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catena-Poly[[diaquacadmium(II)]-μ-benzene-1,4-dioxyacetato-$\kappa^4O,O':O'',O'''$]

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Key indicators

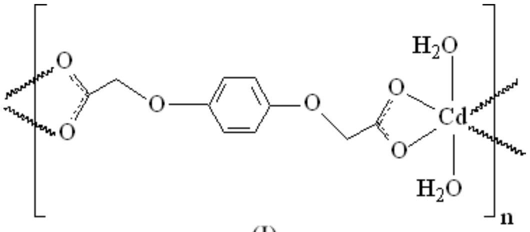
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.009 Å
R factor = 0.046
wR factor = 0.150
Data-to-parameter ratio = 14.2

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

In the title coordination polymer {systematic name: *catena*-poly[[diaquacadmium(II)]-μ-*p*-phenylenebis(oxyacetato)-$\kappa^4O,O':O'',O'''$]}, $[Cd(C_{10}H_8O_6)(H_2O)_2]_n$, the Cd^{II} atom displays a trigonal prismatic coordination geometry, involving four carboxyl O atoms from two different benzene-1,4-dioxyacetate ligands and two water molecules. The Cd^{II} atom and the benzene-1,4-dioxyacetate ligand lie on special positions with twofold rotation and inversion symmetry, respectively. Adjacent Cd^{II} ions are linked by carboxylate groups with the tetradentate coordination mode, forming a one-dimensional chain structure with an adjacent Cd$\cdots$Cd distance of 15.263 (5) Å. These chains are further linked by O—H$\cdots$O hydrogen bonds, forming a supramolecular network.

Comment

Special attention has been devoted to the self-assembly of coordination polymers in recent years, within which the judicious choice of suitable ligands is an important factor that greatly influences the structure of the coordination architecture and functionality of the complex formed (Kim *et al.*, 2003; Iglesias *et al.*, 2003). Benzene-1,4-dioxyacetic acid (1,4-BDOAH$_2$), which has versatile binding modes, is regarded as an excellent candidate for the construction of supramolecular architectures. Recently, we have reported the structures of some one- or two-dimensional polymers incorporating this ligand (Gao *et al.*, 2004, 2004*a*,*b*,*d*). In the case of the one-dimensional Cd^{II} polymer, $[Cd(1,4\text{-BDOA})(\text{imidazole})_3]_n$, the Cd^{II} atom exists in a distorted octahedral coordination geometry and the 1,4-BDOA^{2-} ligand acts in a tridentate bridging mode (Gao *et al.*, 2004*c*). In the present work, a new one-dimensional chain Cd^{II} polymer, $[Cd(1,4\text{-BDOA})(H_2O)_2]_n$, (I), has been obtained from the self-assembly reaction of cadmium nitrate tetrahydrate and 1,4-BDOAH$_2$. Its crystal structure is reported here.



(I)

As shown in Fig. 1, the Cd^{II} ion displays a distorted trigonal prismatic coordination, comprising four carboxyl O atoms from two 1,4-BDOA^{2-} ligands [Cd—O = 2.364 (5) and 2.347 (4) Å] and two coordinated water molecules [Cd—O*w* = 2.196 (5) Å]. The Cd^{II} atom and the 1,4-BDOA^{2-} ligand lie on special positions with twofold rotation and inversion symmetry, respectively.

The two C—O bond distances of the carboxyl group are nearly identical (Table 1), suggesting delocalization of electrons. The coordinated oxyacetate group and benzene ring are almost coplanar, the C3—O3—C2—C1 torsion angle being 172.7 (6)°.

Each 1,4-BDOA^{2-} group acts in a tetradentate mode to bridge two Cd^{II} atom, forming a one-dimensional chain along the *c* axis. In the chain, the adjacent Cd···Cd distance is 15.263 (5) Å. Furthermore, the chains are connected through intermolecular hydrogen bonds involving the water molecules and O atoms of 1,4-BDOA^{2-} groups, forming a hydrogen-bonding supramolecular network (Table 2).

