

catena-Poly[[diaquacadmium(II)]- μ -4,4'-sulfonyldibenzoato- κ^2 O¹:O^{1'}]

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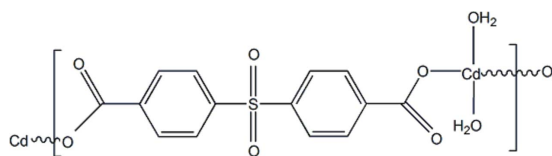
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.032; wR factor = 0.102; data-to-parameter ratio = 12.4.

The title compound, $[\text{Cd}(\text{C}_{14}\text{H}_8\text{O}_6\text{S})(\text{H}_2\text{O})_2]_n$, comprises zigzag chains parallel to $[111]$ of alternating $[\text{Cd}(\text{H}_2\text{O})_2]^{2+}$ and sulfonyldibenzoate units, with the Cd and S atoms lying on crystallographic twofold axes. The central Cd^{II} ion is in a slightly distorted octahedral geometry, coordinated by six O atoms from two carboxylate groups and two water O atoms. An intramolecular C—H \cdots O hydrogen bond occurs. In the crystal, intermolecular hydrogen bonds between carboxylate O atoms and coordinated water molecules in adjacent chains lead to the formation of a three-dimensional network structure. The compound is isotypic with the Zn analog.

Related literature

For related compounds based on 4,4'-sulfonyldibenzoic acid, see: Xiao *et al.* (2007); Wu *et al.* (2007); Miyazawa *et al.* (2009); Wang *et al.* (2009). For the isotypic Zn analog, see: Pan *et al.* (2007). For potential application of metal-organic frameworks, see: Eddaoudi *et al.* (2001); Ferey *et al.* (2005); Kitagawa *et al.* (2004).



Experimental

Crystal data

$[\text{Cd}(\text{C}_{14}\text{H}_8\text{O}_6\text{S})(\text{H}_2\text{O})_2]$	$a = 13.293$ (3) Å
$M_r = 452.72$	$b = 5.2742$ (12) Å
Monoclinic, $P2_1/c$	$c = 12.156$ (3) Å

$\beta = 116.145$ (2)°
 $V = 765.1$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 1.61$ mm⁻¹
 $T = 298$ K
 $0.21 \times 0.19 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	3574 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	1364 independent reflections
$T_{\min} = 0.721$, $T_{\max} = 0.786$	1325 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.073$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	3 restraints
$wR(F^2) = 0.102$	H-atom parameters constrained
$S = 1.24$	$\Delta\rho_{\text{max}} = 0.82$ e Å ⁻³
1361 reflections	$\Delta\rho_{\text{min}} = -1.00$ e Å ⁻³
110 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4B \cdots O1 ⁱ	0.85	1.97	2.7479 (14)	151
O4—H4A \cdots O2 ⁱⁱ	0.85	2.00	2.7364 (15)	145
C6—H6 \cdots O3	0.93	2.55	2.9208 (16)	104

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

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008) and DIAMOND (Brandenburg, 1999); software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2311).

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supporting information

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catena-Poly[[diaquacadmium(II)]- μ -4,4'-sulfonyldibenzoato- κ^2 O¹:O^{1'}]**Chang-mei Jiao****S1. Comment**

In recent years, much attention has been focused on the construction of metal organic frameworks (MOFs) not only because of their fascinating structures and topologies but also owing to their potential application in many fields such as magnetism, catalysis, nonlinear optics. (Eddaoudi, *et al.*, 2001; Kitagawa *et al.*, 2004; Ferey *et al.*, 2005.). The main method to construct such complexes is to use multidentate organic ligands. The organic aromatic polycarboxylate ligands are an important family of multidentate ligands. The 4,4'-sulfonyldibenzoic acid has been widely used in the construction of metal organic frameworks because of two carboxylate functions and its structural flexibility.(Xiao *et al.*, 2007; Wu *et al.*, 2007; Miyazawa *et al.*, 2009; Wang *et al.*, 2009.) We report here the synthesis and crystal structure of the title compound (I) based on 4,4'-sulfonyldibenzoic acid which is isostructural to the reported compound by Pan *et al.*, 2007.

