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[*N*,*N*′-Bis(3-aminopropyl)ethylenediamine]disaccharinatocadmium(II) 0.25-hydrate

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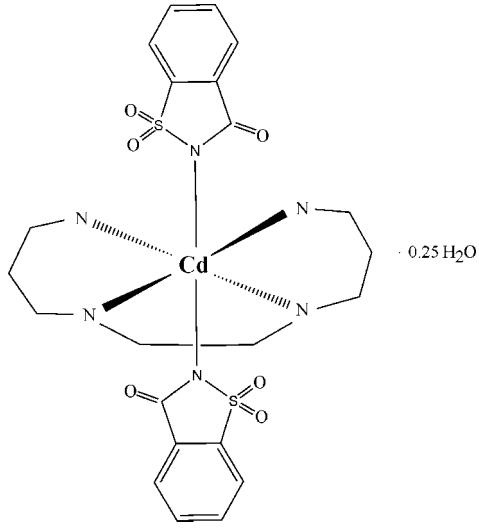
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.036; wR factor = 0.084; data-to-parameter ratio = 14.5.

The asymmetric unit of the title compound, $[Cd(C_7H_4NO_3S)_2(C_8H_{22}N_4)]\cdot 0.25H_2O$, consists of two $[Cd(sac)_2(paen)]$ molecules [sac is saccharinate ($C_7H_4NO_3S$) and paen is *N*,*N*′-bis(3-propylamine)ethylenediamine ($C_8H_{22}N_4$)], and a partial-occupancy water molecule. Each Cd^{II} ion is octahedrally coordinated. The equatorial plane of the octahedron is formed by N atoms of the paen ligands, and the axial positions are occupied by the N atoms of the sac ligands. In one of the molecules, the sulfonyl group of a sac ligand is disordered over two different orientations, with site-occupancy factors of 0.83 and 0.17. N—H···O hydrogen bonding is observed between the independent molecules. Neighbouring $[Cd(sac)_2(paen)]$ units are linked by N—H···O hydrogen bonds into chains running parallel to the *a* axis.

Related literature

For related structures, see: Yeşilel *et al.* (2006); Yilmaz *et al.* (2002, 2006); Paşaoğlu *et al.* (2007).



Experimental

Crystal data

$[Cd(C_7H_4NO_3S)_2(C_8H_{22}N_4)]\cdot 0.25H_2O$
M_r = 653.04
Monoclinic, $P2_1/c$
a = 14.540 (5) Å
b = 24.005 (5) Å
c = 15.701 (5) Å
β = 93.840 (5)°
V = 5468 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 296 K
0.27 × 0.26 × 0.24 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.790, T_{max} = 0.867
78541 measured reflections
10742 independent reflections
6287 reflections with $I > 2\sigma(I)$
R_{int} = 0.077

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.084
S = 0.83
10742 reflections
740 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N6	2.303 (4)	Cd2—N10	2.294 (4)
Cd1—N5	2.306 (3)	Cd2—N12	2.306 (4)
Cd1—N4	2.363 (4)	Cd2—N9	2.346 (4)
Cd1—N3	2.397 (4)	Cd2—N11	2.373 (4)
Cd1—N1	2.443 (3)	Cd2—N7	2.458 (3)
Cd1—N2	2.464 (3)	Cd2—N8	2.470 (3)
N6—Cd1—N4	161.19 (15)	N10—Cd2—N9	160.43 (17)
N5—Cd1—N3	162.43 (14)	N12—Cd2—N11	163.22 (16)
N1—Cd1—N2	165.37 (10)	N7—Cd2—N8	163.28 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5A···O9^{i}	0.87 (5)	2.26 (5)	3.011 (5)	144 (4)
N9—H9···O3^{ii}	0.88 (5)	2.34 (6)	3.142 (5)	151 (5)
N3—H3A···O12	0.99 (6)	2.29 (6)	3.198 (5)	152 (5)
N4—H4A···O2	0.96 (5)	2.17 (5)	3.095 (5)	161 (4)
N5—H5B···O5A	0.98 (5)	2.39 (5)	3.151 (10)	134 (4)
N12—H12A···O12	0.88 (5)	2.20 (5)	2.960 (6)	144 (5)
N12—H12B···O7	0.81 (5)	2.35 (5)	3.094 (5)	152 (5)
N10—H10B···O6	0.80 (5)	2.22 (5)	2.901 (5)	143 (4)
N10—H10A···O8	0.94 (6)	2.22 (6)	3.076 (5)	151 (5)
N6—H6B···O1W	0.98 (4)	2.21 (5)	3.047 (12)	142 (4)

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2495).

