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catena-Poly[[triaquacadmium(II)]-μ-4-carboxylatophenoxyacetato-$\kappa^4O,O':O'',O'''$]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.031
wR factor = 0.083
Data-to-parameter ratio = 14.8

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

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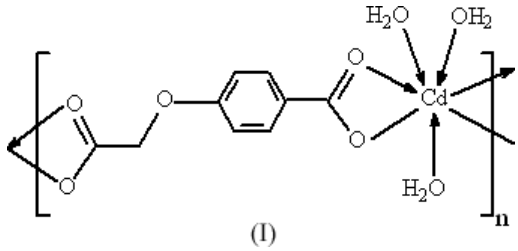
In the title coordination polymer, $[Cd(4\text{-}CPOA)(H_2O)_3]_n$ (where 4-CPOA^{2-} is the 4-carboxylatophenoxyacetate dianion, $C_9H_6O_5$), the Cd^{II} ion is seven-coordinate, involving four O atoms of two different 4-CPOA^{2-} ligands and three water molecules, arranged in a pentagonal–bipyramidal geometry. Adjacent Cd^{II} ions are linked by the 4-CPOA^{2-} groups in bidentate mode, giving rise to a zigzag chain with a closest Cd···Cd distance of 10.310 (5) Å. The chains are further linked by O—H···O hydrogen bonds to form a supramolecular three-dimensional network.

Comment

Supramolecular architectures constructed from the deliberate selection of metals and multifunctional organic carboxylate ligands have aroused considerable interest in recent decades (Burrows *et al.*, 1997; Harry *et al.*, 2004). As a multifunctional flexible ligand, 4-carboxyphenoxyacetic acid (4-CPOAH$_2$) can coordinate to metals in a variety of modes and, in addition, form regular hydrogen bonds by functioning as either a hydrogen-bond donor or acceptor. Thus, 4-CPOAH$_2$ could be considered as an excellent candidate for the construction of supramolecular complexes. Recently, we reported the crystal structures of the manganese, nickel, cobalt and zinc complexes, in which the 4-CPOA^{2-} group is present in bi-, tri- and tetradentate bridging modes (Gu, Gao, Huo *et al.*, 2004; Gu, Gao, Zhao *et al.*, 2004; Gao *et al.*, 2004*a*,*b*). In order to gain further insight into the metal-binding modes of the 4-CPOAH$_2$ ligand, we have introduced the Cd^{II} ion into the coordination system of the 4-CPOAH$_2$ ligand, and produced a new one-dimensional chain polymer, $[Cd(4\text{-}CPOA)(H_2O)_3]_n$, (I), the crystal structure of which is reported here.



(I)

Part of the structure of (I) is shown in Fig. 1. The Cd^{II} ion shows a distorted pentagonal–bipyramidal coordination geometry, defined by four carboxyl O atoms from two bidentate chelate 4-CPOA^{2-} ligands and three coordinated water molecules. The equatorial pentagonal plane is defined by atoms O1, O2, O4, O5 and O1*W*, and the mean deviation from this plane is 0.06 (4) Å. The other two water molecules occupy the axial sites. The Cd^{II} centre has O—Cd—O angles

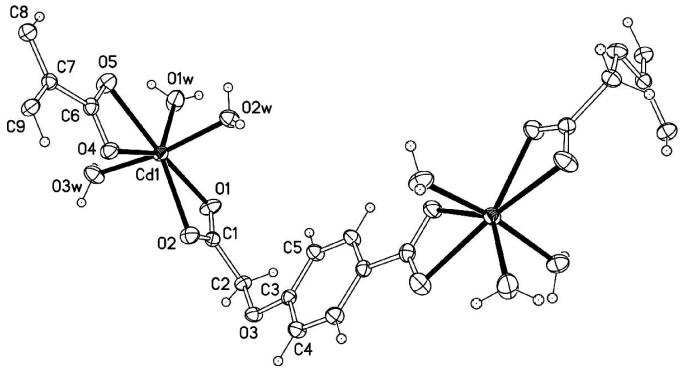


Figure 1
ORTEPII plot (Johnson, 1976) of part of the one-dimensional chain of the title complex, with displacement ellipsoids drawn at the 30% probability level. Only the atoms of the asymmetric unit are labelled.

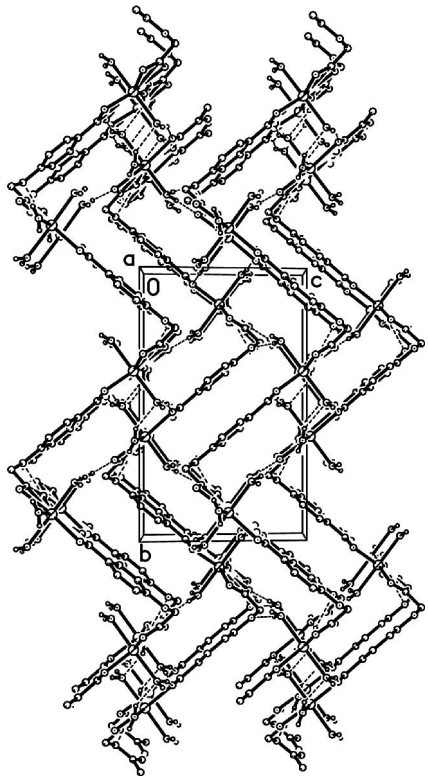


Figure 2
Packing diagram of the title complex, viewed along the *a* axis. Hydrogen bonds are indicated by dashed lines (H atoms bonded to C atoms have been omitted).

as small as 54.20 (7), the smallest being attributed to the bis-chelate coordination of the 4-CPOA^{2-} ligand that forms two four-membered rings.

