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Tetraaquabis(*N*-phenylsulfonyl-L-leucinato)cadmium(II) dihydrate

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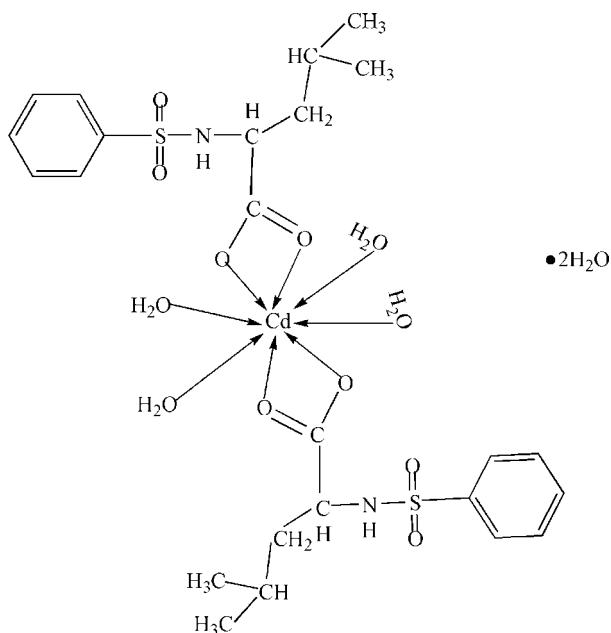
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.018$ Å; disorder in main residue; R factor = 0.068; wR factor = 0.214; data-to-parameter ratio = 14.7.

In the title compound, $[\text{Cd}(\text{C}_{12}\text{H}_{16}\text{NO}_4\text{S})_2(\text{H}_2\text{O})] \cdot 2\text{H}_2\text{O}$, the Cd atom is located on a twofold rotation axis and a distorted CdO_8 dodecahedral arrangement arises from the coordination of the two chelating ligands and four water molecules. A network of $\text{N}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{O}$ and $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds help to establish the crystal packing. Both coordinated and uncoordinated water molecules are disordered with an approximate half-occupation for each of the water molecules.

Related literature

For background to the design and synthesis of metal complexes, see: Zhang *et al.* (2007).



Experimental

Crystal data

$[\text{Cd}(\text{C}_{12}\text{H}_{16}\text{NO}_4\text{S})_2(\text{H}_2\text{O})] \cdot 2\text{H}_2\text{O}$
 $M_r = 725.10$
 Orthorhombic, $P2_12_12_1$
 $a = 17.733$ (2) Å
 $b = 17.2930$ (19) Å
 $c = 5.6051$ (11) Å
 $V = 1718.9$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.81$ mm⁻¹
 $T = 298$ (2) K
 $0.50 \times 0.40 \times 0.36$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.687$, $T_{\max} = 0.759$
 9050 measured reflections
 3033 independent reflections
 1954 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.068$
 $wR(F^2) = 0.214$
 $S = 1.03$
 3033 reflections
 207 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.70$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.56$ e Å⁻³
 Absolute structure: Flack (1983),
 1247 Friedel pairs
 Flack parameter: 0.00 (8)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N1}-\text{H1} \cdots \text{O1}$	0.90	2.29	2.776 (11)	113
$\text{N1}-\text{H1} \cdots \text{O2}^{\text{ii}}$	0.90	2.35	3.121 (12)	143
$\text{O5}-\text{H5E} \cdots \text{O1}^{\text{ii}}$	0.85	1.85	2.639 (19)	154
$\text{O5}-\text{H5F} \cdots \text{O1}^{\text{iii}}$	0.85	1.79	2.605 (18)	161
$\text{O7}-\text{H7C} \cdots \text{O3}^{\text{iv}}$	0.85	2.20	2.99 (2)	155
$\text{O7}-\text{H7D} \cdots \text{O4}^{\text{v}}$	0.85	2.22	3.00 (2)	152
$\text{C2}-\text{H2} \cdots \text{O3}$	0.98	2.46	2.903 (13)	107
$\text{C2}-\text{H2} \cdots \text{O4}^{\text{ii}}$	0.98	2.58	3.457 (13)	149
$\text{C12}-\text{H12} \cdots \text{O3}$	0.93	2.52	2.871 (14)	102

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2702).

