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catena-Poly[[aqua(1,10-phenanthroline-κ^2N,N')-cadmium(II)]-μ-4-carboxylatophenoxyacetato-κ^3O,O':O'']

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Key indicators

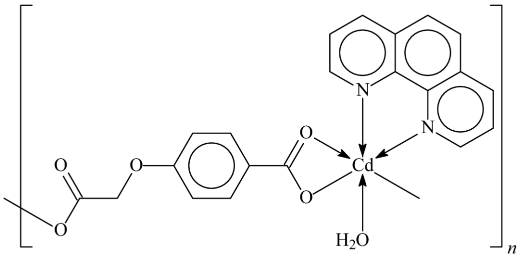
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.006 Å
R factor = 0.040
wR factor = 0.062
Data-to-parameter ratio = 15.3

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

The Cd^{II} atom in the title coordination polymer, $[Cd(4\text{-CPOA})(1,10\text{-phen})(H_2O)]_n$ (1,10-phen is 1,10-phenanthroline, $C_{12}H_8N_2$, and 4-$CPOA^{2-}$ is the 4-carboxyphenoxyacetate dianion, $C_9H_6O_5$), shows a distorted octahedral geometry, defined by three carboxyl O-atom donors from two independent 4-$CPOA^{2-}$ groups, two N-atom donors from one 1,10-phen ligand, and one water molecule. The Cd^{II} ions are bridged by carboxylate groups in mono- and bidentate modes, forming a chain structure. The polymeric chains are connected *via* O—H···O hydrogen bonds and π–π stacking interactions into a two-dimensional layer structure.

Comment

4-Carboxyphenoxyacetic acid (4-$CPOAH_2$) is an excellent bridging ligand with both rigid and flexible parts, which not only has multiple coordination possibilities, but can also form regular hydrogen bonds by functioning as both a hydrogen-bond donor and acceptor. However, the coordination chemistry of 4-$CPOAH_2$ still remains largely unexplored to date. Recently, we have reported the structures of three polymers, $[Ni(4\text{-CPOA})(2,2'\text{-bipy})(H_2O)]_n$ (2,2′-bipy is 2,2′ bipyridine), (II), $\{[Co(4\text{-CPOA})(3\text{-PyOH})_2(H_2O)_2]\cdot H_2O\}_n$ (PyOH is 3-3-hydroxypyridine), (III) and $[Mn(4\text{-CPOA})(H_2O)_3]_n$, (IV), within which the 4-$CPOA^{2-}$ ligand shows various coordination modes, including bi-, tri- and tetradentate (Gu, Gao, Huo *et al*., 2004; Gu, Gao, Zhao *et al*., 2004; Gao *et al*., 2004). Here, we report the crystal structure of the title Cd^{II} coordination polymer, $[Cd(4\text{-CPOA})(1,10\text{-phen})(H_2O)]_n$, (I), which was obtained by the hydrothermal reaction of 4-carboxyphenoxyacetic acid, cadmium dinitrate tetrahydrate and 1,10-phenanthroline in an aqueous solution.


(I)

As illustrated in Fig. 1, the Cd^{II} centre of (I) is in a distorted octahedral geometry. The Cd—$O_{carboxyl}$ distances are somewhat longer than the Cd—$O_{oxycarboxyl}$ distances (Table 1). There are similarities between complexes (I), (II) and (III), in that the metal ions of these three complexes have the same distorted octahedral configuration.

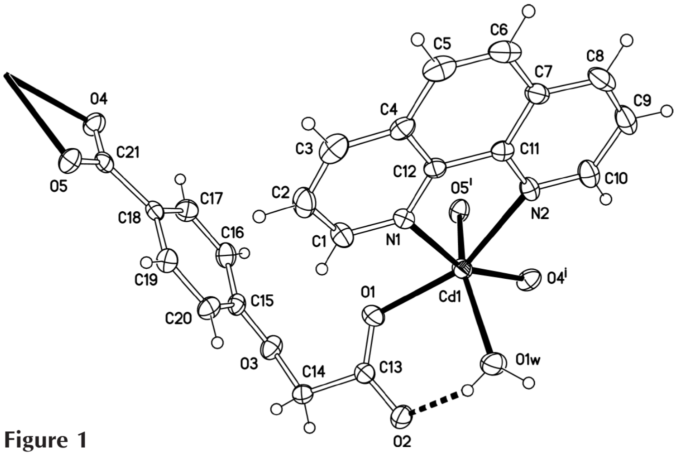


Figure 1
A plot of the title complex, with displacement ellipsoids drawn at the 30% probability level. The dashed line indicates a hydrogen bond. (Symmetry codes are as given in Table 1).

It is noteworthy that the oxyacetate group functions in a monodentate mode through atom O1, while the carboxyl group chelates the Cd^{II} centre through carboxyl atoms O4 and O5. The oxyacetate group is twisted out of the plane of the aromatic ring, the C15—O3—C14—C13 torsion angle being −81.8 (4)°, whereas the carboxyl group, O4—C21—O5, and benzene ring are almost coplanar [dihedral angle 8.3 (3)°].

The 4-$CPOA^{2-}$ ligands which adopt a tridentate coordinating mode link neighbouring Cd^{II} atoms to form a chain structure, the adjacent Cd···Cd separation being 10.455 (2) Å (Fig. 2). In addition, the chains are connected through an intermolecular hydrogen bond between the water molecule and carboxyl atom O5 (Table 2). There are π–π stacking interactions between the phen rings, with a separation of 3.558 (3) Å. The polymeric chains align in a manner which facilitates both hydrogen-bonding and π–π interactions, leading to a two-dimensional layer structure (Fig. 3).

