

Poly[[tetraaquabis(μ -hydroxyacetato- $\kappa^4 O^1, O^2: O^1, O^1'$)- μ_2 -sulfato- $\kappa^2 O: O'$ -dicadmium(II)] monohydrate]

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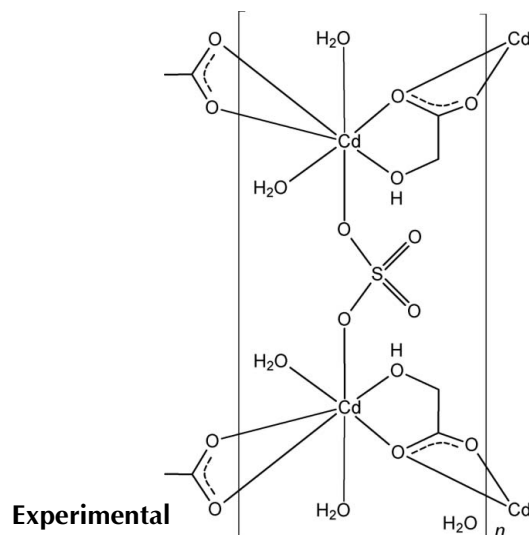
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.015; wR factor = 0.038; data-to-parameter ratio = 16.8.

The title compound, $\{[Cd_2(C_2H_3O_3)_2(SO_4)(H_2O)_4] \cdot H_2O\}_n$, was obtained unintentionally in a transmetallation reaction. The crystal structure contains a two-dimensional metal-organic framework based on $Cd^{II}-(\mu$ -hydroxyacetato- $\kappa^4 O^1, O^2: O^1, O^1')$ - Cd^{II} zigzag chains joined together by bridging SO_4 anions. The resulting layers are shifted with respect to each other and are stacked along the c axis. Their construction is supported by hydrogen bonds between water molecules and between water molecules and carboxylate or sulfate groups. Neighbouring layers are bridged by hydrogen bonds between the hydroxyl substituent and a sulfate anion. The sulfate anion and solvent water molecule are located on twofold axes. The results demonstrate that care must be taken when preparing ethylenediaminetetraacetic acid-type complexes by transmetallation, in order to avoid precipitation of metal complexes with the α -hydroxyacetate ligand.

Related literature

For examples of the successful application of transmetallation reactions in the synthesis of metal(II) complexes with hexadentate 1,3-propanediaminetetraacetate and 1,4-butanediaminetetraacetate ligands, see: Radanović *et al.* (2003, 2004, 2007); Rychlewska *et al.* (2000, 2005, 2007).



Experimental

Crystal data

$[Cd_2(C_2H_3O_3)_2(SO_4)(H_2O)_4] \cdot H_2O$
 $M_r = 561.03$
 Monoclinic, $C2/c$
 $a = 13.5750$ (3) Å
 $b = 8.5777$ (1) Å
 $c = 13.7734$ (3) Å
 $\beta = 107.528$ (2)°

$V = 1529.34$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 2.99$ mm⁻¹
 $T = 295$ K
 0.30 × 0.30 × 0.20 mm

Data collection

Kuma KM4 CCD κ -geometry diffractometer
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
 $T_{min} = 0.388$, $T_{max} = 0.550$

8842 measured reflections
 1710 independent reflections
 1602 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.015$
 $wR(F^2) = 0.038$
 $S = 1.13$
 1710 reflections