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supplementary materials

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Tetraaquabis(*N*-phenylsulfonyl-L-leucinato)cadmium(II) dihydrate

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Comment

During the last decade, the design and synthesis of metal complexes have attracted considerable attention due to their potential uses as biological activities (Zhang *et al.*, 2007). The synthesis and structure of the title compound (I) is reported.

In the title compound, the Cd atom is located on an inversion center. Two O-bidentate ligands and four water molecules are attached to the cadmium atom, resulting in a distorted CdO₈ trigonal dodecahedral arrangement (Fig. 1). The identical S1=O3 [1.407 (7) Å], S1=O4 [1.430 (8) Å] and C1=O2 [1.235 (13) Å] bonds lengths imply double-bond character. The dihedral angle between the two benzene ring mean planes (C7—C12 and C7A—C12A) is 58.2 °.

Two molecules of water complete the structure of (I) and a network of hydrogen bonds helps to establish the crystal packing (Table 1).

Experimental

1 mmol of cadmium chloride was added to a solution of 2-phenylsulfonyl chloride-L-leucine (2 mmol) in 10 ml of CH₃OH/H₂O (*v/v* 1:1). The mixture was continuously stirred for 4 h at refluxing temperature, evaporating some methanol, then, upon cooling, the solid product was collected by filtration and dried *in vacuo* (yield 69%). Clear blocks of (I) were obtained by evaporation from a methanol solution after a week.

Refinement

The water H atoms were located in a difference map and refined as riding in their as-found relative positions with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. Other H atoms were placed geometrically (C—H = 0.93–0.98 Å, O—H = 0.82 Å, N—H = 0.90 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C},\text{N})$ or $1.5U_{\text{eq}}(\text{C},\text{O})$.

Figures

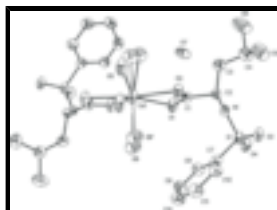


Fig. 1. The complex molecule, with 30% probability ellipsoids.

Tetraaquabis(*N*-phenylsulfonyl-L-leucinato)cadmium(II) dihydrate

Crystal data

$[\text{Cd}(\text{C}_{12}\text{H}_{16}\text{NO}_4\text{S})_2(\text{H}_2\text{O})] \cdot 2\text{H}_2\text{O}$	$F_{000} = 748$
$M_r = 725.10$	$D_x = 1.401 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12$	Mo $K\alpha$ radiation
Hall symbol: P 2 2ab	$\lambda = 0.71073 \text{ \AA}$
$a = 17.733 (2) \text{ \AA}$	Cell parameters from 2267 reflections
$b = 17.2930 (19) \text{ \AA}$	$\theta = 2.3\text{--}19.6^\circ$
$c = 5.6051 (11) \text{ \AA}$	$\mu = 0.81 \text{ mm}^{-1}$
$V = 1718.9 (4) \text{ \AA}^3$	$T = 298 (2) \text{ K}$
$Z = 2$	Block, colourless
	$0.50 \times 0.40 \times 0.36 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	3033 independent reflections
Radiation source: fine-focus sealed tube	1954 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.051$
$T = 298(2) \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.6^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -21 \rightarrow 19$
$T_{\text{min}} = 0.687$, $T_{\text{max}} = 0.759$	$k = -18 \rightarrow 20$
9050 measured reflections	$l = -6 \rightarrow 6$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.1333P)^2 + 0.5509P]$
$wR(F^2) = 0.214$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} = 0.001$
3033 reflections	$\Delta\rho_{\text{max}} = 0.70 \text{ e \AA}^{-3}$
207 parameters	$\Delta\rho_{\text{min}} = -0.56 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none
Secondary atom site location: difference Fourier map	Absolute structure: Flack (1983), 1247 Freidel pairs
	Flack parameter: 0.00 (8)

