Poly[bis[μ_2-2-(2-pyridylmethylamino)-ethanesulfonato]cadmium(II)]

Zhong-Xiang Du* and Xin-Hong Chang

Department of Chemistry, Luoyang Normal University, Luoyang, Henan 471022, People's Republic of China
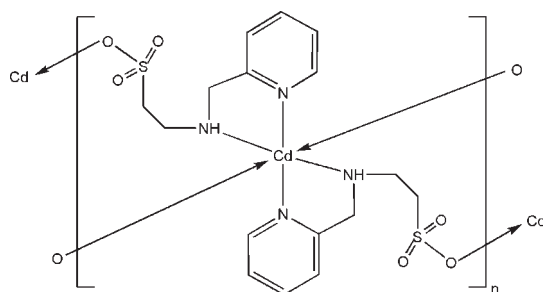Correspondence e-mail: dzx6281@126.com

The title compound $[Cd(C_8H_{11}N_2O_3S)_2]_n$, is a two-dimensional coordination polymer based on a Cd^{2+} atom and deprotonated 2-(2-pyridylmethylamino)ethanesulfonic acid (Hpmt). The complex has molecular symmetry C_i as a consequence of the Cd^{II} being located on an inversion centre. Two N atoms of each pmt^- ligand coordinate to the Cd^{2+} ion and its sulfonate O atom bonds to an adjacent Cd^{2+} ion. 24-membered $(-Cd-N-C-C-S-O-)_4$ rings are formed between neighbouring Cd^{2+} ions; these are interconnected, forming a two-dimensional layer structure. In respect to stereogenic amino N atom and the inversion symmetry of the complex, the compound is a 1:1 racemate. The crystal packing is stabilized by intermolecular $N-H \cdots O$ hydrogen bonds and further connected by $\pi-\pi$ stacking interactions between the pyridyl rings [average interplanar distance and centroid–centroid separation = 3.582 (1) and 3.634 (1)Å, respectively], forming a three-dimensional supramolecular architecture.

Related literature

For different coordination modes of the pmt^- ligand in complexes derived from Hpmt, see: Du & Zhang (2009); Li *et al.* (2006, 2007*a,b*, 2008*a,b*); Liao *et al.* (2007).

Experimental

Crystal data

$[Cd(C_8H_{11}N_2O_3S)_2]$	V = 958.52 (15) Å^3
M_r = 542.90	Z = 2
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 8.8982 (8) Å	μ = 1.40 mm^{-1}
b = 14.0206 (12) Å	T = 291 K
c = 7.9040 (7) Å	0.22 × 0.16 × 0.12 mm
β = 103.579 (1)°	

Data collection

Bruker APEXII CCD area-detector diffractometer	5691 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2178 independent reflections
	2008 reflections with $I > 2\sigma(I)$
T_{min} = 0.749, T_{max} = 0.849	R_{int} = 0.011

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019	133 parameters
$wR(F^2)$ = 0.049	H-atom parameters constrained
S = 1.03	$\Delta\rho_{max}$ = 0.48 e Å^{-3}
2178 reflections	$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N1	2.2853 (14)	Cd1—N2	2.3979 (15)
Cd1—O2^i	2.3496 (14)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2$\cdots$O3^{ii}	0.91	2.26	3.089 (2)	152

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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*.

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Du, Z.-X. & Zhang, G.-Y. (2009). *Acta Cryst.* E**65**, m706.
Li, J.-X., Jiang, Y.-M. & Chen, M.-J. (2008*a*). *J. Coord. Chem.* **61**, 1765–1773.
Li, J.-X., Jiang, Y.-M. & Li, H.-Y. (2006). *Acta Cryst.* E**62**, m2984–m2986.
Li, J.-X., Jiang, Y.-M. & Lian, B.-R. (2008*b*). *J. Chem. Crystallogr.* **38**, 711–715.
Li, J.-X., Jiang, Y.-M. & Wang, J.-G. (2007*a*). *Acta Cryst.* E**63**, m213–m215.
Li, J.-X., Jiang, Y.-M. & Wang, J.-G. (2007*b*). *Acta Cryst.* E**63**, m601–m603.
Liao, B.-L., Li, J.-X. & Jiang, Y.-M. (2007). *Acta Cryst.* E**63**, m1974.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Poly[bis[*μ*₂-2-(2-pyridylmethylamino)ethanesulfonato]cadmium(II)]