Experimental

The title complex was prepared by the addition of 1,10-phenanthroline (1.99 g, 10 mmol) and cadmium dinitrate tetrahydrate (3.08 g, 10 mmol) to a hot aqueous solution of 4-carboxyphenoxyacetic acid (1.96 g, 10 mmol); the pH was adjusted to 6 with 0.1*M* sodium hydroxide. The mixture was sealed in a 20 ml Teflon-lined stainless steel bomb and held at 423 K for 4 d. The bomb was cooled naturally to room temperature, and colourless prismatic crystals were obtained after several days. CHN analysis, calculated for $C_{21}H_{16}N_2O_6Cd$: C 49.97, H 3.19, N 5.55%; found: C 45.13, H 3.22, N 5.51%.

Crystal data

$[Cd(C_9H_6O_5)(C_{12}H_8N_2)(H_2O)]$
$M_r = 504.77$
Orthorhombic, $P2_12_12_1$
$a = 6.9025$ (14) Å
$b = 16.504$ (3) Å
$c = 16.770$ (3) Å
$V = 1910.4$ (6) Å^3
$Z = 4$
$D_x = 1.755$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 16 504 reflections
$\theta = 3.2$–27.3°
$\mu = 1.19$ mm^{-1}
$T = 296$ (2) K
Prism, colourless
0.36 × 0.24 × 0.18 mm

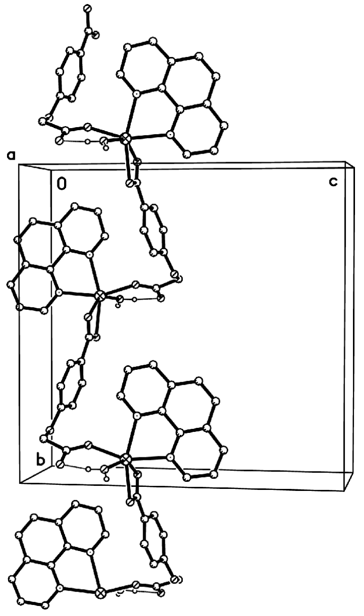


Figure 2
The chain structure of the title complex. Hydrogen bonds are shown as dashed lines. H atoms bound to C atoms have been omitted.

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.675$, $T_{max} = 0.815$
16 533 measured reflections

4259 independent reflections
3477 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
$\theta_{max} = 27.3°$
$h = -8 \rightarrow 7$
$k = -21 \rightarrow 21$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.062$
$S = 1.03$
4259 reflections
278 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0285P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.86$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}
Extinction correction: none
Absolute structure: Flack (1983), with 1812 Friedel pairs
Flack parameter: 0.47 (2)

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.343 (3)	Cd1—O4^i	2.298 (2)
Cd1—N2	2.363 (3)	Cd1—O5^i	2.490 (3)
Cd1—O1	2.239 (3)	Cd1—O1*W*	2.289 (3)
N1—Cd1—N2	71.22 (10)	N2—Cd1—O1*W*	103.83 (11)
N1—Cd1—O1	87.61 (11)	O1—Cd1—O4^i	107.72 (12)
N1—Cd1—O4^i	159.76 (10)	O1—Cd1—O5^i	89.74 (10)
N1—Cd1—O5^i	113.96 (12)	O1—Cd1—O1*W*	88.03 (11)
N1—Cd1—O1*W*	99.85 (14)	O4^i—Cd1—O5^i	54.70 (8)
N2—Cd1—O1	157.07 (12)	O4^i—Cd1—O1*W*	93.95 (12)
N2—Cd1—O4^i	91.21 (11)	O5^i—Cd1—O1*W*	146.00 (12)
N2—Cd1—O5^i	90.93 (11)		

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

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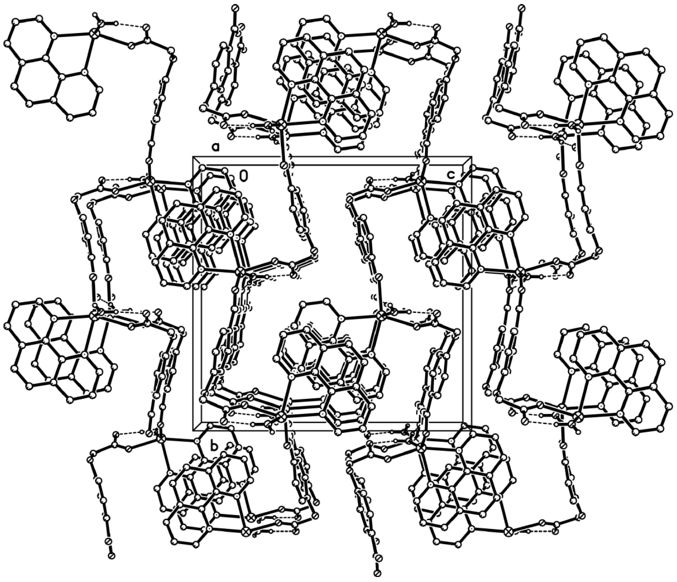

Figure 3
A packing diagram of the title complex. Hydrogen bonds are shown as dashed lines. H atoms bound to C atoms have been omitted.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O5^{ii}	0.85 (4)	1.93 (4)	2.758 (4)	166 (5)
O1W—H1W2···O2	0.85 (2)	1.83 (4)	2.631 (4)	158 (4)

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

C-bound H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C), and were refined in the riding-model approximation. Water H atoms were located in a difference Fourier map and refined with O—H and H···H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(O). The absolute structure parameter could not be reliably determined. The crystal is a racemic twin. The ratio of the two components refined to 0.47 (2):0.53 (2).

Data collection: *RAPID AUTO* (Rigaku, 1998); cell refinement: *RAPID AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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