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Bis[2-(2-pyridylmethyleneamino)-benzenesulfonato-κ^3N,N',O]cadmium(II) dihydrate

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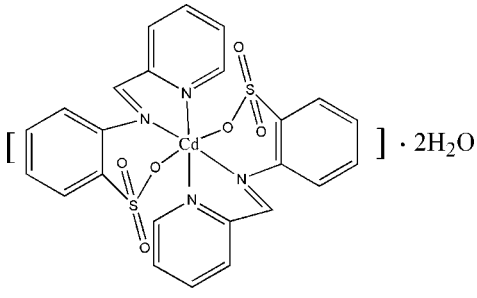
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.034; wR factor = 0.075; data-to-parameter ratio = 13.8.

The title complex, $[Cd(Paba)_2]\cdot 2H_2O$ or $[Cd(C_{12}H_9N_2O_3S)_2]\cdot 2H_2O$, was synthesized by the reaction of the potassium salt of 2-(2-pyridylmethyleneamino)benzenesulfonic acid (PabaK) with $CdCl_2\cdot 2.5H_2O$ in methanol. The Cd^{II} atom lies on a crystallographic twofold axis and is coordinated by four N atoms and two O atoms from two deprotonated tridentate 2-(2-pyridylmethyleneamino)benzenesulfonate ligands in a slightly distorted octahedral environment. There are extensive hydrogen bonds of the type O—H···O between the uncoordinated water molecules and the sulfonate O atoms, through which the complex forms a layered structure parallel to (001).

Related literature

For the isostructural Zn compound, see: Cai *et al.* (2008). For synthesis of the ligand, see: Casella & Gullotti (1986).



$[\ ]\cdot 2H_2O$

Experimental

Crystal data

$[Cd(C_{12}H_9N_2O_3S)_2]\cdot 2H_2O$
M_r = 670.98
Orthorhombic, *Pbcn*
a = 20.255 (4) Å
b = 7.8924 (17) Å
c = 16.475 (3) Å
V = 2633.7 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 291 (2) K
0.23 × 0.08 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.798, T_{max} = 0.950
18106 measured reflections
2443 independent reflections
1672 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.075
S = 1.04
2443 reflections
177 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H2W···O3^{i}	0.83	2.27	2.968 (5)	142
O4—H1W···O1	0.85	2.01	2.863 (5)	179

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

Data collection: *SMART* (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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2123).

References

Bruker (2004). *SMART* and *SAINT*. Bruker AXS inc., Madison, Wisconsin, USA.
Cai, C.-X., Ou-Yang, M., Zhao, Z.-Y. & Jiang, Y.-M. (2008). *Acta Cryst.* E**64**, m1195.
Casella, L. & Gullotti, M. (1986). *Inorg. Chem.* **25**, 1293–1303.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, m1461 [doi:10.1107/S1600536808034387]

Bis[2-(2-pyridylmethyleneamino)benzenesulfonato-κ^3N,N',O]cadmium(II) dihydrate

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S1. Comment

The title complex (Fig. 1) is isostructural with $[Zn(Paba)_2].2H_2O$, whose structure has been described in detail (Cai, *et al.*, 2008). The six-coordinated Cd^{II} lies on a crystallographic 2-fold axis of rotation and two deprotonated PabaH anions coordinate to Cd^{II} in a facial arrangement as N,*N*′,*O*-tridentate donor ligands.

The O—H donor group of the guest waters and the S=O acceptor group of the Paba ligands participate in the hydrogen bonding and form a two-dimensional network in the *ab* plane (Fig. 2).

S2. Experimental

The potassium salt of 2-(2- pyridylmethyleneamino)benzenesulfonic acid(PabaK) was synthesized according to the literature methods (Casella & Gullotti, 1986).