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S1. Comment

In the previous literatures, several complexes derived from Hpmt have been reported. Among them, pmt⁻ ligand displays different coordination modes, such as tridentate chelate (Du & Zhang, 2009; Li *et al.*, 2006, 2008*a*; Liao *et al.*, 2007), μ_2 bridge(Li *et al.*, 2007*a*, 2008*b*) and μ_3 bridge (Li *et al.*, 2007*b*). In this paper, we describe another new complex of pmt⁻, (I), Figure 1.

Compound 1 is a two-dimensional coordination polymer and the repeating unit comprises one Cd^{2+} ion and two pmt⁻ ligands(Fig. 1, Table 1). Cd^{2+} ion situates on a centre of symmetry and is six-coordinated with four N atoms from two pmt⁻ ligands along with two sulfonate O atoms belonging to another two ligands, showing a distorted octahedral geometry (Table 1). The four N atoms from two pmt⁻ ligands define the equatorial plane with the Cd centre located in the plane, and two O atoms are at the axial positions with O2A—Cd1—O2B angle of just 180°[Symmetry codes: (A)1 - *x*, -1/2 + *y*, 0.5 - *z*; (B)*x*, 0.5 - *y*, -1/2 + *z*]. Each pmt⁻ plays as a μ_2 bridge to connect two Cd^{2+} ions and each Cd^{2+} ion links four pmt⁻ ligands, forming an infinite two-dimensional layer structure with (4, 4) topology (Figure 2). The network is based on (Cd(pmt))₄ rhombus, a 24-membered metal-ligand ring (–Cd—N—C—C—S—O–)₄ formed by four pmt⁻ and four quadruply connected Cd^{2+} ions. The edge Cd···Cd distance of the rhombus is 8.048 (3)Å and the Cd···Cd separations through the diagonal of the rhombus are 7.904 (2)Å and 14.021 (1) Å, respectively (Figure 2).

The two-dimensional layer is stabilized by intermolecular N—H···O hydrogen bonds (Figure 3 & Table 2). The interlayers are further connected by *π*-*π* stacking interactions of parallel pyridine rings of adjacent layers. The interplanar average distance and ringcentroid separation distance are 3.582 (1)Å and 3.634 (1) Å, respectively. Thus, the three-dimensional supramolecular architecture of (I) is formed (Figure 4).

S2. Experimental

The ligand Hpmt was prepared according to the method of Li *et al.*, 2006. A water solution (5 ml) of ligand Hpmt (2 mmol, 0.432 g) was added dropwise to a solution of CdCl₂. 2.5H₂O (0.228 g, 1.0 mmol) in methanol (8 ml), then the obtained mixture was stirred at 333 K for 3 h. After that, the mixture was basified with KOH (1 mol/l) to a pH of 7.5–8.0 and continued stirring for another 4 h, filtrated. Two weeks later, colourless claviform crystals were grown from the filtrate by slow evaporation. Analysis, found: C 35.40, H 4.02, N 10.36, S 11.36%; $C_{16}H_{22}CdN_4O_6S_2$ requires: C 35.36, H 4.05, N 10.31, S 11.42%. IR (KBr, *v*, cm⁻¹): 771.2[*γ*(CC—H)], 745.7(*γ*CH₂); 1188.3, 1157.4, 1040.6(*v* SO₃⁻); 1607.7, 1571.7(*v* CC + *v* CN); 3266.2(*v* N—H). CCDC 614219.