As shown in Fig. 1, the Cd centres in (I) are six-coordinate in a highly distorted octahedral geometry, involving four O atom donors of two 4,4'-sulfonyldibenzoic acid ligands and two coordinated water molecules, while the carboxylate group of 4,4'-sulfonyldibenzoic acid adopts μ_2 - η^1 : η^1 - chelating mode in this structure. The structure of (I) comprises zigzag chains of alternating $[\text{Cd}(\text{H}_2\text{O})_2]^{2+}$ and sulfonyldibenzoate unit, with their respective Cd and S atoms lying on crystallographic twofold axes. In the crystal structure there are three hydrogen bonds, two O—H \cdots O intermolecular and one C—H \cdots O intramolecular interactions, lead to the formation of a three dimensional network structure. Fig 2, Table 1.

S2. Experimental

The title compound, (I), was prepared by the hydrothermal reaction of $\text{Cd}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (34.5 mg, 0.1 mmol), 4,4'-sulfonyldibenzoic (30 mg, 0.1 mmol), 1,4-Bis(1,2,4-triazol-1-yl)butane (19.2 mg, 0.1 mmol), and NaOH (8.0 mg, 0.2 mmol) in H_2O (10 ml) was sealed in a 16 ml Teflon-lined stainless steel container and heated at 180 °C for 72 h. After cooling to room temperature, block colorless crystals of (I) were collected by filtration and washed by water and ethanol several times. (yield 47.25%, based on Cd). Elemental analysis for $\text{C}_{14}\text{H}_{12}\text{CdO}_8\text{S}$ (Mr = 452.72): C 37.14, H 2.67; found: 43.61, H 2.69.

S3. Refinement

H atoms bonded to coordinated water oxygen atom were located in a difference Fourier map and fixed in the refinement, with $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{O})$. All C-bound H atoms were positioned in calculated positions and refined using a riding model, with C—H = 0.93(Å)(aromatic) and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

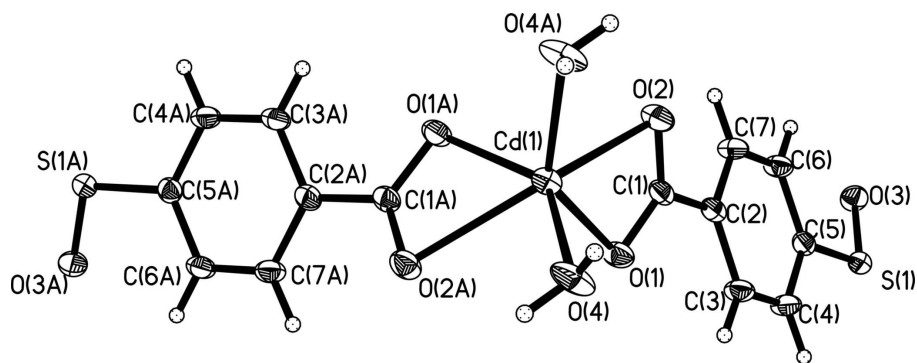


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 30% probability level. [Symmetry codes: (A) $-x, y, 3/2 - z$]