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supplementary materials

Acta Cryst. (2007). E**63**, m2953-m2954 [**doi:10.1107/S1600536807055481**]

[*N*,*N*'-Bis(3-aminopropyl)ethylenediamine]disaccharinatocadmium(II) 0.25-hydrate

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Comment

The title compound has two [Cd(sac)$_2$(paen)] molecules (sac is saccharinate and paen is *N*,*N*'-bis(3-propylamine)ethylenediamine) and a partially occupied water molecule in the asymmetric unit. In each complex molecule, the Cd^{II} atom is octahedrally coordinated by N atoms of paen and sac ligands. The equatorial plane of the octahedron are defined by the N atoms of paen ligands, whereas the axial positions are occupied by the N atoms of the sac ligands (Fig. 1). In the present structure the sac ligand is N-bonded to the Cd^{II} ion whereas O-coordination has been observed in a previously reported structure (Paşaoğlu *et al.*, 2007). The sulfonyl group of the sac ligand in one of the independent molecule is disordered over two different orientations. However, the bond lengths and angles of the sac ligands are similiar to those observed in related structures (Yeşilel *et al.*, 2006; Yilmaz *et al.*, 2002, 2006). The Cd—N$_{sac}$ bonds are slightly longer than the Cd—N$_{paen}$ bonds, and the *trans*-(N—Cd—N) angles deviate significantly from linearity (Table 1).

N—H···O hydrogen bonding is observed between the independent molecules (Table 2). Neighbouring [Cd(sac)$_2$(paen)] units are linked by N—H···O hydrogen bonds (Fig. 2) into chains running parallel to the *a* axis.

Experimental

A solution of *N*,*N*'-bis(3-propylamine)ethylenediamine (2 mmol, 0.36 g) in water (10 ml) was added drop wise with stirring to a solution of [Cd(saccharinate)$_2$(H$_2$O)$_4$]·2H$_2$O (2.0 mmol, 1.17 g) in hot water (20 ml). The mixture was heated to 323 K in a temperature-controlled bath and stirred for 2 h. The reaction mixture was then cooled to room temperature. The crystals formed were filtered and washed with 10 ml of water and ethanol and dried in air.

Refinement

The sulfonyl group of one of the sacharinate ligands is disordered over two different orientations (S2A,O4A,O5A/S2B,O4B,O5B) with refined occupancies of 0.83 (2) and 0.17 (2). The H atoms of the partially occupied water molecule could not be located. H atoms bonded to N3, N4, N5, N6, N9, N10 and N12 were located in a difference map and refined freely. The remaining H atoms were placed in geometrically idealized positions (N—H = 0.91 Å and C—H = 0.93–0.97 Å) and were refined as riding atoms, with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

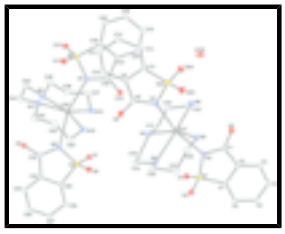

Fig. 1. The molecular structure of the title compound, with atom labels and displacement ellipsoids drawn at the 20% probability level. Only the major disorder component is shown. H atoms have been omitted for clarity.

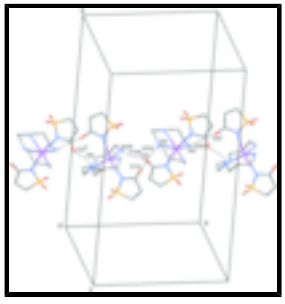

Fig. 2. Part of the crystal packing of the title compound, showing a chain structure along the *a* axis. Benzene rings and some hydrogen bonds have been omitted for clarity [Symmetry codes: (i) $x+1, y, z$; (ii) $x-1, y, z$.]