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>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cd1	0.5000	0.5000	0.05213 (18)	0.0754 (4)	
N1	0.3790 (4)	0.7120 (5)	0.5321 (16)	0.067 (2)	
H1	0.3992	0.6707	0.6057	0.081*	
O1	0.4512 (4)	0.5829 (4)	0.3465 (14)	0.079 (2)	
O2	0.4394 (4)	0.6239 (4)	-0.0210 (14)	0.077 (2)	
O3	0.2573 (4)	0.7608 (4)	0.4174 (14)	0.080 (2)	
O4	0.2793 (4)	0.7154 (5)	0.8283 (13)	0.085 (2)	
O5	0.5451 (10)	0.5261 (9)	-0.333 (3)	0.099 (5)	0.50
H5E	0.5163	0.5567	-0.4087	0.119*	0.50
H5F	0.5517	0.4850	-0.4128	0.119*	0.50
O6	0.379 (2)	0.446 (3)	0.075 (15)	0.110 (12)	0.57 (13)
H6E	0.3791	0.3977	0.0942	0.132*	0.57 (13)
H6F	0.3768	0.4554	-0.0740	0.132*	0.57 (13)
O6'	0.396 (3)	0.428 (3)	0.191 (19)	0.110 (16)	0.43 (13)
H6'C	0.3941	0.3821	0.1354	0.132*	0.43 (13)
H6'B	0.4170	0.4296	0.3270	0.132*	0.43 (13)
O7	0.6587 (11)	0.6808 (11)	0.976 (4)	0.128 (7)	0.50
H7C	0.6778	0.6880	0.8389	0.153*	0.50
H7D	0.6855	0.7054	1.0766	0.153*	0.50
S1	0.29018 (13)	0.70772 (14)	0.5767 (5)	0.0649 (6)	
C1	0.4350 (6)	0.6338 (6)	0.197 (2)	0.068 (3)	
C2	0.4090 (6)	0.7135 (6)	0.2887 (19)	0.069 (3)	
H2	0.3714	0.7354	0.1798	0.083*	
C3	0.4805 (6)	0.7630 (7)	0.285 (2)	0.085 (3)	
H3A	0.5139	0.7441	0.4090	0.102*	
H3B	0.5056	0.7546	0.1336	0.102*	
C4	0.4717 (8)	0.8475 (8)	0.319 (3)	0.101 (4)	
H4	0.4474	0.8621	0.4690	0.122*	
C5	0.4321 (9)	0.8787 (9)	0.095 (4)	0.129 (6)	
H5A	0.4440	0.8463	-0.0392	0.194*	
H5B	0.4491	0.9305	0.0636	0.194*	
H5C	0.3786	0.8789	0.1199	0.194*	
C6	0.5520 (11)	0.8810 (9)	0.286 (4)	0.151 (8)	
H6A	0.5840	0.8629	0.4117	0.227*	
H6B	0.5497	0.9365	0.2897	0.227*	
H6C	0.5719	0.8646	0.1346	0.227*	
C7	0.2568 (6)	0.6164 (6)	0.498 (2)	0.074 (3)	
C8	0.2721 (7)	0.5536 (7)	0.651 (2)	0.083 (3)	