S3. Refinement

H atoms bonded to C were positioned geometrically with C—H distance of 0.93–0.97 Å, and treated as riding atoms, with $U_{iso}(H)=1.2U_{eq}(C)$. The N—H hydrogen atom was located in a difference Fourier map and refined isotropically.
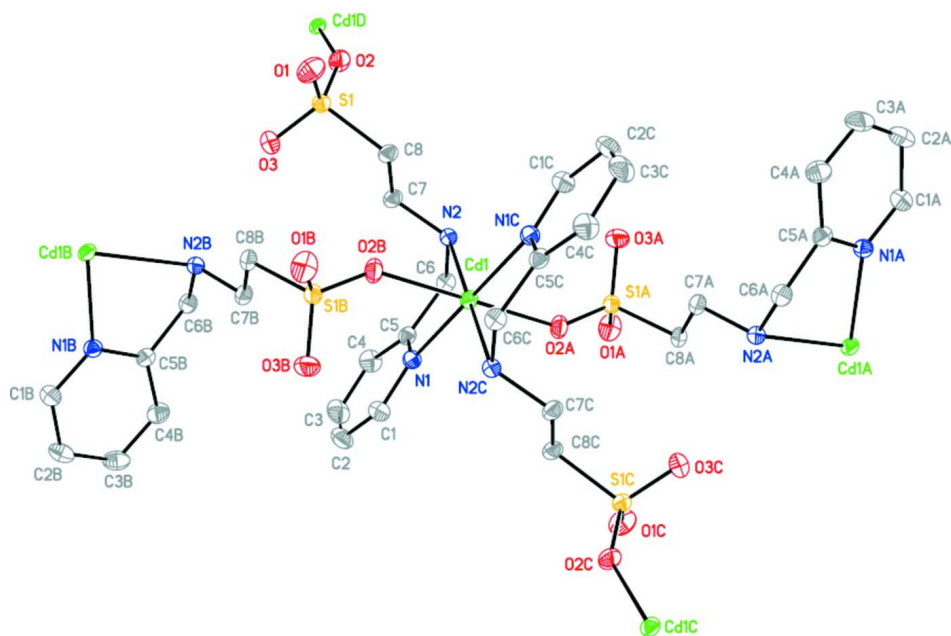
Figure 1

The coordination of Cd^{2+} ion of (I) with the atom-numbering scheme. Displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted. [Symmetry codes: (A)1 - *x*, -1/2 + *y*, 0.5 - *z*; (B)*x*, 0.5 - *y*, -1/2 + *z*; (C)1 - *x*, -*y*, -*z*; (D)1 - *x*, 1/2 + *y*, 0.5 - *z*]
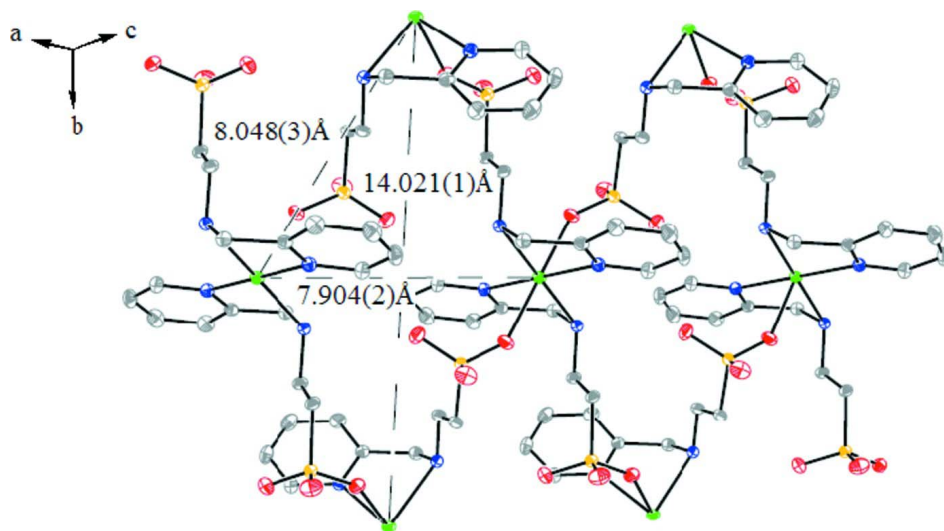
Figure 2