[*N*,*N*'-Bis(3-aminopropyl)ethylenediamine]disaccharinatocadmium(II) 0.25-hydrate

Crystal data

$[Cd(C_7H_4NO_3S)_2(C_8H_{22}N_4)]\cdot 0.25H_2O)$	$F_{000} = 2664$
$M_r = 653.04$	$D_x = 1.587$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 17796 reflections
$a = 14.540$ (5) Å	$\theta = 1.4$–$27.0°$
$b = 24.005$ (5) Å	$\mu = 1.00$ mm^{-1}
$c = 15.701$ (5) Å	$T = 296$ K
$\beta = 93.840$ (5)°	Prism', colourless
$V = 5468$ (3) Å^3	0.27 × 0.26 × 0.24 mm
$Z = 8$	

Data collection

Stoe IPDS II diffractometer	10742 independent reflections
Radiation source: fine-focus sealed tube	6287 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.077$
$T = 296$ K	$\theta_{max} = 26.0°$
ω–scan	$\theta_{min} = 1.4°$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -17\rightarrow17$
$T_{min} = 0.790$, $T_{max} = 0.867$	$k = -29\rightarrow29$
78541 measured reflections	$l = -19\rightarrow19$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.084$	$(\Delta/\sigma)_{max} = 0.009$
$S = 0.83$	$\Delta\rho_{max} = 0.45$ e Å^{-3}
10742 reflections	$\Delta\rho_{min} = -0.58$ e Å^{-3}
740 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00061 (5)
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.

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cd1	0.719145 (19)	0.424731 (11)	0.245527 (17)	0.05342 (9)	
S1	0.78820 (7)	0.57059 (4)	0.27203 (6)	0.0590 (2)	
S2A	0.7253 (3)	0.2771 (2)	0.2090 (3)	0.0699 (9)	0.83 (2)
S2B	0.747 (2)	0.2777 (11)	0.191 (2)	0.109 (11)	0.17 (2)
O1	0.71451 (18)	0.58945 (11)	0.32103 (19)	0.0727 (8)	
O2	0.7740 (2)	0.57911 (11)	0.18148 (17)	0.0761 (8)	
O3	0.93263 (19)	0.45493 (12)	0.35214 (19)	0.0777 (8)	
O4A	0.7579 (5)	0.26783 (18)	0.2995 (6)	0.090 (2)	0.83 (2)
O4B	0.790 (3)	0.2669 (12)	0.258 (3)	0.090 (2)	0.17 (2)
O5A	0.8004 (7)	0.2777 (4)	0.1536 (7)	0.096 (3)	0.83 (2)
O5B	0.783 (3)	0.2837 (19)	0.107 (3)	0.094 (14)	0.17 (2)
O6	0.5144 (2)	0.35423 (12)	0.1666 (2)	0.0920 (10)	
N1	0.6648 (2)	0.33248 (12)	0.1998 (2)	0.0650 (9)	
N2	0.8126 (2)	0.50603 (12)	0.2928 (2)	0.0578 (8)	
N3	0.5770 (3)	0.45627 (16)	0.2978 (2)	0.0724 (10)	