For the preparation of the title complex, the ligand PabaK (1 mmol, 0.30 g) was dissolved in methanol (10 ml) at 333 K and an aqueous solution (10 ml) containing $CdCl_2.2.5H_2O$ (0.5 mmol, 0.12 g) was added. The resulting mixture was stirred at 333 K for 4 h. Then the mixture was filtrated and the filtrate was left to stand at room temperature. Yellow crystals suitable for X-ray diffraction were obtained after a week in a yield of 35%. Elemental analysis,.found (%): C, 46.91; H, 3.36; N, 8.30; S, 9.45; calc (%): C, 42.96; H, 3.31; N, 8.35; S, 9.56.

S3. Refinement

H atoms bonded to C were positioned geometrically with C—H distance 0.93 Å, and treated as riding atoms,with U_{iso}(H)= 1.2U_{eq}(*C*). Water hydrogens were placed in fixed positions and assigned U_{iso} values of 1.5 U_{eq} of the water oxygen atom.

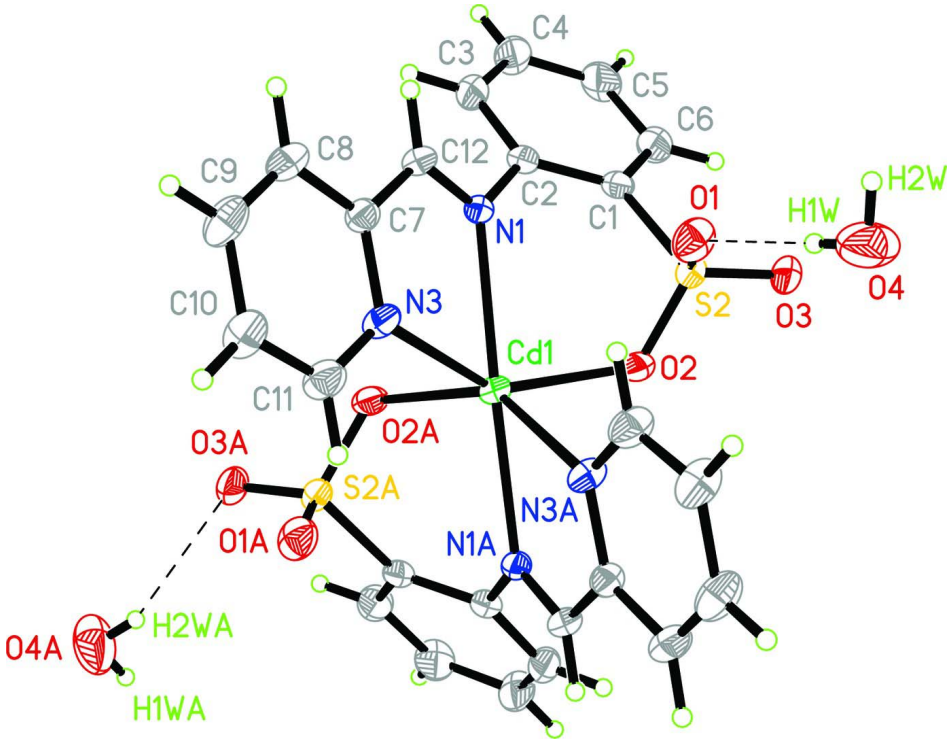

Figure 1

An ellipsoid plot (30% probability) showing the numbering scheme. Dashed lines indicate hydrogen bonds. Symmetry code: 1# -*x* + 1, *y*, -*z* + 3/2.