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H8	0.2995	0.5616	0.7905	0.099*
C9	0.2469 (7)	0.4809 (7)	0.596 (3)	0.093 (4)
H9	0.2571	0.4398	0.6977	0.111*
C10	0.2057 (8)	0.4681 (8)	0.384 (3)	0.094 (4)
H10	0.1882	0.4189	0.3462	0.113*
C11	0.1923 (7)	0.5283 (7)	0.239 (3)	0.093 (4)
H11	0.1650	0.5202	0.1000	0.112*
C12	0.2186 (7)	0.6048 (7)	0.292 (2)	0.083 (3)
H12	0.2096	0.6454	0.1871	0.099*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0923 (8)	0.0840 (7)	0.0497 (6)	0.0321 (6)	0.000	0.000
N1	0.075 (5)	0.069 (4)	0.058 (5)	0.015 (4)	-0.007 (4)	-0.005 (4)
O1	0.095 (5)	0.077 (4)	0.064 (5)	0.024 (4)	-0.006 (4)	0.004 (4)
O2	0.090 (5)	0.079 (4)	0.062 (5)	0.026 (4)	0.002 (4)	0.000 (4)
O3	0.084 (4)	0.080 (5)	0.076 (5)	0.030 (4)	-0.004 (4)	0.003 (4)
O4	0.099 (5)	0.102 (5)	0.056 (4)	0.030 (5)	0.010 (4)	-0.010 (4)
O5	0.149 (14)	0.083 (11)	0.066 (10)	0.054 (9)	0.002 (9)	0.006 (8)
O6	0.115 (16)	0.120 (16)	0.09 (3)	0.017 (12)	-0.012 (19)	0.005 (18)
O6'	0.11 (2)	0.12 (2)	0.09 (3)	0.017 (17)	-0.01 (2)	0.00 (3)
O7	0.133 (15)	0.133 (14)	0.117 (17)	-0.040 (12)	0.014 (13)	-0.052 (14)
S1	0.0736 (14)	0.0714 (14)	0.0498 (13)	0.0225 (12)	-0.0001 (13)	-0.0047 (13)
C1	0.074 (6)	0.071 (6)	0.058 (7)	0.015 (5)	-0.006 (5)	0.008 (6)
C2	0.077 (7)	0.071 (6)	0.060 (6)	0.009 (5)	-0.004 (5)	0.003 (5)
C3	0.087 (8)	0.088 (8)	0.080 (8)	0.003 (6)	-0.008 (6)	0.006 (6)
C4	0.102 (9)	0.103 (10)	0.099 (10)	-0.002 (7)	-0.018 (8)	0.005 (9)
C5	0.142 (13)	0.119 (11)	0.126 (15)	-0.002 (9)	-0.027 (13)	0.022 (12)
C6	0.147 (15)	0.137 (14)	0.17 (2)	-0.037 (12)	-0.029 (15)	0.013 (15)
C7	0.083 (6)	0.080 (6)	0.060 (8)	0.008 (5)	-0.001 (5)	0.003 (5)
C8	0.095 (8)	0.085 (8)	0.069 (8)	0.004 (6)	-0.008 (6)	0.002 (6)
C9	0.104 (8)	0.089 (9)	0.085 (9)	0.002 (6)	-0.004 (7)	0.011 (7)
C10	0.106 (9)	0.091 (8)	0.086 (10)	-0.008 (7)	0.003 (8)	0.003 (8)
C11	0.105 (9)	0.099 (10)	0.075 (9)	-0.006 (7)	-0.008 (7)	0.000 (7)
C12	0.096 (8)	0.086 (8)	0.067 (8)	-0.002 (6)	-0.003 (7)	0.003 (6)

Geometric parameters (\AA , $^\circ$)

Cd1—O5 ⁱ	2.343 (16)	S1—C7	1.742 (12)
Cd1—O5	2.343 (16)	C1—C2	1.543 (15)
Cd1—O6	2.35 (3)	C2—C3	1.531 (15)
Cd1—O6 ⁱ	2.35 (3)	C2—H2	0.9800
Cd1—O1 ⁱ	2.351 (7)	C3—C4	1.481 (17)
Cd1—O1	2.351 (7)	C3—H3A	0.9700
Cd1—O6 ⁱ	2.36 (4)	C3—H3B	0.9700
Cd1—O6'	2.36 (4)	C4—C5	1.54 (2)
Cd1—O2 ⁱ	2.433 (7)	C4—C6	1.55 (2)