N4	0.6483 (3)	0.47838 (16)	0.1333 (2)	0.0727 (10)
N5	0.8367 (3)	0.40708 (18)	0.1577 (3)	0.0693 (10)
N6	0.7589 (3)	0.39118 (19)	0.3804 (3)	0.0904 (13)
C1	0.8984 (3)	0.49998 (16)	0.3302 (2)	0.0566 (9)
C2	0.9484 (2)	0.55429 (16)	0.3421 (2)	0.0546 (9)
C3	1.0357 (3)	0.56411 (18)	0.3783 (3)	0.0688 (11)
H3	1.0725	0.5350	0.3998	0.083*
C4	1.0670 (3)	0.6180 (2)	0.3818 (3)	0.0806 (13)
H4	1.1261	0.6252	0.4056	0.097*
C5	1.0137 (3)	0.66141 (18)	0.3512 (3)	0.0814 (13)
H5	1.0369	0.6975	0.3543	0.098*
C6	0.9256 (3)	0.65202 (17)	0.3158 (3)	0.0708 (11)
H6	0.8887	0.6813	0.2951	0.085*
C7	0.8944 (2)	0.59838 (15)	0.3119 (2)	0.0556 (9)
C8	0.5758 (3)	0.31942 (16)	0.1756 (3)	0.0625 (10)
C9	0.5607 (3)	0.25861 (16)	0.1611 (3)	0.0613 (10)
C10	0.4798 (3)	0.23143 (19)	0.1390 (3)	0.0809 (13)
H10	0.4247	0.2509	0.1296	0.097*
C11	0.4828 (4)	0.1736 (2)	0.1311 (3)	0.0877 (14)
H11	0.4285	0.1541	0.1176	0.105*
C12	0.5641 (4)	0.14522 (19)	0.1430 (3)	0.0835 (14)
H12	0.5644	0.1068	0.1360	0.100*
C13	0.6452 (3)	0.17213 (16)	0.1650 (3)	0.0754 (12)
H13	0.7006	0.1529	0.1734	0.091*
C14	0.6410 (3)	0.22930 (15)	0.1743 (3)	0.0620 (10)
C15	0.7214 (4)	0.4245 (2)	0.4533 (3)	0.1023 (17)
H15B	0.7390	0.4057	0.5065	0.123*
H15A	0.7510	0.4608	0.4553	0.123*
C16	0.6201 (4)	0.4331 (2)	0.4481 (3)	0.0979 (16)
H16A	0.5910	0.3974	0.4356	0.117*
H16B	0.6028	0.4444	0.5042	0.117*
C17	0.5804 (4)	0.4741 (2)	0.3852 (3)	0.0924 (15)
H17B	0.5183	0.4829	0.3997	0.111*
H17A	0.6164	0.5081	0.3906	0.111*
C18	0.5401 (3)	0.49984 (17)	0.2381 (3)	0.0792 (13)
H18B	0.4750	0.5049	0.2457	0.095*
H18A	0.5710	0.5348	0.2520	0.095*
C19	0.5523 (3)	0.48605 (19)	0.1482 (3)	0.0834 (13)
H19B	0.5186	0.4522	0.1331	0.100*
H19A	0.5270	0.5158	0.1120	0.100*
C20	0.6663 (4)	0.4581 (2)	0.0470 (3)	0.0942 (16)
H20B	0.6364	0.4824	0.0043	0.113*
H20A	0.6406	0.4210	0.0387	0.113*
C21	0.7707 (4)	0.4564 (2)	0.0354 (3)	0.1011 (17)
H21B	0.7797	0.4600	−0.0250	0.121*
H21A	0.7987	0.4886	0.0639	0.121*
C22	0.8193 (4)	0.4073 (3)	0.0668 (3)	0.1048 (17)
H22A	0.7833	0.3746	0.0499	0.126*
H22B	0.8776	0.4049	0.0404	0.126*