The two-dimensional layer structure of (I). H atoms have been omitted.
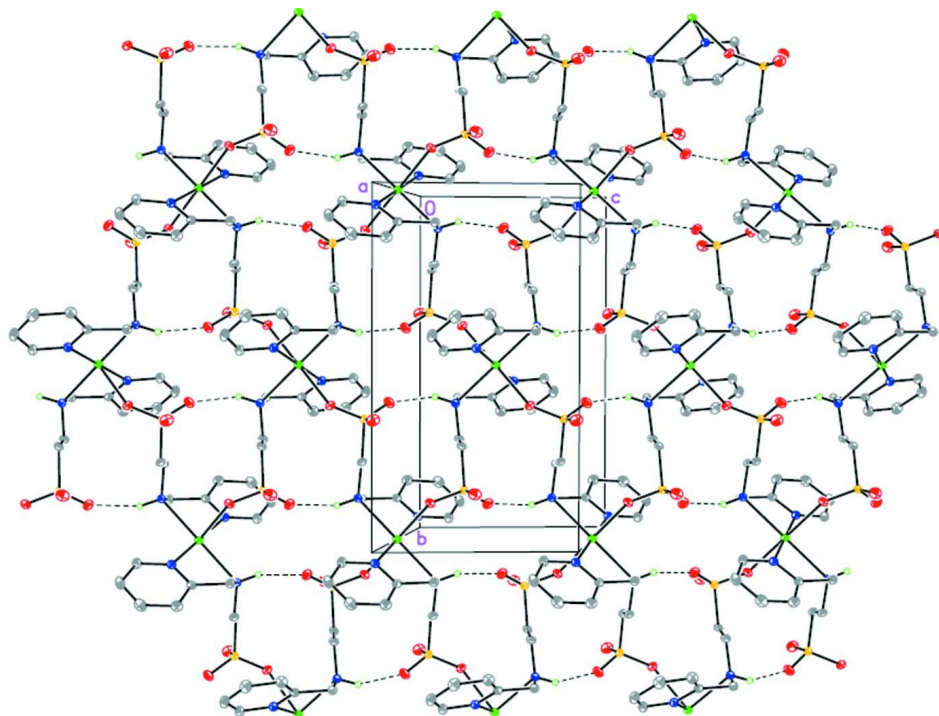
Figure 3

The hydrogen bonding interactions in (I)(dashed lines) projected in the plane *bc*. H atoms on C atoms have been omitted.
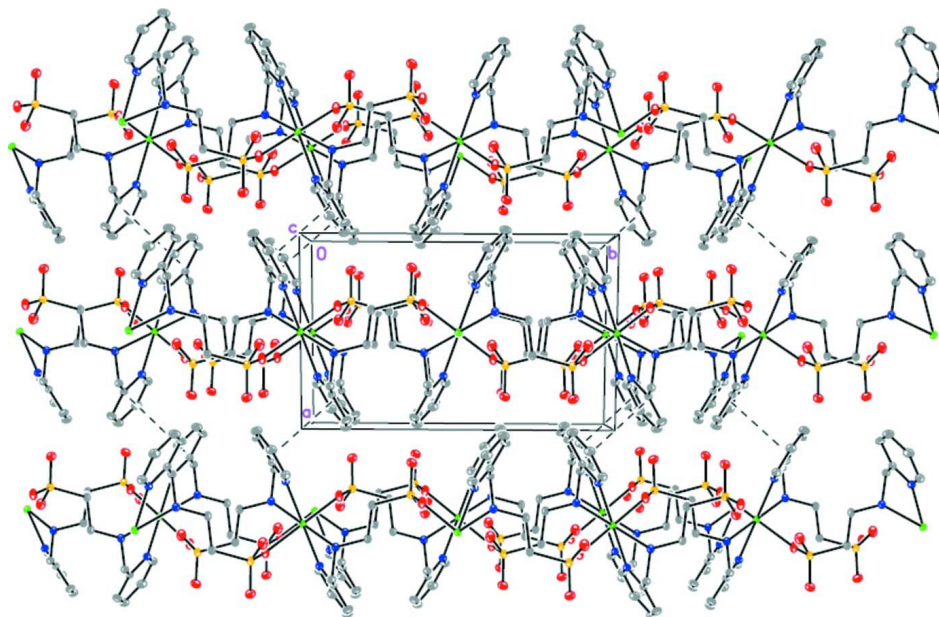
Figure 4

Packing diagram for (I), showing *π*-*π* stacking as dashed lines in the plane *ab*. H atoms on C have been deleted.