Cd1—O2	2.433 (7)	C4—H4	0.9800
Cd1—C1 ⁱ	2.709 (11)	C5—H5A	0.9600
N1—C2	1.464 (14)	C5—H5B	0.9600
N1—S1	1.597 (8)	C5—H5C	0.9600
N1—H1	0.8999	C6—H6A	0.9600
O1—C1	1.249 (12)	C6—H6B	0.9600
O2—C1	1.235 (13)	C6—H6C	0.9600
O3—S1	1.407 (7)	C7—C12	1.356 (16)
O4—S1	1.430 (8)	C7—C8	1.409 (16)
O5—H5E	0.8500	C8—C9	1.371 (17)
O5—H5F	0.8500	C8—H8	0.9300
O6—H6E	0.8500	C9—C10	1.408 (19)
O6—H6F	0.8501	C9—H9	0.9300
O6—H6'C	1.1951	C10—C11	1.343 (16)
O6'—H6E	0.8094	C10—H10	0.9300
O6'—H6'C	0.8500	C11—C12	1.432 (17)
O6'—H6'B	0.8501	C11—H11	0.9300
O7—H7C	0.8500	C12—H12	0.9300
O7—H7D	0.8499		
O5 ⁱ —Cd1—O5	46.1 (9)	H6E—O6—H6'C	15.9
O5 ⁱ —Cd1—O6	70 (2)	H6F—O6—H6'C	117.1
O5—Cd1—O6	116 (2)	Cd1—O6'—H6E	114.2
O5 ⁱ —Cd1—O6 ⁱ	116 (2)	Cd1—O6'—H6'C	113.8
O5—Cd1—O6 ⁱ	70 (2)	H6E—O6'—H6'C	30.9
O6—Cd1—O6 ⁱ	174 (4)	Cd1—O6'—H6'B	86.3
O5 ⁱ —Cd1—O1 ⁱ	130.8 (4)	H6E—O6'—H6'B	141.9
O5—Cd1—O1 ⁱ	129.6 (4)	H6'C—O6'—H6'B	112.3
O6—Cd1—O1 ⁱ	93 (2)	H7C—O7—H7D	107.7
O6 ⁱ —Cd1—O1 ⁱ	82.2 (9)	O3—S1—O4	120.6 (5)
O5 ⁱ —Cd1—O1	129.6 (4)	O3—S1—N1	106.2 (5)
O5—Cd1—O1	130.8 (4)	O4—S1—N1	106.4 (5)
O6—Cd1—O1	82.2 (9)	O3—S1—C7	106.9 (5)
O6 ⁱ —Cd1—O1	93 (2)	O4—S1—C7	106.7 (5)
O1 ⁱ —Cd1—O1	90.8 (4)	N1—S1—C7	109.7 (5)
O5 ⁱ —Cd1—O6 ⁱ	132 (3)	O2—C1—O1	123.5 (10)
O5—Cd1—O6 ⁱ	86 (3)	O2—C1—C2	118.2 (10)
O6—Cd1—O6 ⁱ	155 (4)	O1—C1—C2	118.3 (9)
O6 ⁱ —Cd1—O6 ⁱ	19.3 (9)	N1—C2—C3	108.8 (9)
O1 ⁱ —Cd1—O6 ⁱ	78.7 (11)	N1—C2—C1	113.8 (9)
O1—Cd1—O6 ⁱ	75 (3)	C3—C2—C1	104.4 (9)
O5 ⁱ —Cd1—O6'	86 (3)	N1—C2—H2	109.9
O5—Cd1—O6'	132 (3)	C3—C2—H2	109.9
O6—Cd1—O6'	19.3 (9)	C1—C2—H2	109.9
O6 ⁱ —Cd1—O6'	155 (4)	C4—C3—C2	117.6 (10)