Cd2	0.223114 (19)	0.388307 (11)	0.258670 (17)	0.05582 (9)
S3	0.23685 (7)	0.53591 (4)	0.22569 (6)	0.0557 (2)
S4	0.28813 (7)	0.24494 (4)	0.30894 (7)	0.0625 (3)
O7	0.25839 (19)	0.54825 (10)	0.31489 (16)	0.0671 (7)
O8	0.31629 (17)	0.52983 (11)	0.17642 (18)	0.0707 (7)
O9	0.02169 (19)	0.46385 (12)	0.16454 (19)	0.0775 (8)
O10	0.2174 (2)	0.23164 (12)	0.3642 (2)	0.0854 (9)
O11	0.2679 (2)	0.23039 (12)	0.22060 (19)	0.0791 (8)
O12	0.4422 (2)	0.36187 (13)	0.3612 (2)	0.0930 (10)
N7	0.3165 (2)	0.30991 (12)	0.3165 (2)	0.0632 (8)
N8	0.1701 (2)	0.48235 (12)	0.21432 (19)	0.0557 (7)
N9	0.0830 (3)	0.3655 (2)	0.3159 (3)	0.0929 (14)
N10	0.3312 (3)	0.40248 (19)	0.1609 (3)	0.0704 (10)
N11	0.1472 (3)	0.32990 (15)	0.1542 (3)	0.0842 (11)
H11A	0.1711	0.2953	0.1647	0.101*
N12	0.2748 (4)	0.42835 (17)	0.3865 (3)	0.0916 (14)
C23	0.0852 (3)	0.49682 (16)	0.1782 (2)	0.0563 (9)
C24	0.0781 (3)	0.55779 (15)	0.1581 (2)	0.0538 (9)
C25	0.0021 (3)	0.58737 (18)	0.1250 (3)	0.0717 (11)
H25	−0.0537	0.5696	0.1109	0.086*
C26	0.0117 (4)	0.6440 (2)	0.1136 (3)	0.0890 (14)
H26	−0.0389	0.6648	0.0925	0.107*
C27	0.0936 (4)	0.67025 (19)	0.1326 (3)	0.0868 (14)
H27	0.0980	0.7083	0.1229	0.104*
C28	0.1701 (3)	0.64179 (17)	0.1659 (3)	0.0719 (11)
H28	0.2260	0.6597	0.1788	0.086*
C29	0.1597 (3)	0.58505 (15)	0.1791 (2)	0.0552 (9)
C30	0.4039 (3)	0.31674 (17)	0.3493 (3)	0.0644 (10)
C31	0.4517 (3)	0.26224 (16)	0.3693 (2)	0.0609 (10)
C32	0.5402 (3)	0.2529 (2)	0.4028 (3)	0.0829 (13)
H32	0.5790	0.2825	0.4183	0.099*
C33	0.5698 (3)	0.1989 (2)	0.4128 (3)	0.0930 (15)
H33	0.6293	0.1920	0.4356	0.112*
C34	0.5131 (3)	0.1551 (2)	0.3898 (3)	0.0886 (14)
H34	0.5356	0.1189	0.3961	0.106*
C35	0.4238 (3)	0.16317 (18)	0.3578 (3)	0.0767 (12)
H35	0.3848	0.1334	0.3434	0.092*
C36	0.3952 (3)	0.21765 (16)	0.3481 (2)	0.0603 (10)
C37	0.2366 (6)	0.4030 (3)	0.4625 (3)	0.133 (2)
H37B	0.2578	0.4244	0.5125	0.159*
H37A	0.2610	0.3656	0.4697	0.159*
C38	0.1331 (6)	0.4001 (3)	0.4586 (4)	0.148 (3)
H38A	0.1094	0.4356	0.4371	0.178*
H38B	0.1147	0.3964	0.5166	0.178*
C39	0.0860 (5)	0.3546 (3)	0.4056 (5)	0.131 (3)
H39A	0.1183	0.3197	0.4171	0.157*
H39B	0.0235	0.3502	0.4227	0.157*
C40	0.0390 (3)	0.3188 (2)	0.2654 (5)	0.110 (2)
H40A	0.0664	0.2838	0.2848	0.132*