102 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.46$ e Å⁻³
 $\Delta\rho_{min} = -0.31$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cd1—O1	2.3584 (14)	Cd1—O2W	2.3245 (14)
Cd1—O2	2.3013 (14)	Cd1—O2 ⁱ	2.5937 (14)
Cd1—O4	2.2386 (16)	Cd1—O3 ⁱ	2.3379 (17)
Cd1—O1W	2.2731 (15)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H1W ⁱⁱ ···O2W ⁱⁱ	0.85	1.94	2.784 (2)	170
O1W—H2W ⁱⁱⁱ ···O3 ⁱⁱⁱ	0.85	1.88	2.723 (2)	172
O2W—H3W ⁱⁱⁱ ···O3W	0.85	1.88	2.720 (2)	172
O2W—H4W ⁱⁱⁱ ···O5 ⁱ	0.85	1.82	2.648 (2)	162
O1—H1O ^{iv} ···O5 ^{iv}	0.85	1.81	2.659 (2)	175
O3W—H5W ^v ···O4 ^v	0.85	2.25	2.813 (3)	124

Symmetry codes: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z$; (iii) $x, y - 1, z$; (iv) $x, -y + 2, z - \frac{1}{2}$; (v) $x + \frac{1}{2}, y + \frac{1}{2}, z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Siemens, 1989) and *Mercury* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2209).

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supplementary materials

Acta Cryst. (2009). E65, m648-m649 [doi:10.1107/S1600536809017255]

Poly[[tetraaquabis(μ -hydroxyacetato- $\kappa^4 O^1, O^2:O^1, O^1'$)- μ_2 -sulfato- $\kappa^2 O:O'$ -dicadmium(II)] mono-hydrate]

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Comment

Research concerning metal–organic frameworks (MOF) has recently become important due to their potential application in a number of areas, including gas storage and catalysis. Prominent in this class of materials are frameworks that involve α -hydroxycarboxylate ligands spanning network nodes. We have recently obtained one such MOF by serendipity, when trying to synthesize cadmium(II) homometallic complex with 1,4-bdta ligand (1,4-bdta stands for 1,4-butanediaminetetraacetate) by the process of transmetalation. So far we have successfully used this strategy for obtaining M (II) complexes with both 1,3-pdta (1,3-propanediaminetetraacetate) (Rychlewska *et al.*, 2000; Radanović *et al.*, 2003; Radanović *et al.*, 2004; Rychlewska *et al.*, 2005, 2007) and 1,4-bdta ligands (Radanović *et al.*, 2007). In this procedure, barium(II) cations, forming the homometallic barium 1,3-pdta or 1,4-bdta complex, are being exchanged by much smaller in size metal(II) cations. At the very first step of this reaction we synthesize the ligands by reacting 1,3-propanediamine (or 1,4-butanediamine) with sodium chloracetate. It turned out that, when trying to synthesize 1,4-bdta ligand, we have obtained, in the reaction mixture, besides the expected H_4 -1,4-bdta, some amount of α -hydroxycarboxylic acid. Most probably, this α -hydroxycarboxylic acid has originated from the chloroacetic acid when heated at $pH > 10$. Consequent addition of $BaCl_2$ to the solution resulted in formation of two types of barium(II) salts, one formed by H_4 -1,4-bdta and the other by $HOCH_2COOH$. An attempt to exchange barium(II) by cadmium(II) cations by addition of $CdSO_4$ resulted in precipitation of two-dimensional homometallic MOF formed by Cd^{II} cations, hydroxyacetate and sulfate anions, instead of the expected Cd^{II} 1,4-bdta complex. This has been unequivocally established by the X-ray crystal structure analysis, the results of which are reported in this paper. We next attempted to verify this hypothetical synthetic route by synthesizing the very same Cd^{II} complex starting from $(HOCH_2COO)_2Ba$ salt. For both samples we have performed elemental microanalyses and NMR measurements which confirmed their identity.