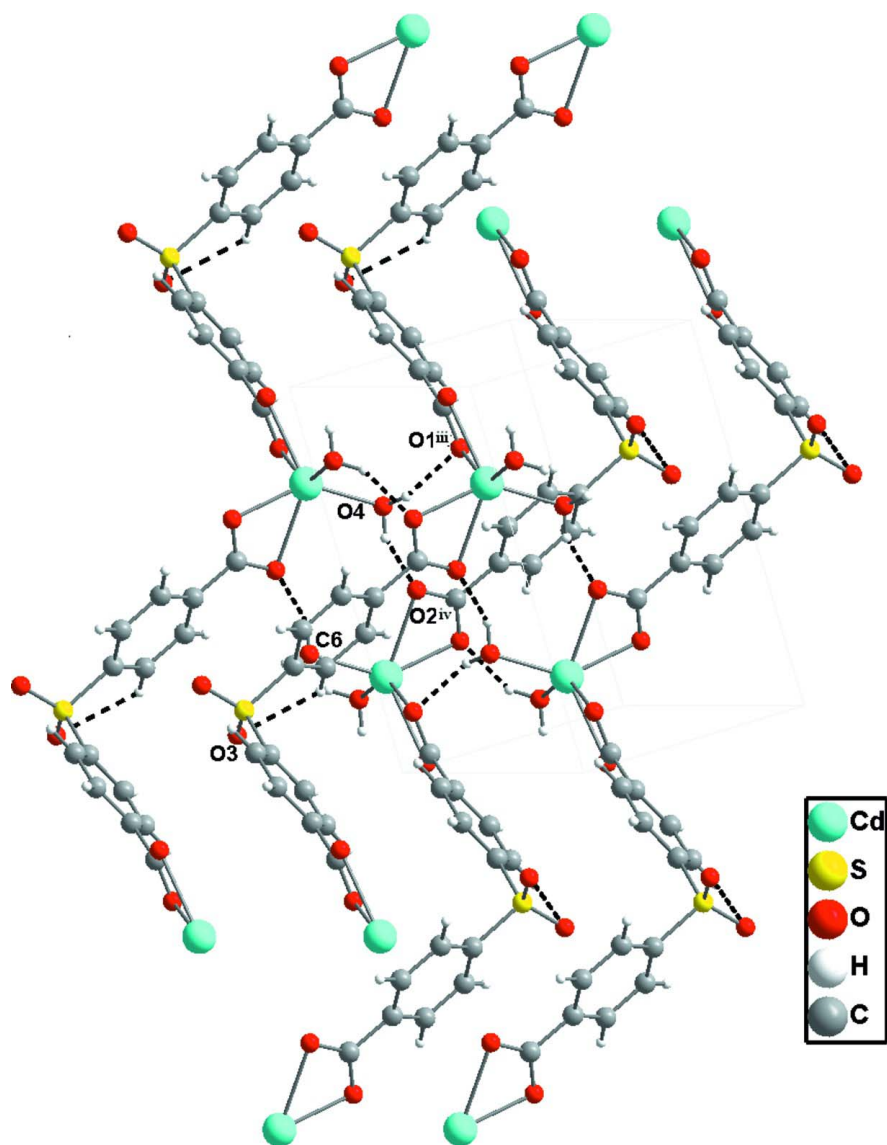


Figure 2

A view of (I), showing the three-dimensional framework constructed *via* O—H \cdots O hydrogen bonds. Hydrogen bonds are depicted as dashed lines. [Symmetry codes: (iii) $x, y - 1, z$; (iv) $x, -y, -1/2 + z$]

catena-Poly[[diaquacadmium(II)]- μ -4,4'-sulfonyldibenzoato- κ^2 O¹:O¹']

Crystal data

[Cd(C₁₄H₈O₆S)(H₂O)₂]

$M_r = 452.72$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 13.293\ (3)\ \text{\AA}$

$b = 5.2742\ (12)\ \text{\AA}$

$c = 12.156\ (3)\ \text{\AA}$

$\beta = 116.145\ (2)^\circ$

$V = 765.1\ (3)\ \text{\AA}^3$

$Z = 2$

$F(000) = 448$

$D_x = 1.965\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 4318 reflections

$\theta = 2.2\text{--}27.2^\circ$

$\mu = 1.61\ \text{mm}^{-1}$

$T = 298\ \text{K}$

Block, white

$0.21 \times 0.19 \times 0.15\ \text{mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2000)
 $T_{\min} = 0.721$, $T_{\max} = 0.786$

3574 measured reflections
1364 independent reflections
1325 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.073$
 $\theta_{\max} = 25.1^\circ$, $\theta_{\min} = 1.7^\circ$
 $h = -8 \rightarrow 15$
 $k = -6 \rightarrow 6$
 $l = -14 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.102$
 $S = 1.24$
1361 reflections
110 parameters
3 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0652P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 0.82 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.00 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.0000	0.06452 (2)	0.7500	0.03071 (4)
S1	0.5000	1.11217 (9)	1.2500	0.02880 (11)
O1	0.14145 (7)	0.34261 (18)	0.81726 (7)	0.0355 (2)
O2	0.08657 (7)	0.25919 (19)	0.95927 (7)	0.0382 (2)
O3	0.45660 (6)	1.24838 (18)	1.32215 (7)	0.0379 (2)
O4	0.07556 (8)	-0.2236 (2)	0.67828 (7)	0.0504 (3)
H4A	0.0490	-0.2211	0.6006	0.060*
H4B	0.0724	-0.3725	0.7034	0.060*
C1	0.14914 (9)	0.3776 (3)	0.92426 (9)	0.0286 (2)
C2	0.23354 (12)	0.5638 (2)	1.00469 (11)	0.0304 (4)
C3	0.32577 (10)	0.6180 (3)	0.98250 (11)	0.0354 (3)
H3	0.3327	0.5418	0.9172	0.043*
C4	0.40667 (9)	0.7851 (3)	1.05787 (10)	0.0365 (3)
H4	0.4693	0.8180	1.0449	0.044*
C5	0.39451 (10)	0.9035 (2)	1.15258 (11)	0.0290 (3)
C6	0.30158 (9)	0.8548 (3)	1.17385 (10)	0.0351 (3)

