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Aqua(4,4′-oxydibenzoato-*κO*)-cadmium(II)

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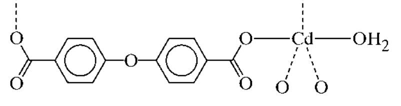
The Cd atom in the polymeric title compound, [Cd($C_{14}H_8O_5$)(H_2O)]$_n$, is linked to four carboxyl O atoms and a water molecule in a five-coordinate coordination polyhedron that is midway between a square pyramid and a trigonal bipyramid. The Cd atom and the water molecules both lie on the same twofold axis and the central O atom of the 4,4′-oxydibenzoate moiety lies on another twofold axis. Covalent Cd—O bonds lead to the formation of a layer architecture perpendicular to the twofold axis, the layers being held together by hydrogen bonds in the third direction.

Comment

The study of diaqua[4,4′-(ethylenedioxy)dibenzoato]cadmium has documented the chelating mode of the two carboxyl ends of the dicarboxylate group [Cd—O = 2.241 (3) and 2.537 (3) Å], which links the six-coordinate Cd atoms into a zigzag chain (Liu *et al.*, 2001). The omission of the flexible –CH_2CH_2O– linkage in the dicarboxylate unit furnishes the more tightly packed title compound, (I) (Fig. 1). The Cd atom and the water molecules both lie on the same twofold axis and the central O atom (O3) lies on another twofold axis. Both carboxyl O atoms are engaged in bonding to one metal atom [Cd—O = 2.198 (2) and 2.394 (2) Å] to furnish a layer structure. The layers are held together by hydrogen bonds [$O_{water}\cdots O$ = 2.690 (3) Å]. The five-coordinate geometry is completed by the water ligand [Cd—O = 2.231 (3) Å].



(I)

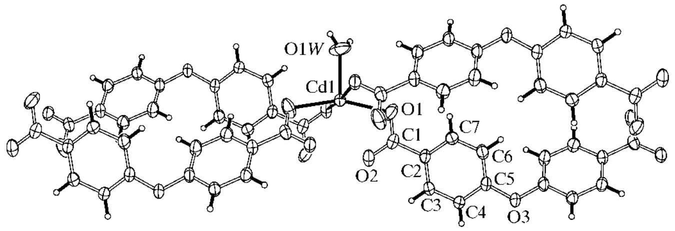


Figure 1
*ORTEP*II plot (Johnson, 1976) of the title compound at the 50% probability level, illustrating the five-coordinate geometry of the Cd atom. H atoms are drawn as small spheres of arbitrary radii.

A search using the Cambridge Structural Database (Allen *et al.*, 1983) did not locate the parent carboxylic acid; only two metal complexes have been documented, namely a cobalt(II) and a copper(II) derivative. The dicarboxylate group functions as a bichelate in the cobalt complex, which adopts a chain structure (Skakle *et al.*, 2001). In the copper complex, both carboxyl ends are monodentate to Cu atoms; the double-bonded O atoms are engaged in hydrogen bonding with the lattice methanol molecules (Burger *et al.*, 1995). As no cadmium derivative of the parent acid appears to have been synthesized, the structure of (I) can only be compared with related structures, such as, for example, the malonate analog. The Cd—O distances are similar to distances found in these carboxylates. On the other hand, the Cd—O_{water} distance compares well with the distances in the trigonal [2.277 (7) Å; Post & Trotter, 1974] and rhombohedral modifications [2.283 (3) Å; Naumov *et al.*, 2001] of cadmium malonate.

The d^{10} electron configuration of cadmium(II) allows the ion to exist in a variety of stereochemical environments, with the six-coordinate geometry accounting for 56% of examples; the five-coordinate geometry is found in only 8% of examples (Siegel & Martin, 1994). The geometry of the Cd atom in (I), as calculated by *PLATON* (Spek, 1990), is approximately midway between a square pyramid and a trigonal bipyramid. Additionally, two somewhat long interactions of 2.824 (2) Å indicate a trigonal-prismatic geometry whose rectangular face is capped (Fig. 2). A five-coordinate geometry is found in the anionic complexes [{(C_2H_5)$_2$NCS$_2$}Cd*X*] (*X* = NCS, Cl or Br). The geometry of the *X* = Cl derivative also lies midway along the Berry pseudorotation pathway. However, there are no important contacts (Baggio *et al.*, 1996) that could raise the coordination number. The unambiguous seven-coordinate

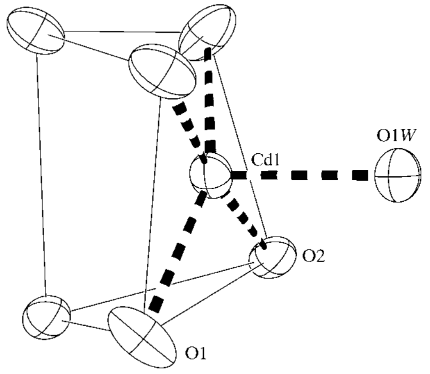


Figure 2
*ORTEP*II plot (Johnson, 1976) showing the five-coordinate square-pyramidal/trigonal-bipyramidal intermediate geometry distorted to a seven-coordinate geometry, in which one rectangular face of the trigonal prism is capped. Symmetry-related atoms are not labeled.

geometry found in cadmium diacetate dihydrate shows a smaller spread of distances for the square-base trigonal-cap polyhedron [2.294 (4)–2.597 (4) Å; Harrison & Trotter, 1972].

Experimental

Cadmium nitrate tetrahydrate (0.31 g, 1 mmol) and 4,4′-oxydibenzoic acid (0.26 g, 1 mmol) were heated in a small volume of methanol/water (50:50) until they dissolved completely. Ammonium hydroxide was then added dropwise until the solution had a pH of 6.0. Colorless crystals were deposited from the solution after it had been set aside for several weeks.

Crystal data

$[Cd(C_{14}H_8O_5)(H_2O)]$
M_r = 386.62
Monoclinic, *P*2/*a*
a = 7.307 (3) Å
b = 6.453 (3) Å
c = 14.423 (8) Å
β = 101.83 (3)°
V = 665.6 (6) $Å^3$
Z = 2

D_x = 1.929 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 7.5–15°
μ = 1.67 mm^{-1}
T = 298 (2) K
Block, colorless
0.45 × 0.33 × 0.27 mm

Data collection

Siemens *R*3*m* four-circle diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.408, T_{max} = 0.433
2078 measured reflections
1939 independent reflections
1776 reflections with $I > 2\sigma(I)$

R_{int} = 0.017
θ_{max} = 30.0°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 9$
$l = -20 \rightarrow 19$
2 standard reflections every 200 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.067
S = 1.05
1939 reflections
101 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.3373P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.58 e $Å^{-3}$

The aqua H atom was refined with the distance restraints O—H = 0.85 (1) Å and H···H = 1.39 (1) Å. The remaining H atoms were treated as riding (C—H = 0.93 Å).

Data collection: *XSCANS* (Siemens, 1990); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.198 (2)	Cd1—O1*W*	2.231 (3)
Cd1—O2^{i}	2.394 (2)		
O1—Cd1—O1^{ii}	157.4 (1)	O1—Cd1—O2^{iii}	85.1 (1)
O1—Cd1—O1*W*	101.3 (1)	O2^{i}—Cd1—O1*W*	86.2 (1)
O1—Cd1—O2^{i}	96.4 (1)	O2^{i}—Cd1—O2^{iii}	172.4 (1)

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

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1548). Services for accessing these data are described at the back of the journal.

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