In the crystal the Cd^{II} nodes bind together by a singly deprotonated hydroxyacetate and doubly deprotonated sulfate linkers. The hydroxyacetate acts as a tetradentate ligand with α -hydroxyacetate group $O1-C1-C2-O2$ acting as a bidentate chelate to $Cd1$, and carboxylate group $O2-C2-O3$ acting as a bidentate chelate to $Cd1$ at $1/2 - x, 1/2 + y, 1/2 - z$. The two Cd^{II} centers sharing the same (O2) carboxylate oxygen and bridged by the $O2-C2-O3$ carboxylate group are 4.736 (1) Å apart, and extend in a *zigzag* manner along the *b*-direction. Each Cd^{II} cation is chelated by a hydroxyacetate residue and a carboxylate group, and is coordinated by two water molecules, and one sulfate anion, resulting in a sevenfold coordination mode (Fig. 1). The hydroxyacetate anions and one coordinated water molecule (O1W) lie in the equatorial plane while the other water molecule (O2W) and the sulfate anion take the axial positions. Hence, the coordination polyhedron formed around $Cd1$ is a distorted pentagonal bipyramid with the in-plane *cis* bond angles in the range 52.37 (4)–83.68 (5)°, the smallest angle reflecting chelation by the carboxylate ligand, and with the out-of-plane *trans* angle of 170.76 (6)°. Sulfate anions lie on the twofold axis and connect the neighbouring Cd^{II} centers, related by this symmetry axis *via* O4 oxygen atoms. Separation of the two Cd^{II} metal centers bridged by the sulfate group measures 6.773 (1) Å. The sulfate bridges help

supplementary materials

to extend the basic structural motif in the *a*-direction, thus forming a (001) layer (Fig. 2). This polymeric two-dimensional construction is additionally supported by hydrogen bonds (Table 2) that involve crystalline water molecule, which also occupies the twofold axis (O3w). This water molecule acts as a double hydrogen bond donor to two coordinated sulfate O atoms (O4 and its symmetry equivalent) and a double hydrogen bond acceptor from the axially coordinated water molecule (O2W and its twofold equivalent). The equatorially coordinated water molecule (O1W) acts as a hydrogen bond donor to carboxylate O3 and the axially coordinated water O2W. The neighbouring two-dimensional layers are bridged by a hydrogen bond formed between a hydroxyl group (O1) acting as a hydrogen-bond donor and the uncoordinated oxygen atom (O5) from the sulfate anion. The hydrogen bond parameters are provided in Table 2.

The reported X-ray analysis allowed us to identify and structurally characterize the unintentionally synthesized two-dimensional MOF and to demonstrate that care must be taken when preparing the edta-type complexes by transmetallation to avoid precipitation of metal complexes with α -hydroxyacetate bridges. To remove the excess of Ba(II) α -hydroxyacetate, a water washing procedure should be repeated several times.

Experimental

2.56 g (0.003 mol) of $\text{CdSO}_4 \cdot 8\text{H}_2\text{O}$ were dissolved in 50 cm^3 of distilled water at 70°C . To this solution, 6.27 g of solid $\text{Ba}[\text{Ba}(1,4\text{-bdta})] \cdot 2\text{H}_2\text{O}$ containing $\text{Ba}(\text{HOCH}_2\text{COO})_2$ in ratio 3:1, respectively, was added and the reaction mixture was heated at 90°C with stirring for 6 h. The precipitated BaSO_4 was removed by filtration and the filtrate was evaporated to *ca* 10 cm^3 and then left in a refrigerator for several days. Colorless crystals of the title compound were collected, washed with ethanol, and air-dried. Yield 0.98 g (59.5%). The complex was recrystallized from hot water while cooling in a refrigerator. Analysis calculated for $\text{C}_4\text{H}_{14}\text{Cd}_2\text{O}_{14}\text{S} \cdot \text{H}_2\text{O}$ (FW = 561.03; m. p. 416 K): C 8.84, H 2.87, S 5.90%; found: C 8.93, H 2.83, S 6.28%.

Refinement

All H atoms attached to C atoms were placed in their idealized positions, the hydroxyl and water H atoms were located on difference Fourier maps. All H atoms were refined as riding on their carrier atoms with constraints imposed on the bond lengths and displacement parameters, *i.e.* C—H = 0.96 Å O—H = 0.85 Å with $U_{\text{iso}}(\text{H})$ 20% higher than U_{eq} of the carrier atom.