H6	0.2937	0.9353	1.2377	0.042*
C7	0.22143 (9)	0.6857 (3)	1.09904 (10)	0.0349 (3)
H7	0.1588	0.6533	1.1121	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03760 (6)	0.02817 (8)	0.02969 (5)	0.000	0.01787 (4)	0.000
S1	0.03045 (16)	0.03051 (18)	0.02660 (15)	0.000	0.01361 (12)	0.000
O1	0.0430 (3)	0.0402 (4)	0.0285 (2)	-0.0069 (3)	0.0206 (2)	-0.0069 (3)
O2	0.0473 (3)	0.0419 (5)	0.0299 (3)	-0.0117 (3)	0.0211 (2)	-0.0022 (3)
O3	0.0406 (3)	0.0381 (5)	0.0387 (4)	0.0037 (4)	0.0208 (3)	-0.0066 (3)
O4	0.0902 (5)	0.0382 (5)	0.0411 (3)	0.0184 (4)	0.0456 (3)	0.0079 (4)
C1	0.0348 (4)	0.0289 (5)	0.0234 (3)	0.0038 (4)	0.0140 (2)	0.0057 (4)
C2	0.0345 (5)	0.0342 (8)	0.0240 (5)	0.0000 (4)	0.0143 (4)	0.0034 (4)
C3	0.0375 (5)	0.0461 (6)	0.0309 (4)	-0.0039 (5)	0.0226 (3)	-0.0076 (5)
C4	0.0348 (4)	0.0464 (7)	0.0378 (4)	-0.0055 (5)	0.0248 (3)	-0.0056 (5)
C5	0.0305 (5)	0.0305 (6)	0.0253 (5)	0.0004 (4)	0.0116 (4)	0.0028 (4)
C6	0.0394 (5)	0.0426 (6)	0.0314 (4)	-0.0039 (6)	0.0231 (3)	-0.0065 (5)
C7	0.0375 (4)	0.0405 (7)	0.0364 (4)	-0.0060 (5)	0.0252 (3)	-0.0035 (5)

Geometric parameters (Å, °)

Cd1—O4	2.2023 (11)	O4—H4A	0.8500
Cd1—O4 ⁱ	2.2023 (11)	O4—H4B	0.8499
Cd1—O1	2.2362 (10)	C1—C2	1.4871 (16)
Cd1—O1 ⁱ	2.2362 (9)	C2—C7	1.385 (2)
Cd1—O2	2.5040 (9)	C2—C3	1.396 (2)
Cd1—O2 ⁱ	2.5040 (10)	C3—C4	1.3801 (18)
Cd1—C1 ⁱ	2.7283 (12)	C3—H3	0.9300
S1—O3	1.4367 (10)	C4—C5	1.380 (2)
S1—O3 ⁱⁱ	1.4367 (10)	C4—H4	0.9300
S1—C5	1.7655 (12)	C5—C6	1.393 (2)
S1—C5 ⁱⁱ	1.7655 (12)	C6—C7	1.3798 (17)
O1—C1	1.2725 (15)	C6—H6	0.9300
O2—C1	1.2550 (17)	C7—H7	0.9300
O4—Cd1—O4 ⁱ	92.73 (6)	C1—O1—Cd1	98.32 (8)
O4—Cd1—O1	98.09 (4)	C1—O2—Cd1	86.34 (7)
O4 ⁱ —Cd1—O1	139.87 (3)	Cd1—O4—H4A	113.0
O4—Cd1—O1 ⁱ	139.87 (3)	Cd1—O4—H4B	113.1
O4 ⁱ —Cd1—O1 ⁱ	98.09 (4)	H4A—O4—H4B	110.5
O1—Cd1—O1 ⁱ	98.02 (5)	O2—C1—O1	120.51 (10)
O4—Cd1—O2	126.84 (3)	O2—C1—C2	121.76 (11)
O4 ⁱ —Cd1—O2	88.07 (4)	O1—C1—C2	117.73 (12)
O1—Cd1—O2	54.80 (3)	C7—C2—C3	119.83 (11)
O1 ⁱ —Cd1—O2	92.21 (3)	C7—C2—C1	121.45 (14)
O4—Cd1—O2 ⁱ	88.07 (4)	C3—C2—C1	118.72 (13)