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Crystal data

[Cd(C₈H₁₁N₂O₃S)₂]	$F(000) = 548$
$M_r = 542.90$	$D_x = 1.881$ Mg m⁻³
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3852 reflections
$a = 8.8982$ (8) Å	$\theta = 2.4$–28.2°
$b = 14.0206$ (12) Å	$\mu = 1.40$ mm⁻¹
$c = 7.9040$ (7) Å	$T = 291$ K
$\beta = 103.579$ (1)°	Claviform, colourless
$V = 958.52$ (15) Å³	$0.22 \times 0.16 \times 0.12$ mm
$Z = 2$	

Data collection

Bruker APEXII CCD area-detector diffractometer	5691 measured reflections
Radiation source: fine-focus sealed tube	2178 independent reflections
Graphite monochromator	2008 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.011$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
	$h = -7 \rightarrow 11$
	$k = -18 \rightarrow 15$
$T_{min} = 0.749$, $T_{max} = 0.849$	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.019$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.049$	
$S = 1.03$	H-atom parameters constrained
2178 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 0.5977P]$ where $P = (F_o^2 + 2F_c^2)/3$
133 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.48$ e Å⁻³
	$\Delta\rho_{min} = -0.38$ e Å⁻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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.0000	0.0000	0.02456 (7)
S1	0.33469 (5)	0.35013 (3)	0.12343 (6)	0.02701 (10)
O1	0.17221 (17)	0.35246 (12)	0.0384 (2)	0.0474 (4)

O2	0.36412 (18)	0.38778 (10)	0.30088 (18)	0.0382 (3)
O3	0.43417 (19)	0.39430 (11)	0.0247 (2)	0.0446 (4)
N1	0.72897 (17)	0.05064 (11)	−0.05239 (19)	0.0265 (3)
N2	0.60386 (17)	0.11240 (10)	0.22587 (19)	0.0260 (3)
H2	0.5777	0.0929	0.3250	0.031*
C1	0.7692 (2)	0.04398 (15)	−0.2058 (2)	0.0342 (4)
H1	0.7061	0.0096	−0.2957	0.041*
C2	0.9010 (2)	0.08650 (17)	−0.2341 (3)	0.0409 (5)
H2A	0.9275	0.0800	−0.3406	0.049*
C3	0.9923 (2)	0.13852 (18)	−0.1025 (3)	0.0456 (5)
H3	1.0805	0.1688	−0.1196	0.055*
C4	0.9522 (2)	0.14571 (16)	0.0561 (3)	0.0393 (5)
H4	1.0134	0.1805	0.1468	0.047*
C5	0.8193 (2)	0.10009 (13)	0.0778 (2)	0.0270 (4)
C6	0.7732 (2)	0.10068 (13)	0.2504 (2)	0.0289 (4)
H6A	0.8052	0.0413	0.3111	0.035*
H6B	0.8260	0.1525	0.3217	0.035*
C7	0.5616 (2)	0.21429 (13)	0.1977 (2)	0.0301 (4)
H7A	0.6054	0.2395	0.1055	0.036*
H7B	0.6048	0.2499	0.3031	0.036*
C8	0.3876 (2)	0.22747 (12)	0.1489 (2)	0.0289 (4)
H8A	0.3435	0.1996	0.2386	0.035*
H8B	0.3451	0.1940	0.0409	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02285 (10)	0.02064 (10)	0.03077 (10)	−0.00396 (6)	0.00747 (7)	−0.00131 (7)
S1	0.0320 (2)	0.0237 (2)	0.0260 (2)	0.00119 (16)	0.00802 (17)	−0.00138 (16)
O1	0.0355 (8)	0.0447 (9)	0.0561 (10)	0.0066 (6)	−0.0011 (7)	−0.0040 (7)
O2	0.0547 (9)	0.0275 (7)	0.0328 (7)	−0.0018 (6)	0.0109 (6)	−0.0074 (6)
O3	0.0567 (9)	0.0389 (8)	0.0447 (8)	0.0005 (7)	0.0249 (7)	0.0101 (7)
N1	0.0246 (7)	0.0267 (8)	0.0287 (7)	−0.0016 (6)	0.0071 (6)	0.0000 (6)
N2	0.0295 (7)	0.0237 (7)	0.0263 (7)	−0.0002 (6)	0.0098 (6)	0.0002 (6)
C1	0.0332 (10)	0.0393 (11)	0.0309 (9)	0.0007 (8)	0.0092 (8)	−0.0007 (8)
C2	0.0353 (10)	0.0545 (13)	0.0375 (10)	0.0039 (9)	0.0178 (9)	0.0075 (10)
C3	0.0289 (10)	0.0554 (14)	0.0563 (14)	−0.0057 (9)	0.0176 (9)	0.0085 (11)
C4	0.0274 (9)	0.0428 (11)	0.0468 (12)	−0.0094 (8)	0.0071 (8)	−0.0037 (9)
C5	0.0234 (8)	0.0245 (8)	0.0324 (9)	0.0015 (6)	0.0052 (7)	0.0018 (7)
C6	0.0271 (9)	0.0294 (9)	0.0277 (8)	−0.0013 (7)	0.0018 (7)	−0.0015 (7)
C7	0.0336 (9)	0.0217 (8)	0.0361 (9)	−0.0005 (7)	0.0103 (8)	−0.0035 (7)
C8	0.0332 (9)	0.0226 (8)	0.0316 (9)	−0.0006 (7)	0.0089 (7)	−0.0056 (7)