Figures

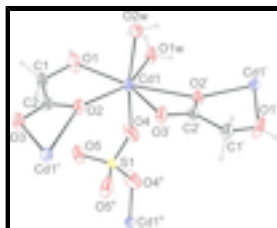


Fig. 1. Basic supramolecular motif showing pentagonal bipyramidal coordination around Cd^{II} . Displacement ellipsoids are drawn at the 40% probability level. Symmetry codes: *i* = $-x + 1/2, y - 1/2, -z + 1/2$; *ii* = $-x + 1/2, y + 1/2, -z + 1/2$; *iii* = $-x, y, -z + 1/2$.

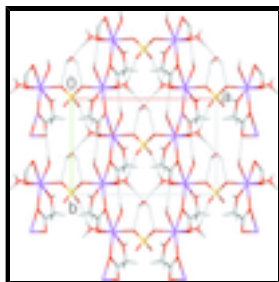


Fig. 2. View down the monoclinic *c*-direction showing hydrogen bonding (dashed lines), water channels and two-dimensional structure of the complex.

Poly[[tetraaquabis(μ_2 -hydroxyacetato- $\kappa^4 O^1, O^2: O^1, O^1$)- μ_2 -sulfato- $\kappa^2 O: O^1$ -dicadmium(II)] monohydrate]

Crystal data

[Cd₂(C₂H₃O₃)₂(SO₄)(H₂O)₄].H₂O

M_r = 561.03

Monoclinic, *C2/c*

Hall symbol: -*C* 2yc

a = 13.5750 (3) Å

b = 8.57770 (10) Å

c = 13.7734 (3) Å

β = 107.528 (2)°

V = 1529.34 (5) Å³

Z = 4

*F*₀₀₀ = 1088

D_x = 2.437 Mg m⁻³

Melting point: 416 K

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 5972 reflections

θ = 2.9–28.0°

μ = 2.99 mm⁻¹

T = 295 K

Prismatic, colourless

0.30 × 0.30 × 0.20 mm

Data collection

Kuma KM4 CCD κ -geometry diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 295 K

ω and φ scans

Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)

*T*_{min} = 0.388, *T*_{max} = 0.550

8842 measured reflections

1710 independent reflections

1602 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.018

θ_{\max} = 28.0°

θ_{\min} = 2.9°

h = -17→17

k = -10→10

l = -17→17

Refinement

Refinement on *F*²

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.015$

wR(*F*²) = 0.038

S = 1.13

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2 + 0.9781P]$$

where $P = (F_o^2 + 2F_c^2)/3$

(Δ/σ)_{max} = 0.001

$\Delta\rho_{\max} = 0.46 \text{ e } \text{Å}^{-3}$

supplementary materials

1710 reflections

$$\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$$

102 parameters

Extinction correction: SHELXL97 (Sheldrick, 2008),

$$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.00703 (18)