supplementary materials

O1 ⁱ —Cd1—O6'	75 (3)	C4—C3—H3A	107.9
O1—Cd1—O6'	78.7 (11)	C2—C3—H3A	107.9
O6 ⁱ —Cd1—O6'	142 (5)	C4—C3—H3B	107.9
O5 ⁱ —Cd1—O2 ⁱ	80.0 (4)	C2—C3—H3B	107.9
O5—Cd1—O2 ⁱ	82.2 (4)	H3A—C3—H3B	107.2
O6—Cd1—O2 ⁱ	93.9 (10)	C3—C4—C5	107.0 (13)
O6 ⁱ —Cd1—O2 ⁱ	87.2 (16)	C3—C4—C6	104.9 (12)
O1 ⁱ —Cd1—O2 ⁱ	54.4 (3)	C5—C4—C6	101.0 (15)
O1—Cd1—O2 ⁱ	144.9 (3)	C3—C4—H4	114.2
O6 ⁱ —Cd1—O2 ⁱ	100 (2)	C5—C4—H4	114.2
O6'—Cd1—O2 ⁱ	86.3 (13)	C6—C4—H4	114.2
O5 ⁱ —Cd1—O2	82.2 (4)	C4—C5—H5A	109.5
O5—Cd1—O2	80.0 (4)	C4—C5—H5B	109.5
O6—Cd1—O2	87.2 (16)	H5A—C5—H5B	109.5
O6 ⁱ —Cd1—O2	93.9 (10)	C4—C5—H5C	109.5
O1 ⁱ —Cd1—O2	144.9 (3)	H5A—C5—H5C	109.5
O1—Cd1—O2	54.4 (3)	H5B—C5—H5C	109.5
O6 ⁱ —Cd1—O2	86.3 (13)	C4—C6—H6A	109.5
O6'—Cd1—O2	100 (2)	C4—C6—H6B	109.5
O2 ⁱ —Cd1—O2	160.6 (4)	H6A—C6—H6B	109.5
O5 ⁱ —Cd1—C1 ⁱ	104.8 (4)	C4—C6—H6C	109.5
O5—Cd1—C1 ⁱ	107.1 (4)	H6A—C6—H6C	109.5
O6—Cd1—C1 ⁱ	92.2 (18)	H6B—C6—H6C	109.5
O6 ⁱ —Cd1—C1 ⁱ	86.0 (9)	C12—C7—C8	120.0 (11)
O1 ⁱ —Cd1—C1 ⁱ	27.4 (3)	C12—C7—S1	121.3 (9)
O1—Cd1—C1 ⁱ	117.9 (3)	C8—C7—S1	118.7 (9)
O6 ⁱ —Cd1—C1 ⁱ	91.2 (11)	C9—C8—C7	120.4 (12)
O6'—Cd1—C1 ⁱ	77 (2)	C9—C8—H8	119.8
O2 ⁱ —Cd1—C1 ⁱ	27.1 (3)	C7—C8—H8	119.8
O2—Cd1—C1 ⁱ	172.3 (3)	C8—C9—C10	120.3 (12)
C2—N1—S1	120.3 (7)	C8—C9—H9	119.8
C2—N1—H1	107.3	C10—C9—H9	119.8
S1—N1—H1	106.5	C11—C10—C9	118.5 (12)
C1—O1—Cd1	92.5 (6)	C11—C10—H10	120.7
C1—O2—Cd1	89.0 (6)	C9—C10—H10	120.7
Cd1—O5—H5E	112.2	C10—C11—C12	122.3 (12)
Cd1—O5—H5F	111.9	C10—C11—H11	118.8
H5E—O5—H5F	109.8	C12—C11—H11	118.8
Cd1—O6—H6F	84.7	C7—C12—C11	118.4 (12)
H6E—O6—H6F	107.7	C7—C12—H12	120.8
Cd1—O6—H6'C	99.8	C11—C12—H12	120.8
O5 ⁱ —Cd1—O1—C1	-40.1 (10)	Cd1—O1—C1—C2	-171.1 (9)
O5—Cd1—O1—C1	21.6 (9)	S1—N1—C2—C3	146.7 (7)