Geometric parameters (Å, º)

Cd1—N1	2.2853 (14)	C1—C2	1.380 (3)
Cd1—N1[i]	2.2853 (14)	C1—H1	0.9300
Cd1—O2[ii]	2.3496 (14)	C2—C3	1.370 (3)

Cd1—O2ⁱⁱⁱ	2.3497 (14)	C2—H2A	0.9300
Cd1—N2	2.3979 (15)	C3—C4	1.385 (3)
Cd1—N2ⁱ	2.3979 (15)	C3—H3	0.9300
S1—O1	1.4447 (15)	C4—C5	1.390 (3)
S1—O3	1.4496 (15)	C4—H4	0.9300
S1—O2	1.4635 (14)	C5—C6	1.514 (2)
S1—C8	1.7821 (18)	C6—H6A	0.9700
O2—Cd1ⁱᵛ	2.3497 (14)	C6—H6B	0.9700
N1—C5	1.341 (2)	C7—C8	1.516 (3)
N1—C1	1.346 (2)	C7—H7A	0.9700
N2—C7	1.481 (2)	C7—H7B	0.9700
N2—C6	1.483 (2)	C8—H8A	0.9700
N2—H2	0.9100	C8—H8B	0.9700
N1—Cd1—N1ⁱ	180	N1—C1—H1	118.9
N1—Cd1—O2ⁱⁱ	89.37 (5)	C2—C1—H1	118.9
N1ⁱ—Cd1—O2ⁱⁱ	90.63 (5)	C3—C2—C1	118.77 (19)
N1—Cd1—O2ⁱⁱⁱ	90.63 (5)	C3—C2—H2A	120.6
N1ⁱ—Cd1—O2ⁱⁱⁱ	89.37 (5)	C1—C2—H2A	120.6
O2ⁱⁱ—Cd1—O2ⁱⁱⁱ	179.999 (1)	C2—C3—C4	119.59 (19)
N1—Cd1—N2	74.13 (5)	C2—C3—H3	120.2
N1ⁱ—Cd1—N2	105.87 (5)	C4—C3—H3	120.2
O2ⁱⁱ—Cd1—N2	83.89 (5)	C3—C4—C5	119.02 (19)
O2ⁱⁱⁱ—Cd1—N2	96.11 (5)	C3—C4—H4	120.5
N1—Cd1—N2ⁱ	105.87 (5)	C5—C4—H4	120.5
N1ⁱ—Cd1—N2ⁱ	74.13 (5)	N1—C5—C4	121.17 (17)
O2ⁱⁱ—Cd1—N2ⁱ	96.11 (5)	N1—C5—C6	116.99 (15)
O2ⁱⁱⁱ—Cd1—N2ⁱ	83.89 (5)	C4—C5—C6	121.80 (17)
N2—Cd1—N2ⁱ	180.0	N2—C6—C5	111.41 (14)
O1—S1—O3	114.25 (10)	N2—C6—H6A	109.3
O1—S1—O2	111.86 (9)	C5—C6—H6A	109.3
O3—S1—O2	111.57 (9)	N2—C6—H6B	109.3
O1—S1—C8	106.47 (9)	C5—C6—H6B	109.3
O3—S1—C8	107.12 (9)	H6A—C6—H6B	108.0
O2—S1—C8	104.88 (9)	N2—C7—C8	111.36 (15)
S1—O2—Cd1ⁱᵛ	146.26 (9)	N2—C7—H7A	109.4
C5—N1—C1	119.27 (16)	C8—C7—H7A	109.4
C5—N1—Cd1	114.90 (11)	N2—C7—H7B	109.4
C1—N1—Cd1	125.37 (13)	C8—C7—H7B	109.4
C7—N2—C6	109.95 (14)	H7A—C7—H7B	108.0
C7—N2—Cd1	118.81 (11)	C7—C8—S1	111.93 (12)
C6—N2—Cd1	103.10 (10)	C7—C8—H8A	109.2
C7—N2—H2	108.2	S1—C8—H8A	109.2
C6—N2—H2	108.2	C7—C8—H8B	109.2
Cd1—N2—H2	108.2	S1—C8—H8B	109.2
N1—C1—C2	122.17 (19)	H8A—C8—H8B	107.9
O1—S1—O2—Cd1ⁱᵛ	−124.02 (16)	Cd1—N1—C1—C2	171.82 (15)