Secondary atom site location: difference Fourier map

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.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.215433 (10)	0.885016 (14)	0.174423 (9)	0.02516 (7)
O1W	0.15455 (14)	0.67573 (17)	0.07284 (12)	0.0463 (4)
H1W	0.1546	0.6610	0.0118	0.056*
H2W	0.1641	0.5894	0.1046	0.056*
O2W	0.36889 (11)	0.85773 (16)	0.13399 (12)	0.0344 (3)
H3W	0.4134	0.9233	0.1669	0.041*
H4W	0.3970	0.7714	0.1573	0.041*
O1	0.14443 (14)	1.02774 (17)	0.02309 (11)	0.0499 (4)
H1O	0.1128	1.0004	-0.0376	0.060*
C1	0.12548 (16)	1.1879 (2)	0.03179 (14)	0.0323 (4)
H1A	0.0528	1.2052	0.0191	0.039*
H1B	0.1474	1.2454	-0.0178	0.039*
C2	0.18369 (14)	1.2435 (2)	0.13702 (13)	0.0254 (4)
O2	0.23446 (11)	1.14930 (16)	0.20257 (11)	0.0310 (3)
O4	0.07190 (15)	0.87150 (18)	0.22208 (19)	0.0617 (6)
S1	0.0000	0.97501 (7)	0.2500	0.02325 (13)
O5	0.05131 (16)	1.0737 (2)	0.33543 (12)	0.0570 (5)
O3W	0.5000	1.0723 (3)	0.2500	0.0749 (10)
H5W	0.5380	1.1144	0.2183	0.090*
O3	0.17860 (15)	1.38542 (15)	0.15667 (12)	0.0396 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03149 (10)	0.02054 (9)	0.02099 (9)	0.00182 (4)	0.00418 (6)	-0.00095 (5)
O1W	0.0858 (12)	0.0209 (7)	0.0251 (7)	-0.0006 (7)	0.0062 (7)	-0.0006 (6)
O2W	0.0402 (8)	0.0289 (7)	0.0334 (8)	0.0051 (6)	0.0098 (6)	0.0019 (6)
O1	0.0872 (12)	0.0260 (8)	0.0193 (7)	0.0107 (7)	-0.0098 (7)	-0.0061 (6)
C1	0.0445 (11)	0.0231 (9)	0.0224 (9)	0.0022 (8)	-0.0001 (8)	0.0011 (7)
C2	0.0323 (9)	0.0211 (9)	0.0218 (8)	-0.0040 (7)	0.0067 (7)	0.0000 (7)
O2	0.0416 (7)	0.0226 (6)	0.0214 (6)	-0.0032 (5)	-0.0018 (6)	0.0001 (5)

O3	0.0629 (10)	0.0208 (7)	0.0274 (8)	-0.0011 (6)	0.0021 (7)	-0.0030 (5)
O4	0.0565 (11)	0.0353 (9)	0.1112 (18)	0.0121 (7)	0.0524 (13)	0.0067 (9)
S1	0.0263 (3)	0.0186 (3)	0.0233 (3)	0.000	0.0051 (2)	0.000
O5	0.0940 (15)	0.0310 (8)	0.0250 (8)	-0.0193 (8)	-0.0139 (8)	0.0032 (7)
O3W	0.0500 (15)	0.0271 (12)	0.140 (3)	0.000	0.0168 (17)	0.000

Geometric parameters (Å, °)