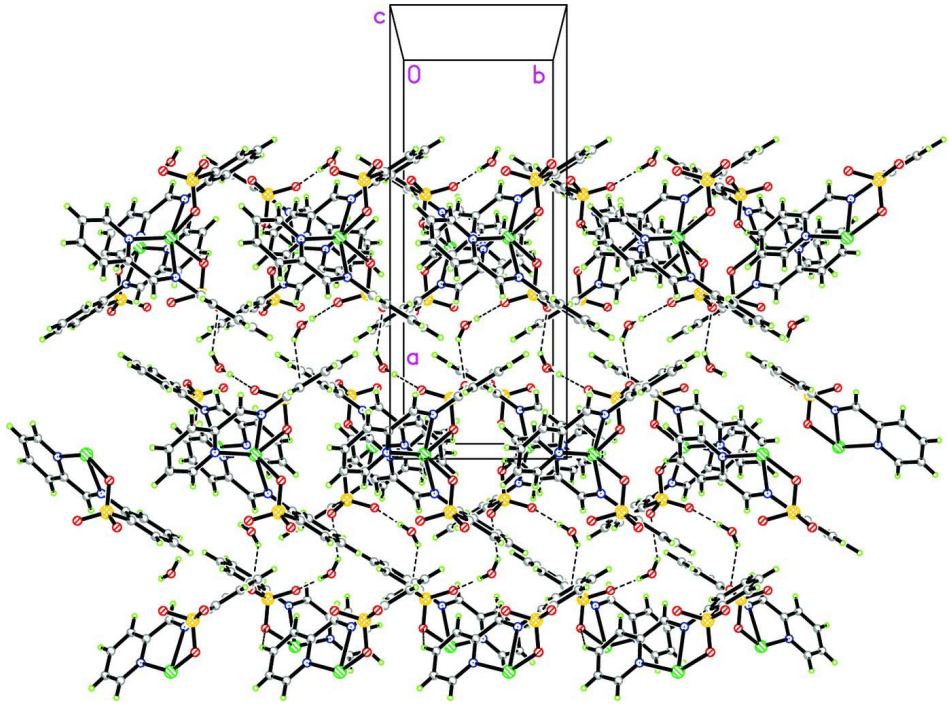

Figure 2

2-D network, as viewed down the *c* axis. Dashed lines indicate hydrogen bonds.

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$b = 7.8924$ (17) Å
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$V = 2633.7$ (9) Å^3
$Z = 4$
$F(000) = 1352$
$D_x = 1.692$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2541 reflections
$\theta = 2.5$–$23.2°$
$\mu = 1.04$ mm^{-1}
$T = 291$ K
Block, colourless
0.23 × 0.08 × 0.05 mm