H40B	−0.0262	0.3175	0.2747	0.132*	
C41	0.0511 (4)	0.3256 (2)	0.1727 (4)	0.1069 (18)	
H41A	0.0236	0.2940	0.1421	0.128*	
H41B	0.0188	0.3589	0.1523	0.128*	
C42	0.1615 (5)	0.3407 (2)	0.0647 (3)	0.114 (2)	
H42B	0.1285	0.3744	0.0474	0.137*	
H42A	0.1349	0.3103	0.0307	0.137*	
C43	0.2618 (5)	0.3473 (3)	0.0451 (4)	0.124 (2)	
H43A	0.2966	0.3171	0.0726	0.149*	
H43B	0.2657	0.3431	−0.0160	0.149*	
C44	0.3059 (4)	0.3991 (3)	0.0706 (3)	0.1065 (18)	
H44B	0.3608	0.4037	0.0396	0.128*	
H44A	0.2645	0.4296	0.0548	0.128*	
O1W	0.7901 (12)	0.2850 (5)	0.4846 (8)	0.108 (5)	0.25
H3A	0.531 (4)	0.426 (2)	0.296 (4)	0.14 (2)*	
H4A	0.677 (3)	0.514 (2)	0.140 (3)	0.098 (16)*	
H9	0.054 (4)	0.398 (2)	0.314 (3)	0.12 (2)*	
H5B	0.859 (3)	0.370 (2)	0.176 (3)	0.098 (16)*	
H12A	0.334 (4)	0.424 (2)	0.379 (4)	0.118*	
H12B	0.261 (4)	0.461 (2)	0.384 (3)	0.118*	
H5A	0.877 (3)	0.431 (2)	0.177 (3)	0.097 (17)*	
H10B	0.371 (3)	0.383 (2)	0.181 (3)	0.088 (18)*	
H10A	0.349 (4)	0.440 (2)	0.173 (3)	0.13 (2)*	
H6A	0.805 (5)	0.374 (3)	0.362 (4)	0.156*	
H6B	0.738 (3)	0.3587 (19)	0.412 (3)	0.086 (14)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.05049 (17)	0.05383 (16)	0.05555 (16)	0.00683 (13)	0.00069 (12)	0.00101 (12)
S1	0.0504 (5)	0.0537 (5)	0.0710 (6)	−0.0022 (4)	−0.0094 (5)	0.0021 (5)
S2A	0.0454 (19)	0.0487 (11)	0.115 (2)	0.0051 (13)	0.0012 (16)	−0.0089 (9)
S2B	0.047 (10)	0.041 (5)	0.24 (3)	0.003 (5)	0.035 (13)	−0.010 (10)
O1	0.0475 (16)	0.0698 (17)	0.101 (2)	0.0050 (13)	0.0063 (14)	−0.0072 (15)
O2	0.077 (2)	0.0789 (19)	0.0693 (18)	−0.0143 (15)	−0.0192 (15)	0.0115 (14)
O3	0.0621 (18)	0.0602 (18)	0.109 (2)	0.0129 (15)	−0.0057 (16)	0.0018 (16)
O4A	0.100 (4)	0.069 (2)	0.096 (5)	0.013 (2)	−0.034 (4)	−0.007 (3)
O4B	0.100 (4)	0.069 (2)	0.096 (5)	0.013 (2)	−0.034 (4)	−0.007 (3)
O5A	0.054 (4)	0.073 (4)	0.165 (8)	0.007 (3)	0.029 (5)	−0.014 (5)
O5B	0.07 (2)	0.085 (16)	0.14 (3)	−0.003 (14)	0.05 (2)	0.01 (2)
O6	0.0571 (18)	0.0647 (19)	0.154 (3)	0.0128 (16)	0.0034 (18)	−0.0160 (19)
N1	0.052 (2)	0.0432 (17)	0.100 (3)	0.0019 (15)	0.0026 (17)	−0.0047 (16)
N2	0.0528 (19)	0.0464 (17)	0.072 (2)	0.0008 (14)	−0.0078 (15)	−0.0032 (15)
N3	0.067 (2)	0.074 (2)	0.078 (2)	−0.008 (2)	0.0131 (18)	−0.0050 (19)
N4	0.064 (2)	0.066 (2)	0.086 (3)	0.0021 (19)	−0.0110 (19)	−0.0064 (19)
N5	0.055 (2)	0.069 (2)	0.085 (3)	−0.006 (2)	0.0137 (19)	−0.015 (2)
N6	0.109 (4)	0.086 (3)	0.075 (3)	−0.001 (3)	−0.009 (2)	0.018 (2)
C1	0.050 (2)	0.054 (2)	0.066 (2)	0.0076 (19)	0.0007 (18)	−0.0044 (18)