Cd1—O1	2.3584 (14)	O1—H1O	0.8500
Cd1—O2	2.3013 (14)	C1—C2	1.504 (3)
Cd1—O4	2.2386 (16)	C1—H1A	0.9601
Cd1—O1W	2.2731 (15)	C1—H1B	0.9599
Cd1—O2W	2.3245 (14)	C2—O2	1.252 (2)
Cd1—O2 ⁱ	2.5937 (14)	C2—O3	1.253 (2)
Cd1—O3 ⁱ	2.3379 (17)	O2—Cd1 ⁱⁱ	2.5937 (14)
O1W—H1W	0.8500	O4—S1	1.4543 (16)
O1W—H2W	0.8500	S1—O5	1.4468 (16)
O2W—H3W	0.8500	O3W—H5W	0.8500
O2W—H4W	0.8500	O3—Cd1 ⁱⁱ	2.3379 (17)
O1—C1	1.410 (2)		
O4—Cd1—O1W	87.27 (7)	Cd1—O2W—H3W	110.5
O4—Cd1—O2	93.73 (5)	H4W—O2W—H3W	102.0
O1W—Cd1—O2	152.03 (5)	C1—O1—Cd1	117.86 (11)
O4—Cd1—O2W	170.76 (6)	C1—O1—H1O	107.6
O1W—Cd1—O2W	87.65 (6)	Cd1—O1—H1O	132.6
O2—Cd1—O2W	94.38 (5)	O1—C1—C2	109.54 (15)
O4—Cd1—O3 ⁱ	92.14 (8)	O1—C1—H1A	109.8
O1W—Cd1—O3 ⁱ	127.91 (5)	C2—C1—H1A	109.8
O2—Cd1—O3 ⁱ	80.02 (5)	O1—C1—H1B	109.7
O2W—Cd1—O3 ⁱ	84.91 (6)	C2—C1—H1B	109.8
O4—Cd1—O1	97.23 (7)	H1A—C1—H1B	108.2
O1W—Cd1—O1	83.68 (5)	O2—C2—O3	121.68 (18)
O2—Cd1—O1	68.45 (5)	O2—C2—C1	120.37 (17)
O2W—Cd1—O1	89.87 (6)	O3—C2—C1	117.95 (17)
O3 ⁱ —Cd1—O1	147.55 (5)	C2—O2—Cd1	120.32 (12)
O4—Cd1—O2 ⁱ	81.27 (6)	C2—O2—Cd1 ⁱⁱ	86.96 (11)
O1W—Cd1—O2 ⁱ	76.21 (5)	Cd1—O2—Cd1 ⁱⁱ	150.69 (6)
O2—Cd1—O2 ⁱ	131.594 (18)	S1—O4—Cd1	139.34 (10)
O2W—Cd1—O2 ⁱ	90.02 (5)	O5—S1—O5 ⁱⁱⁱ	108.34 (13)
O3 ⁱ —Cd1—O2 ⁱ	52.37 (4)	O5—S1—O4 ⁱⁱⁱ	109.84 (12)
O1—Cd1—O2 ⁱ	159.88 (5)	O5 ⁱⁱⁱ —S1—O4 ⁱⁱⁱ	112.05 (13)
Cd1—O1W—H2W	113.6	O5—S1—O4	112.05 (13)
Cd1—O1W—H1W	128.1	O5 ⁱⁱⁱ —S1—O4	109.84 (12)
H2W—O1W—H1W	109.5	O4 ⁱⁱⁱ —S1—O4	104.74 (14)
Cd1—O2W—H4W	109.2	C2—O3—Cd1 ⁱⁱ	98.98 (12)

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O4—Cd1—O1—C1	74.77 (15)	O2 ⁱ —Cd1—O2—C2	-163.19 (14)
O1W—Cd1—O1—C1	161.19 (16)	O4—Cd1—O2—Cd1 ⁱⁱ	74.85 (14)
O2—Cd1—O1—C1	-16.41 (14)	O1W—Cd1—O2—Cd1 ⁱⁱ	166.05 (11)
O2W—Cd1—O1—C1	-111.16 (15)	O2W—Cd1—O2—Cd1 ⁱⁱ	-100.72 (13)
O3 ⁱ —Cd1—O1—C1	-30.9 (2)	O3 ⁱ —Cd1—O2—Cd1 ⁱⁱ	-16.67 (13)
O2 ⁱ —Cd1—O1—C1	159.13 (13)	O1—Cd1—O2—Cd1 ⁱⁱ	171.15 (15)
Cd1—O1—C1—C2	16.3 (2)	O2 ⁱ —Cd1—O2—Cd1 ⁱⁱ	-6.79 (12)
O1—C1—C2—O2	-3.4 (2)	O1W—Cd1—O4—S1	-144.9 (2)
O1—C1—C2—O3	177.33 (17)	O2—Cd1—O4—S1	7.1 (2)
O3—C2—O2—Cd1	167.52 (14)	O3 ⁱ —Cd1—O4—S1	87.2 (2)
C1—C2—O2—Cd1	-11.7 (2)	O1—Cd1—O4—S1	-61.6 (2)
O3—C2—O2—Cd1 ⁱⁱ	-1.16 (18)	O2 ⁱ —Cd1—O4—S1	138.6 (2)
C1—C2—O2—Cd1 ⁱⁱ	179.64 (15)	Cd1—O4—S1—O5	-57.4 (2)
O4—Cd1—O2—C2	-81.55 (15)	Cd1—O4—S1—O5 ⁱⁱⁱ	63.0 (2)
O1W—Cd1—O2—C2	9.6 (2)	Cd1—O4—S1—O4 ⁱⁱⁱ	-176.5 (3)
O2W—Cd1—O2—C2	102.89 (14)	O2—C2—O3—Cd1 ⁱⁱ	1.3 (2)
O3 ⁱ —Cd1—O2—C2	-173.07 (15)	C1—C2—O3—Cd1 ⁱⁱ	-179.48 (13)
O1—Cd1—O2—C2	14.76 (13)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W \cdots O2W ^{iv}	0.85	1.94	2.784 (2)	170
O1W—H2w \cdots O3 ^v	0.85	1.88	2.723 (2)	172
O2W—H3W \cdots O3W	0.85	1.88	2.720 (2)	172
O2W—H4W \cdots O5 ⁱ	0.85	1.82	2.648 (2)	162
O1—H1O \cdots O5 ^{vi}	0.85	1.81	2.659 (2)	175
O3W—H5W \cdots O4 ^{vii}	0.85	2.25	2.813 (3)	124