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18106 measured reflections
2443 independent reflections
1672 reflections with $I > 2\sigma(I)$
$R_{int} = 0.075$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.5°$
$h = -24\rightarrow24$
$k = -9\rightarrow9$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.075$
$S = 1.04$
2443 reflections
177 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2 + 3.1957P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ 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	0.68040 (5)	0.7500	0.03074 (13)
S2	0.62752 (5)	0.83468 (15)	0.66388 (6)	0.0372 (3)
N1	0.59409 (15)	0.7358 (4)	0.83494 (18)	0.0302 (7)
C12	0.60345 (19)	0.6263 (5)	0.8904 (2)	0.0382 (10)
H12	0.6393	0.6381	0.9253	0.046*
N3	0.50869 (16)	0.4691 (4)	0.84673 (18)	0.0373 (8)
O1	0.64757 (15)	0.6598 (4)	0.67446 (17)	0.0523 (8)
O2	0.55529 (12)	0.8506 (4)	0.66248 (15)	0.0413 (7)
O3	0.65696 (14)	0.9203 (4)	0.59556 (16)	0.0509 (8)
O4	0.69916 (18)	0.4179 (6)	0.5615 (2)	0.1121 (17)
H1W	0.6840	0.4904	0.5948	0.168*
H2W	0.7324	0.3778	0.5833	0.168*
C1	0.65210 (16)	0.9451 (5)	0.7530 (3)	0.0342 (9)
C2	0.63521 (18)	0.8827 (5)	0.8292 (2)	0.0319 (9)
C3	0.6563 (2)	0.9697 (6)	0.8973 (3)	0.0455 (11)
H3	0.6462	0.9281	0.9486	0.055*
C4	0.6920 (2)	1.1170 (6)	0.8899 (3)	0.0552 (13)
H4	0.7057	1.1748	0.9361	0.066*
C5	0.7074 (2)	1.1785 (6)	0.8147 (3)	0.0561 (13)
H5	0.7310	1.2790	0.8099	0.067*
C6	0.6880 (2)	1.0922 (5)	0.7457 (3)	0.0481 (11)
H6	0.6992	1.1333	0.6947	0.058*
C7	0.55885 (19)	0.4823 (5)	0.9002 (2)	0.0334 (9)
C8	0.5667 (2)	0.3684 (5)	0.9628 (2)	0.0445 (11)
H8	0.6020	0.3780	0.9985	0.053*
C9	0.5212 (2)	0.2402 (6)	0.9716 (3)	0.0520 (13)
H9	0.5253	0.1625	1.0138	0.062*
C10	0.4700 (2)	0.2279 (5)	0.9178 (3)	0.0491 (12)
H10	0.4387	0.1424	0.9232	0.059*
C11	0.4654 (2)	0.3423 (6)	0.8565 (3)	0.0465 (11)
H11	0.4308	0.3322	0.8197	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0291 (2)	0.0362 (2)	0.0269 (2)	0.000	−0.00588 (19)	0.000
S2	0.0355 (6)	0.0497 (7)	0.0265 (5)	−0.0025 (6)	−0.0008 (4)	0.0002 (5)
N1	0.0246 (16)	0.0403 (19)	0.0257 (17)	−0.0062 (15)	−0.0016 (14)	0.0016 (16)
C12	0.032 (2)	0.055 (3)	0.027 (2)	0.000 (2)	−0.0072 (18)	−0.001 (2)
N3	0.043 (2)	0.0398 (19)	0.0289 (17)	−0.0012 (18)	−0.0090 (17)	0.0029 (15)
O1	0.065 (2)	0.047 (2)	0.0442 (18)	0.0116 (16)	−0.0022 (15)	−0.0107 (15)
O2	0.0329 (15)	0.059 (2)	0.0322 (15)	−0.0061 (14)	−0.0076 (12)	0.0112 (14)
O3	0.0464 (18)	0.077 (2)	0.0296 (16)	−0.0113 (17)	0.0048 (14)	0.0037 (16)
O4	0.066 (2)	0.168 (4)	0.102 (3)	0.043 (3)	−0.025 (2)	−0.068 (3)
C1	0.0245 (18)	0.044 (2)	0.034 (2)	0.0008 (16)	−0.004 (2)	−0.004 (2)

C2	0.024 (2)	0.037 (2)	0.034 (2)	0.0001 (18)	−0.0021 (18)	−0.0005 (19)
C3	0.042 (3)	0.062 (3)	0.032 (2)	−0.007 (2)	0.001 (2)	−0.004 (2)
C4	0.053 (3)	0.070 (3)	0.043 (3)	−0.020 (3)	−0.002 (2)	−0.019 (2)
C5	0.048 (3)	0.058 (3)	0.062 (3)	−0.026 (3)	0.002 (2)	−0.011 (3)
C6	0.042 (2)	0.057 (3)	0.045 (3)	−0.012 (2)	0.001 (2)	0.000 (3)
C7	0.035 (2)	0.036 (2)	0.029 (2)	−0.0003 (19)	−0.0025 (18)	−0.0014 (18)
C8	0.052 (3)	0.047 (3)	0.035 (2)	0.006 (2)	−0.011 (2)	0.005 (2)
C9	0.081 (4)	0.037 (3)	0.038 (3)	0.002 (2)	−0.007 (2)	0.010 (2)
C10	0.071 (3)	0.036 (3)	0.040 (3)	−0.013 (2)	−0.005 (2)	0.001 (2)
C11	0.055 (3)	0.045 (3)	0.039 (3)	−0.013 (2)	−0.010 (2)	0.004 (2)

Geometric parameters (Å, º)