C2	0.047 (2)	0.058 (2)	0.059 (2)	0.0039 (18)	0.0028 (17)	−0.0057 (17)
C3	0.050 (2)	0.071 (3)	0.084 (3)	0.010 (2)	−0.006 (2)	−0.007 (2)
C4	0.051 (3)	0.085 (3)	0.104 (3)	−0.005 (2)	−0.011 (2)	−0.013 (3)
C5	0.061 (3)	0.064 (3)	0.117 (4)	−0.012 (2)	−0.011 (3)	−0.003 (2)
C6	0.057 (3)	0.058 (3)	0.096 (3)	0.000 (2)	−0.009 (2)	0.003 (2)
C7	0.047 (2)	0.054 (2)	0.065 (2)	−0.0012 (18)	−0.0006 (17)	−0.0007 (18)
C8	0.056 (3)	0.052 (2)	0.081 (3)	0.0045 (19)	0.009 (2)	−0.007 (2)
C9	0.061 (3)	0.053 (2)	0.071 (3)	−0.002 (2)	0.012 (2)	−0.0054 (19)
C10	0.062 (3)	0.079 (3)	0.103 (4)	−0.008 (2)	0.010 (2)	−0.015 (3)
C11	0.085 (4)	0.077 (3)	0.102 (4)	−0.031 (3)	0.014 (3)	−0.019 (3)
C12	0.108 (4)	0.053 (3)	0.089 (3)	−0.007 (3)	0.003 (3)	−0.005 (2)
C13	0.089 (3)	0.048 (2)	0.089 (3)	−0.001 (2)	0.000 (3)	−0.006 (2)
C14	0.066 (3)	0.049 (2)	0.071 (3)	−0.001 (2)	0.007 (2)	−0.0045 (18)
C15	0.109 (4)	0.138 (5)	0.058 (3)	−0.002 (4)	−0.003 (3)	0.008 (3)
C16	0.099 (4)	0.122 (4)	0.075 (3)	−0.018 (3)	0.020 (3)	−0.006 (3)
C17	0.090 (4)	0.094 (4)	0.095 (4)	−0.009 (3)	0.014 (3)	−0.019 (3)
C18	0.044 (2)	0.061 (3)	0.129 (4)	0.013 (2)	−0.015 (2)	−0.016 (3)
C19	0.073 (3)	0.067 (3)	0.107 (4)	−0.007 (2)	−0.016 (3)	0.006 (3)
C20	0.113 (4)	0.107 (4)	0.059 (3)	−0.028 (3)	−0.029 (3)	0.017 (3)
C21	0.114 (5)	0.121 (5)	0.072 (3)	0.005 (4)	0.029 (3)	0.012 (3)
C22	0.098 (4)	0.136 (5)	0.082 (4)	0.003 (4)	0.021 (3)	−0.015 (3)
Cd2	0.05405 (18)	0.05503 (17)	0.05806 (17)	−0.00392 (13)	0.00148 (12)	−0.00233 (13)
S3	0.0501 (6)	0.0484 (5)	0.0678 (6)	−0.0010 (4)	−0.0023 (5)	0.0017 (4)
S4	0.0504 (6)	0.0509 (6)	0.0850 (7)	0.0008 (4)	−0.0039 (5)	0.0068 (5)
O7	0.0793 (19)	0.0541 (15)	0.0653 (16)	−0.0020 (14)	−0.0159 (14)	−0.0025 (13)
O8	0.0451 (15)	0.0739 (18)	0.094 (2)	0.0004 (13)	0.0104 (14)	0.0034 (15)
O9	0.0546 (18)	0.0698 (19)	0.107 (2)	−0.0147 (15)	−0.0063 (15)	0.0085 (16)
O10	0.0582 (18)	0.075 (2)	0.125 (3)	0.0015 (15)	0.0196 (17)	0.0243 (17)
O11	0.078 (2)	0.0689 (19)	0.086 (2)	0.0045 (15)	−0.0261 (16)	−0.0091 (15)
O12	0.080 (2)	0.0629 (19)	0.133 (3)	−0.0175 (17)	−0.0184 (19)	0.0037 (18)
N7	0.059 (2)	0.0457 (18)	0.083 (2)	0.0020 (15)	−0.0080 (17)	0.0074 (15)
N8	0.0480 (19)	0.0464 (17)	0.0720 (19)	−0.0024 (14)	−0.0013 (15)	0.0007 (14)
N9	0.072 (3)	0.083 (3)	0.128 (4)	0.019 (2)	0.038 (2)	0.024 (3)
N10	0.063 (2)	0.072 (3)	0.077 (3)	0.015 (2)	0.0134 (19)	0.003 (2)
N11	0.076 (3)	0.069 (2)	0.104 (3)	−0.003 (2)	−0.025 (2)	−0.002 (2)
N12	0.139 (4)	0.069 (2)	0.063 (2)	0.016 (3)	−0.018 (3)	−0.005 (2)
C23	0.047 (2)	0.060 (2)	0.062 (2)	−0.0039 (19)	0.0041 (18)	0.0013 (18)
C24	0.052 (2)	0.058 (2)	0.052 (2)	0.0032 (18)	0.0052 (17)	−0.0006 (17)
C25	0.063 (3)	0.079 (3)	0.071 (3)	0.008 (2)	−0.009 (2)	0.006 (2)
C26	0.104 (4)	0.073 (3)	0.085 (3)	0.022 (3)	−0.027 (3)	0.008 (2)
C27	0.110 (4)	0.058 (3)	0.087 (3)	0.009 (3)	−0.027 (3)	0.010 (2)
C28	0.080 (3)	0.059 (3)	0.074 (3)	−0.006 (2)	−0.010 (2)	0.008 (2)
C29	0.060 (2)	0.051 (2)	0.054 (2)	0.0010 (18)	−0.0018 (18)	0.0027 (16)
C30	0.059 (3)	0.058 (3)	0.075 (3)	−0.002 (2)	−0.003 (2)	0.004 (2)
C31	0.053 (2)	0.064 (3)	0.064 (2)	0.000 (2)	−0.0033 (19)	0.0052 (19)
C32	0.065 (3)	0.079 (3)	0.102 (4)	0.000 (2)	−0.014 (3)	0.005 (3)
C33	0.055 (3)	0.102 (4)	0.119 (4)	0.015 (3)	−0.017 (3)	0.008 (3)
C34	0.070 (3)	0.073 (3)	0.120 (4)	0.022 (3)	−0.013 (3)	0.007 (3)
C35	0.070 (3)	0.060 (3)	0.098 (3)	0.008 (2)	−0.007 (2)	0.003 (2)