O3—S1—O2—Cd1ⁱᵛ	5.3 (2)	N1—C1—C2—C3	−1.1 (3)
C8—S1—O2—Cd1ⁱᵛ	120.97 (16)	C1—C2—C3—C4	1.3 (3)
O2ⁱⁱ—Cd1—N1—C5	−71.71 (12)	C2—C3—C4—C5	−0.3 (3)
O2ⁱⁱⁱ—Cd1—N1—C5	108.29 (12)	C1—N1—C5—C4	1.0 (3)
N2—Cd1—N1—C5	12.12 (12)	Cd1—N1—C5—C4	−171.65 (15)
N2ⁱ—Cd1—N1—C5	−167.88 (12)	C1—N1—C5—C6	−176.72 (16)
O2ⁱⁱ—Cd1—N1—C1	116.16 (16)	Cd1—N1—C5—C6	10.6 (2)
O2ⁱⁱⁱ—Cd1—N1—C1	−63.84 (16)	C3—C4—C5—N1	−0.9 (3)
N2—Cd1—N1—C1	−160.01 (16)	C3—C4—C5—C6	176.77 (19)
N2ⁱ—Cd1—N1—C1	19.99 (16)	C7—N2—C6—C5	−80.67 (18)
N1—Cd1—N2—C7	90.73 (12)	Cd1—N2—C6—C5	46.99 (15)
N1ⁱ—Cd1—N2—C7	−89.27 (12)	N1—C5—C6—N2	−42.0 (2)
O2ⁱⁱ—Cd1—N2—C7	−178.19 (12)	C4—C5—C6—N2	140.29 (18)
O2ⁱⁱⁱ—Cd1—N2—C7	1.81 (12)	C6—N2—C7—C8	172.59 (14)
N1—Cd1—N2—C6	−31.13 (10)	Cd1—N2—C7—C8	54.25 (18)
N1ⁱ—Cd1—N2—C6	148.87 (10)	N2—C7—C8—S1	177.53 (12)
O2ⁱⁱ—Cd1—N2—C6	59.95 (10)	O1—S1—C8—C7	166.69 (13)
O2ⁱⁱⁱ—Cd1—N2—C6	−120.05 (10)	O3—S1—C8—C7	44.07 (16)
C5—N1—C1—C2	0.0 (3)	O2—S1—C8—C7	−74.60 (15)

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) −*x*+1, *y*−1/2, −*z*+1/2; (iii) *x*, −*y*+1/2, *z*−1/2; (iv) −*x*+1, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3ᵛ	0.91	2.26	3.089 (2)	152

Symmetry code: (v) *x*, −*y*+1/2, *z*+1/2.