O4 ⁱ —Cd1—O2 ⁱ	126.84 (3)	C4—C3—C2	119.75 (13)
O1—Cd1—O2 ⁱ	92.21 (3)	C4—C3—H3	120.1
O1 ⁱ —Cd1—O2 ⁱ	54.80 (3)	C2—C3—H3	120.1
O2—Cd1—O2 ⁱ	131.59 (5)	C5—C4—C3	119.95 (13)
O4—Cd1—C1 ⁱ	114.36 (4)	C5—C4—H4	120.0
O4 ⁱ —Cd1—C1 ⁱ	115.02 (4)	C3—C4—H4	120.0
O1—Cd1—C1 ⁱ	95.34 (4)	C4—C5—C6	120.73 (11)
O1 ⁱ —Cd1—C1 ⁱ	27.48 (4)	C4—C5—S1	119.41 (11)
O2—Cd1—C1 ⁱ	113.08 (4)	C6—C5—S1	119.84 (10)
O2 ⁱ —Cd1—C1 ⁱ	27.33 (4)	C7—C6—C5	119.16 (12)
O3—S1—O3 ⁱⁱ	119.99 (9)	C7—C6—H6	120.4
O3—S1—C5	107.90 (6)	C5—C6—H6	120.4
O3 ⁱⁱ —S1—C5	108.43 (6)	C6—C7—C2	120.54 (13)
O3—S1—C5 ⁱⁱ	108.43 (6)	C6—C7—H7	119.7
O3 ⁱⁱ —S1—C5 ⁱⁱ	107.90 (6)	C2—C7—H7	119.7
C5—S1—C5 ⁱⁱ	102.86 (8)		
O4—Cd1—O1—C1	-130.73 (7)	O2—C1—C2—C3	156.57 (12)
O4 ⁱ —Cd1—O1—C1	-26.66 (10)	O1—C1—C2—C3	-23.92 (16)
O1 ⁱ —Cd1—O1—C1	86.14 (8)	C7—C2—C3—C4	2.62 (18)
O2—Cd1—O1—C1	-0.88 (7)	C1—C2—C3—C4	-178.34 (11)
O2 ⁱ —Cd1—O1—C1	140.90 (7)	C2—C3—C4—C5	-1.87 (19)
C1 ⁱ —Cd1—O1—C1	113.69 (8)	C3—C4—C5—C6	0.49 (19)
O4—Cd1—O2—C1	72.63 (8)	C3—C4—C5—S1	178.80 (10)
O4 ⁱ —Cd1—O2—C1	164.60 (7)	O3 ⁱⁱ —S1—C5—C4	36.48 (11)
O1 ⁱ —Cd1—O2—C1	-97.38 (8)	O3—S1—C5—C4	167.88 (10)
O1—Cd1—O2—C1	0.89 (7)	C5 ⁱⁱ —S1—C5—C4	-77.63 (10)
O2 ⁱ —Cd1—O2—C1	-54.85 (7)	O3 ⁱⁱ —S1—C5—C6	-145.19 (10)
C1 ⁱ —Cd1—O2—C1	-78.93 (9)	O3—S1—C5—C6	-13.78 (12)
Cd1—O2—C1—O1	-1.48 (11)	C5 ⁱⁱ —S1—C5—C6	100.71 (11)
Cd1—O2—C1—C2	178.02 (11)	C4—C5—C6—C7	0.15 (19)
Cd1—O1—C1—O2	1.67 (13)	S1—C5—C6—C7	-178.16 (10)
Cd1—O1—C1—C2	-177.85 (9)	C5—C6—C7—C2	0.61 (18)
O2—C1—C2—C7	-24.41 (18)	C3—C2—C7—C6	-2.00 (18)
O1—C1—C2—C7	155.11 (11)	C1—C2—C7—C6	178.99 (11)

Symmetry codes: (i) $-x, y, -z+3/2$; (ii) $-x+1, y, -z+5/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4B ⁱⁱⁱ —O1 ⁱⁱⁱ	0.85	1.97	2.7479 (14)	151
O4—H4A ^{iv} —O2 ^{iv}	0.85	2.00	2.7364 (15)	145
C6—H6 ⁱⁱⁱ —O3	0.93	2.55	2.9208 (16)	104

Symmetry codes: (iii) $x, y-1, z$; (iv) $x, -y, z-1/2$.