Cd1—O2^{i}	2.267 (3)	C1—C6	1.375 (5)
Cd1—O2	2.267 (3)	C1—C2	1.390 (5)
Cd1—N3^{i}	2.313 (3)	C2—C3	1.383 (5)
Cd1—N3	2.313 (3)	C3—C4	1.374 (6)
Cd1—N1^{i}	2.405 (3)	C3—H3	0.9300
Cd1—N1	2.405 (3)	C4—C5	1.367 (6)
S2—O3	1.442 (3)	C4—H4	0.9300
S2—O1	1.449 (3)	C5—C6	1.381 (6)
S2—O2	1.469 (3)	C5—H5	0.9300
S2—C1	1.779 (4)	C6—H6	0.9300
N1—C12	1.272 (5)	C7—C8	1.377 (5)
N1—C2	1.431 (5)	C8—C9	1.376 (6)
C12—C7	1.461 (5)	C8—H8	0.9300
C12—H12	0.9300	C9—C10	1.368 (6)
N3—C11	1.340 (5)	C9—H9	0.9300
N3—C7	1.349 (5)	C10—C11	1.359 (6)
O4—H1W	0.8502	C10—H10	0.9300
O4—H2W	0.8263	C11—H11	0.9300
O2^{i}—Cd1—O2	107.31 (15)	C6—C1—S2	119.3 (4)
O2^{i}—Cd1—N3^{i}	145.88 (11)	C2—C1—S2	120.2 (3)
O2—Cd1—N3^{i}	91.52 (11)	C3—C2—C1	118.7 (4)
O2^{i}—Cd1—N3	91.52 (11)	C3—C2—N1	121.9 (4)
O2—Cd1—N3	145.88 (11)	C1—C2—N1	119.3 (3)
N3^{i}—Cd1—N3	87.74 (16)	C4—C3—C2	120.7 (4)
O2^{i}—Cd1—N1^{i}	82.58 (10)	C4—C3—H3	119.6
O2—Cd1—N1^{i}	85.04 (10)	C2—C3—H3	119.6
N3^{i}—Cd1—N1^{i}	70.73 (11)	C5—C4—C3	120.0 (4)
N3—Cd1—N1^{i}	126.32 (11)	C5—C4—H4	120.0
O2^{i}—Cd1—N1	85.04 (10)	C3—C4—H4	120.0
O2—Cd1—N1	82.58 (10)	C4—C5—C6	120.4 (4)
N3^{i}—Cd1—N1	126.32 (11)	C4—C5—H5	119.8
N3—Cd1—N1	70.73 (11)	C6—C5—H5	119.8
N1^{i}—Cd1—N1	159.04 (16)	C1—C6—C5	119.6 (5)
O3—S2—O1	115.11 (19)	C1—C6—H6	120.2

O3—S2—O2	111.07 (17)	C5—C6—H6	120.2
O1—S2—O2	111.26 (18)	N3—C7—C8	121.7 (4)
O3—S2—C1	107.40 (18)	N3—C7—C12	117.0 (4)
O1—S2—C1	106.80 (18)	C8—C7—C12	121.3 (4)
O2—S2—C1	104.47 (17)	C9—C8—C7	118.8 (4)
C12—N1—C2	120.8 (3)	C9—C8—H8	120.6
C12—N1—Cd1	114.4 (3)	C7—C8—H8	120.6
C2—N1—Cd1	124.8 (2)	C10—C9—C8	119.4 (4)
N1—C12—C7	121.1 (4)	C10—C9—H9	120.3
N1—C12—H12	119.5	C8—C9—H9	120.3
C7—C12—H12	119.5	C11—C10—C9	119.2 (4)
C11—N3—C7	118.2 (3)	C11—C10—H10	120.4
C11—N3—Cd1	124.8 (3)	C9—C10—H10	120.4
C7—N3—Cd1	116.9 (3)	N3—C11—C10	122.7 (4)
S2—O2—Cd1	115.56 (15)	N3—C11—H11	118.6
H1W—O4—H2W	105.8	C10—C11—H11	118.6
C6—C1—C2	120.5 (4)		

