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catena-Poly[[diaquacadmium(II)]-μ-4-(carboxylatomethylsulfanyl)phenoxyacetato]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
Disorder in main residue
R factor = 0.035
wR factor = 0.094
Data-to-parameter ratio = 13.9

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

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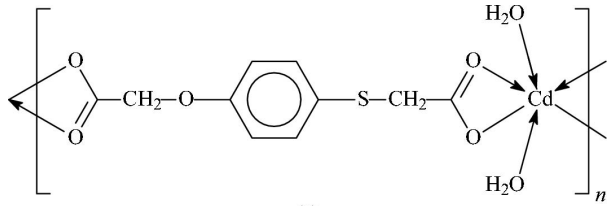
The dicarboxylate dianion in the polymeric title compound, $[Cd(C_{10}H_8O_3S)(H_2O)_2]_n$, links diaquacadmium(II) units into a zigzag chain. Adjacent chains are linked by hydrogen bonds into a layered structure. The coordination geometry of the Cd atom is octahedral, with Cd—O_{COO} distances of 2.395 (3) and 2.359 (3) Å, and a Cd—O_{aqua} distance of 2.193 (4) Å. The Cd atom lies on a twofold rotation axis.

Comment

4-Thioacetic phenoxyacetic acid can be used for the synthesis of metal complexes and its phenylene-1,4-dioxyacetic acid analogue has already been used for the preparation of metal complexes. Anhydrous zinc phenylene-1,4-dioxyacetate (Gao *et al.*, 2004) reveals two symmetrically independent dianions that are disordered over an inversion centre. The diaquazinc analogue adopts a zigzag chain structure in which the carboxyl $-CO_2$ group chelates to the metal atom (Gao *et al.*, 2005). The present diaquacadmium analogue, (I) (Fig. 1), has a structure similar to that of the diaquazinc compound, which was described in detail. The Cd atom lies on a twofold axis and the dianion acts as a bridging ligand to connect adjacent diaquacadmium units into chains. Adjacent chains are linked by hydrogen bonds (Table 2) into layers.



(I)

Experimental

An aqueous solution of cadmium(II) acetate dihydrate (3.08 g, 10 mmol) was added to an aqueous solution of 4-thioacetic phenoxyacetic acid (2.42 g, 10 mmol). The pH of the solution was raised to 6 with 0.1*M* sodium hydroxide. Colourless crystals of (I) were isolated from the filtered solution after several days. Analysis, calculated for C and H in $C_{10}H_{12}O_7S$ Cd: C 30.90, H 3.11%; found: C 30.75, H 3.16%.

Crystal data

$[Cd(C_{10}H_8O_3S)(H_2O)_2]$
M_r = 388.66
Monoclinic, $C2/c$
a = 11.991 (2) Å
b = 5.486 (1) Å
c = 18.894 (4) Å
β = 94.64 (3)°
V = 1238.8 (4) Å^3
Z = 4
D_x = 2.084 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5056 reflections
θ = 3.4–27.5°
μ = 1.96 mm^{-1}
T = 293 (2) K
Block, colourless
0.38 × 0.26 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.556, T_{max} = 0.771
5107 measured reflections
1332 independent reflections
1269 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°
$h = -15 \rightarrow 15$
$k = -6 \rightarrow 7$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
S = 1.11
1332 reflections
96 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 8.8641P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.395 (3)	Cd1—O1*w*	2.193 (4)
Cd1—O2	2.359 (3)		
O1—Cd1—O1^{i}	131.9 (2)	O2—Cd1—O2^{i}	87.1 (2)
O1—Cd1—O2	55.3 (1)	O2—Cd1—O1*w*	106.5 (2)
O1—Cd1—O2^{i}	88.8 (1)	O2^{i}—Cd1—O1*w*	138.3 (1)
O1—Cd1—O1*w*	131.6 (2)	O1*w*—Cd1—O1*w*^{i}	89.3 (2)
O1—Cd1—O1*w*^{i}	85.2 (1)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*w*1···O1^{iii}	0.85 (1)	1.84 (1)	2.678 (6)	175 (8)
O1*W*—H1*w*2···O2^{iv}	0.84 (1)	1.95 (3)	2.743 (6)	157 (8)

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

In the structure of (I), atoms O3 and S1 of the carboxylate dianion are disordered and their occupancies were set to 0.5 in agreement with the formula. For the O atom, the two distances involved to the C atoms were restrained to be equal within 0.01 Å; for the S atom, the corresponding distances were also restrained to be equal within 0.01 Å. The displacement parameters of the O and S atoms were set equal. The disorder affected the aromatic C atoms, and their displacement parameters had to be restrained to be nearly isotropic in order for the refinement to converge. Water H atoms were located and refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å; their displacement parameters were set to $1.2U_{eq}$(O). H atoms attached to C atoms were placed in calculated positions (aromatic distance 0.93 Å, methylene distance 0.97 Å) and were included in the refinement in the riding model, with U_{iso}(H) = $1.2U_{eq}$(C).

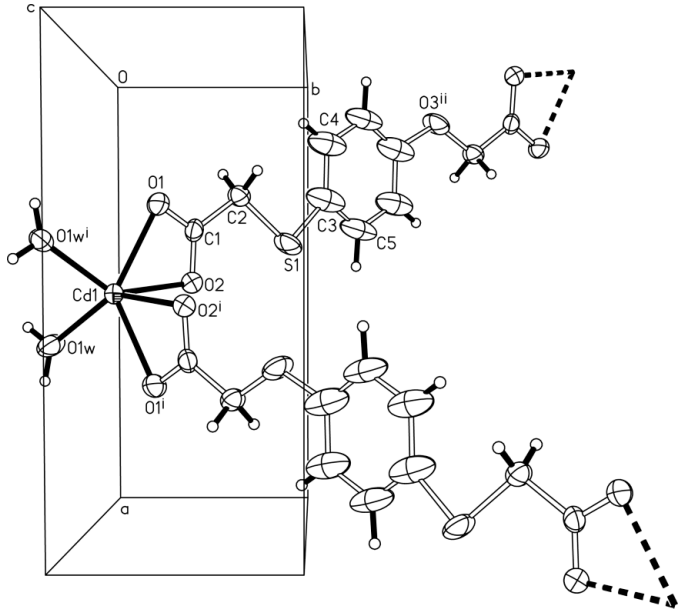


Figure 1
A plot of the polymeric chain structure of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Symmetry codes: (i) $1-x, y, \frac{3}{2}-z$; (ii) $\frac{1}{2}-x, \frac{5}{2}-y, 1-z$.

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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