Symmetry codes: (iv) $-x+1/2, -y+3/2, -z$; (v) $x, y-1, z$; (i) $-x+1/2, y-1/2, -z+1/2$; (vi) $x, -y+2, z-1/2$; (vii) $x+1/2, y+1/2, z$.

Fig. 1

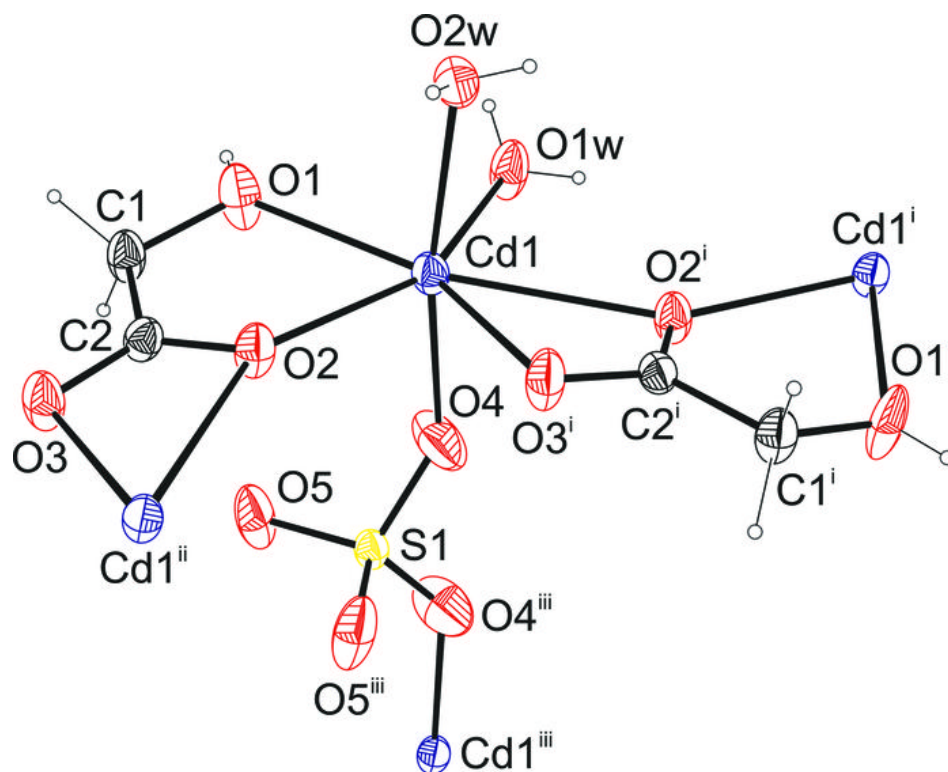


Fig. 2

