $O4^i$.

It should be noted that the C14—O2 and C17—O3 distances are longer than the C14—O1 and C17—O4 distances, appropriate for the monodentate coordination mode of carboxyl groups. Two bidentate $HIDC^{2-}$ groups and one 1,10-phen molecule combine with the Cd^{II} atom to give three five-membered chelate rings. The $HIDC^{2-}$ ligand is essentially planar, with an r.m.s. deviations of 0.05 (4) Å. The dihedral angle between the 1,10-phen and $HIDC^{2-}$ ligands is 77.09 (6)°.

Each $HIDC^{2-}$ ligand serves as a bis-bidentate bridging group to link two Cd^{II} ions, giving rise to a one-dimensional chain running along the *b* axis. The antiparallel 1,10-phen ligands lie on alternate sides of the chain. In the chain, the shortest adjacent Cd···Cd distance is 6.661 (2) Å. In addition, there are strong π–π stacking interactions between 1,10-phen molecules at a centroid–centroid distance of 3.513 (3) Å. In this way, a two-dimensional supramolecular network structure is constructed, as shown in Fig. 2.

Experimental

1*H*-Imidazole-4,5-dicarboxylic acid was prepared following the literature method of Premkumar & Govindarajan (2002). Cadmium dinitrate tetrahydrate (6.16 g, 20 mmol), 1,10-phenanthroline (3.98 g, 20 mmol) and 1*H*-imidazole-4,5-dicarboxylic acid (4.60 g, 20 mmol) were dissolved in a 1:5 (*v*/*v*) ethanol–water mixture. The mixture was sealed in a 25 ml Teflon-lined stainless steel bomb and held at 403 K for 3 d. The bomb was cooled naturally to room temperature, and colorless prismatic crystals were obtained after several days. Analysis calculated for $C_{17}H_{10}CdN_4O_4$: C 45.71, H 2.26, N 12.54%; found: C 45.89, H 2.19, N 12.47%.

Crystal data

$[Cd(C_5H_2N_2O_4)(C_{12}H_8N_2)]$
$M_r = 446.70$
Monoclinic, $P2_1/c$
$a = 10.644$ (2) Å
$b = 10.415$ (2) Å
$c = 13.736$ (3) Å
$\beta = 91.07$ (3)°
$V = 1522.5$ (5) Å^3
$Z = 4$
$D_x = 1.949$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 14467 reflections
$\theta = 3.1$–27.5°
$\mu = 1.47$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.38 × 0.25 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.599$, $T_{\max} = 0.770$
14512 measured reflections
3485 independent reflections
3179 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.014$
$\theta_{\max} = 27.5°$
$h = -13 \rightarrow 13$
$k = -13 \rightarrow 13$
$l = -17 \rightarrow 17$

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.052$
$S = 1.04$
3485 reflections
238 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 0.6528P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.52$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.3399 (16)	Cd1—O4^{i}	2.3675 (15)
Cd1—N2	2.3977 (15)	O1—C14	1.237 (2)
Cd1—N3	2.2490 (15)	O2—C14	1.291 (2)
Cd1—N4^{i}	2.2592 (15)	O3—C17	1.282 (2)
Cd1—O1	2.4324 (15)	O4—C17	1.243 (2)
N1—Cd1—N2	70.40 (5)	N3—Cd1—O4^{i}	105.13 (5)
N1—Cd1—O1	91.99 (6)	N4^{i}—Cd1—N1	99.81 (5)
N1—Cd1—O4^{i}	95.56 (6)	N4^{i}—Cd1—N2	170.11 (5)
N2—Cd1—O1	87.43 (5)	N4^{i}—Cd1—O1	91.61 (5)
N3—Cd1—N1	152.45 (5)	N4^{i}—Cd1—O4^{i}	73.46 (5)
N3—Cd1—N2	85.76 (5)	O4^{i}—Cd1—N2	108.17 (5)
N3—Cd1—N4^{i}	103.36 (5)	O4^{i}—Cd1—O1	164.20 (5)
N3—Cd1—O1	72.79 (5)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H14···O2	0.86 (3)	1.60 (3)	2.462 (3)	174 (3)

The H atoms attached to C atoms were placed in calculated positions, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C), and refined as riding. The H atom of the carboxyl group was located in a difference map and refined with an O—H distance restraint of 0.85 (1) Å, and with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97; molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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