Each 4-CPOA^{2-} group acts as a bis-bidentate ligand to link two Cd^{II} ions through the carboxyl O atoms, resulting in a one-dimensional chain along the *b*-axis direction (Fig. 2). In the chain, the shortest Cd···Cd distance is 10.310 (2) Å, which is somewhat shorter than the *b*-axis repeat Cd···Cd distance of 16.417 (2) Å. Furthermore, the chains are connected through intermolecular hydrogen bonds involving 4-CPOA^{2-} groups and water molecules, yielding an O—H···O hydrogen-bonded three-dimensional supramolecular network (Table 2).

Experimental

The 4-carboxyphenoxyacetic acid ligand was prepared by the reaction of chloroacetic acid with 4-hydroxybenzoic acid (Mirci, 1990). The title complex was prepared by the addition of cadmium nitrate tetrahydrate (6.16 g, 20 mmol) to an aqueous solution of 4-carboxyphenoxyacetic acid (3.92 g, 20 mmol); the pH was adjusted to 6 with 0.2 *M* NaOH solution, and filtered. Colourless prism-shaped single crystals were obtained from the filtrate at room temperature over several days. Analysis calculated for $C_9H_{12}CdO_8$: C 29.98, H 3.35%; found: C 30.16, H 3.31%.

Crystal data

$[Cd(C_9H_6O_5)(H_2O)_3]$	D_x = 2.035 Mg m^{-3}
M_r = 360.60	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 10 102 reflections
a = 7.1306 (14) Å	θ = 3.3–27.5°
b = 16.417 (3) Å	μ = 1.89 mm^{-1}
c = 10.200 (2) Å	T = 295 (3) K
β = 99.74 (3)°	Prism, colourless
V = 1176.8 (4) Å^3	0.37 × 0.26 × 0.18 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	2681 independent reflections
ω scans	2507 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.043
T_{min} = 0.558, T_{max} = 0.714	θ_{max} = 27.5°
10 784 measured reflections	$h = -8 \rightarrow 9$
	$k = -21 \rightarrow 21$
	$l = -12 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.8705P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.031	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.083	$\Delta\rho_{max}$ = 0.89 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.50 e Å^{-3}
2681 reflections	
181 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.362 (2)	Cd1—O3*W*	2.317 (2)
Cd1—O2	2.444 (2)	O1—C1	1.255 (3)
Cd1—O4	2.356 (2)	O2—C1	1.246 (3)
Cd1—O5	2.444 (2)	O4—C6	1.267 (4)
Cd1—O1*W*	2.314 (2)	O5—C6	1.252 (4)
Cd1—O2*W*	2.269 (2)		
O1—Cd1—O2	54.20 (7)	O2*W*—Cd1—O1	90.50 (9)
O1—Cd1—O5	165.49 (7)	O2*W*—Cd1—O2	88.41 (8)
O2—Cd1—O5	140.21 (7)	O2*W*—Cd1—O4	94.05 (8)
O4—Cd1—O1	139.84 (7)	O2*W*—Cd1—O5	91.69 (9)
O4—Cd1—O2	86.03 (7)	O2*W*—Cd1—O1*W*	85.43 (10)
O4—Cd1—O5	54.26 (7)	O2*W*—Cd1—O3*W*	168.46 (8)
O1*W*—Cd1—O1	85.37 (9)	O3*W*—Cd1—O1	90.87 (9)
O1*W*—Cd1—O2	139.05 (9)	O3*W*—Cd1—O2	101.66 (8)
O1*W*—Cd1—O4	134.75 (9)	O3*W*—Cd1—O4	92.28 (9)
O1*W*—Cd1—O5	80.50 (9)	O3*W*—Cd1—O5	84.20 (9)
O1*W*—Cd1—O3*W*	83.26 (10)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O5^{i}	0.84 (3)	2.61 (3)	3.151 (4)	123 (3)
O1W—H1W1···O3W^{i}	0.84 (3)	2.20 (2)	2.956 (4)	149 (4)
O1W—H1W···O2^{ii}	0.84 (3)	2.27 (3)	2.842 (3)	126 (3)
O1W—H1W···O3^{ii}	0.84 (3)	2.39 (3)	3.203 (3)	162 (3)
O2W—H2W1···O3^{iii}	0.84 (3)	2.03 (3)	2.856 (3)	165 (3)
O2W—H2W···O1^{iv}	0.84 (3)	1.83 (3)	2.659 (3)	171 (3)
O3W—H3W1···O4^{v}	0.85 (3)	1.84 (3)	2.682 (3)	171 (3)
O3W—H3W···O5^{i}	0.85 (3)	2.01 (2)	2.756 (3)	146 (3)

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

C-bound H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C), and were refined in the riding-model approximation. The H atoms of water molecules 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_{iso}(H) = 1.5U_{eq}(O).

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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