O6—Cd1—O1—C1	-96 (2)	S1—N1—C2—C1	-97.4 (9)
O6 ⁱ —Cd1—O1—C1	88.2 (11)	O2—C1—C2—N1	158.6 (10)
O1 ⁱ —Cd1—O1—C1	170.4 (8)	O1—C1—C2—N1	-22.2 (14)
O6 ⁱⁱ —Cd1—O1—C1	92.4 (13)	O2—C1—C2—C3	-82.9 (13)
O6 ⁱⁱⁱ —Cd1—O1—C1	-116 (3)	O1—C1—C2—C3	96.3 (12)
O2 ⁱ —Cd1—O1—C1	178.1 (7)	N1—C2—C3—C4	-69.9 (14)
O2—Cd1—O1—C1	-4.2 (7)	C1—C2—C3—C4	168.2 (12)
C1 ⁱ —Cd1—O1—C1	175.4 (4)	C2—C3—C4—C5	-68.8 (16)
O5 ⁱ —Cd1—O2—C1	157.0 (9)	C2—C3—C4—C6	-175.5 (13)
O5—Cd1—O2—C1	-156.3 (9)	O3—S1—C7—C12	11.0 (11)
O6—Cd1—O2—C1	87 (2)	O4—S1—C7—C12	141.3 (10)
O6 ⁱ —Cd1—O2—C1	-87 (2)	N1—S1—C7—C12	-103.7 (10)
O1 ⁱ —Cd1—O2—C1	-5.3 (10)	O3—S1—C7—C8	-170.8 (9)
O1—Cd1—O2—C1	4.2 (7)	O4—S1—C7—C8	-40.5 (10)
O6 ⁱⁱ —Cd1—O2—C1	-69 (3)	N1—S1—C7—C8	74.5 (10)
O6 ⁱⁱⁱ —Cd1—O2—C1	72 (3)	C12—C7—C8—C9	-1.7 (19)
O2 ⁱ —Cd1—O2—C1	-179.7 (7)	S1—C7—C8—C9	-179.9 (10)
C1 ⁱ —Cd1—O2—C1	1(3)	C7—C8—C9—C10	0(2)
C2—N1—S1—O3	-44.3 (9)	C8—C9—C10—C11	0.4 (19)
C2—N1—S1—O4	-174.0 (8)	C9—C10—C11—C12	0(2)
C2—N1—S1—C7	70.9 (9)	C8—C7—C12—C11	2.2 (18)
Cd1—O2—C1—O1	-7.7 (12)	S1—C7—C12—C11	-179.6 (9)
Cd1—O2—C1—C2	171.4 (9)	C10—C11—C12—C7	-1.5 (19)
Cd1—O1—C1—O2	8.0 (13)		

Symmetry codes: (i) $-x+1, -y+1, z$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1 \cdots O1	0.90	2.29	2.776 (11)	113
N1—H1 \cdots O2 ⁱⁱ	0.90	2.35	3.121 (12)	143
O5—H5E \cdots O1 ⁱⁱⁱ	0.85	1.85	2.639 (19)	154
O5—H5F \cdots O1 ^{iv}	0.85	1.79	2.605 (18)	161
O7—H7C \cdots O3 ^v	0.85	2.20	2.99 (2)	155
O7—H7D \cdots O4 ^{vi}	0.85	2.22	3.00 (2)	152
C2—H2 \cdots O3	0.98	2.46	2.903 (13)	107
C2—H2 \cdots O4 ⁱⁱⁱ	0.98	2.58	3.457 (13)	149
C12—H12 \cdots O3	0.93	2.52	2.871 (14)	102

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

Fig. 1