Experimental

Benzene-1,4-dioxyacetic acid was prepared following the method described for the synthesis of benzene-1,2-dioxyacetic acid by Mirci (1990). The title complex was prepared by the addition of cadmium nitrate tetrahydrate (6.16 g, 20 mmol) and NaOH (1.60 g, 40 mmol) to a hot aqueous solution of 1,4-BDOAH$_2$ (4.52 g, 20 mmol) which was then filtered. Colorless prismatic single crystals were obtained from the filtrate at room temperature over a period of several days. Analysis calculated for $C_{10}H_{12}CdO_8$: C 32.23, H 3.25%; found: C 31.49, H 3.32%.

Crystal data

[Cd($C_{10}H_8O_6$)(H_2O)$_2$]
M_r = 372.60
Monoclinic, $C2/c$
a = 11.751 (1) Å
b = 5.510 (1) Å
c = 18.277 (2) Å
β = 96.14 (2)°
V = 1176.6 (3) Å^3
Z = 4
D_x = 2.103 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4187 reflections
θ = 3.4–27.4°
μ = 1.89 mm^{-1}
T = 295 (2) K
Prism, colorless
0.38 × 0.24 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min}$ = 0.583, $T_{\max}$ = 0.717
4210 measured reflections
1321 independent reflections
1249 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.031
$\theta_{\max}$ = 27.4°
$h = -15 \rightarrow 15$
$k = -6 \rightarrow 7$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.150
S = 1.04
1321 reflections
93 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0741P)^2 + 0.7307P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.75 e Å^{-3}
$\Delta\rho_{\min}$ = −0.69 e Å^{-3}

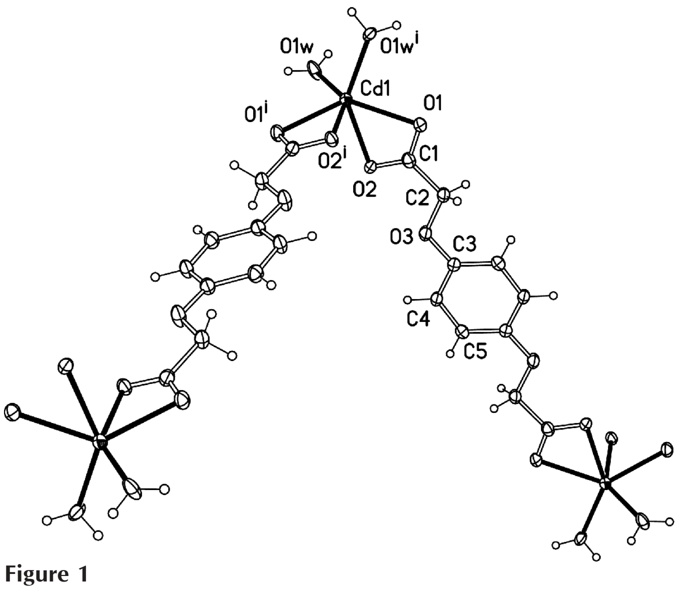


Figure 1
ORTEPII plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level. The symmetry codes are as given in Table 1.

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.364 (4)	O1—C1	1.251 (8)
Cd1—O2	2.347 (4)	O2—C1	1.253 (7)
Cd1—O1*w*	2.196 (5)		
O1^{i}—Cd1—O1	133.3 (2)	O1*w*^{i}—Cd1—O1	88.35 (17)
O2^{i}—Cd1—O1	89.59 (17)	O1*w*—Cd1—O2	102.3 (2)
O2—Cd1—O1	55.24 (15)	O1*w*^{i}—Cd1—O2	142.77 (16)
O2^{i}—Cd1—O2	86.5 (2)	O1*w*—Cd1—O1*w*^{i}	92.3 (3)
O1*w*—Cd1—O1	125.30 (19)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*w*1···O1^{ii}	0.85 (4)	1.84 (4)	2.687 (6)	176 (8)
O1*W*—H1*w*2···O2^{iii}	0.85 (7)	1.91 (5)	2.698 (7)	153 (11)
O1*W*—H1*w*2···O3^{iii}	0.85 (7)	2.61 (8)	3.142 (7)	122 (7)

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

C-bound H atoms were placed in calculated positions, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C), and were refined in the riding-model approximation. The H atoms of water molecules were located in a difference map and refined with with O—H and H···H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and $U_{\rm iso}$(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: *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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