O2^{i}—Cd1—N1—C12	93.5 (3)	O2—S2—C1—C6	−113.1 (3)
O2—Cd1—N1—C12	−158.3 (3)	O3—S2—C1—C2	−174.9 (3)
N3^{i}—Cd1—N1—C12	−71.9 (3)	O1—S2—C1—C2	−50.9 (3)
N3—Cd1—N1—C12	0.1 (3)	O2—S2—C1—C2	67.1 (3)
N1^{i}—Cd1—N1—C12	147.4 (3)	C6—C1—C2—C3	−1.2 (6)
O2^{i}—Cd1—N1—C2	−82.9 (3)	S2—C1—C2—C3	178.6 (3)
O2—Cd1—N1—C2	25.3 (3)	C6—C1—C2—N1	175.8 (3)
N3^{i}—Cd1—N1—C2	111.7 (3)	S2—C1—C2—N1	−4.3 (5)
N3—Cd1—N1—C2	−176.3 (3)	C12—N1—C2—C3	−39.6 (5)
N1^{i}—Cd1—N1—C2	−29.0 (3)	Cd1—N1—C2—C3	136.5 (3)
C2—N1—C12—C7	175.6 (3)	C12—N1—C2—C1	143.4 (4)
Cd1—N1—C12—C7	−0.9 (5)	Cd1—N1—C2—C1	−40.4 (4)
O2^{i}—Cd1—N3—C11	91.9 (3)	C1—C2—C3—C4	1.4 (6)
O2—Cd1—N3—C11	−143.3 (3)	N1—C2—C3—C4	−175.5 (4)
N3^{i}—Cd1—N3—C11	−53.9 (3)	C2—C3—C4—C5	−0.4 (7)
N1^{i}—Cd1—N3—C11	10.0 (4)	C3—C4—C5—C6	−0.9 (7)
N1—Cd1—N3—C11	176.1 (3)	C2—C1—C6—C5	−0.1 (6)
O2^{i}—Cd1—N3—C7	−83.5 (3)	S2—C1—C6—C5	−179.9 (3)
O2—Cd1—N3—C7	41.3 (4)	C4—C5—C6—C1	1.1 (7)
N3^{i}—Cd1—N3—C7	130.7 (3)	C11—N3—C7—C8	0.9 (6)
N1^{i}—Cd1—N3—C7	−165.4 (2)	Cd1—N3—C7—C8	176.6 (3)
N1—Cd1—N3—C7	0.7 (3)	C11—N3—C7—C12	−177.2 (4)
O3—S2—O2—Cd1	168.04 (16)	Cd1—N3—C7—C12	−1.4 (4)
O1—S2—O2—Cd1	38.4 (2)	N1—C12—C7—N3	1.6 (6)
C1—S2—O2—Cd1	−76.5 (2)	N1—C12—C7—C8	−176.5 (4)
O2^{i}—Cd1—O2—S2	118.00 (19)	N3—C7—C8—C9	−1.3 (6)
N3^{i}—Cd1—O2—S2	−90.86 (18)	C12—C7—C8—C9	176.7 (4)
N3—Cd1—O2—S2	−2.6 (3)	C7—C8—C9—C10	0.6 (7)
N1^{i}—Cd1—O2—S2	−161.36 (19)	C8—C9—C10—C11	0.4 (7)
N1—Cd1—O2—S2	35.59 (17)	C7—N3—C11—C10	0.2 (6)

O3—S2—C1—C6	4.9 (4)	Cd1—N3—C11—C10	−175.2 (3)
O1—S2—C1—C6	128.9 (3)	C9—C10—C11—N3	−0.9 (7)

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H2*W*···O3^{ii}	0.83	2.27	2.968 (5)	142
O4—H1*W*···O1	0.85	2.01	2.863 (5)	179

Symmetry code: (ii) −*x*+3/2, *y*−1/2, *z*.