C36	0.054 (2)	0.060 (2)	0.066 (2)	0.0043 (19)	−0.0009 (19)	0.0033 (19)
C37	0.195 (8)	0.146 (6)	0.056 (3)	0.049 (5)	0.001 (4)	0.004 (3)
C38	0.205 (9)	0.163 (7)	0.082 (4)	0.072 (7)	0.050 (5)	0.007 (4)
C39	0.132 (5)	0.134 (6)	0.137 (6)	0.051 (5)	0.080 (5)	0.048 (5)
C40	0.057 (3)	0.066 (3)	0.208 (7)	−0.011 (2)	0.004 (4)	0.034 (4)
C41	0.072 (4)	0.078 (3)	0.167 (6)	0.000 (3)	−0.026 (4)	−0.004 (4)
C42	0.137 (5)	0.121 (5)	0.077 (4)	0.024 (4)	−0.050 (4)	−0.026 (3)
C43	0.155 (6)	0.138 (6)	0.079 (4)	0.023 (5)	0.008 (4)	−0.017 (4)
C44	0.121 (5)	0.123 (5)	0.078 (4)	0.025 (4)	0.025 (3)	0.010 (3)
O1W	0.196 (16)	0.056 (7)	0.072 (8)	0.005 (8)	−0.002 (9)	0.003 (6)

Geometric parameters (Å, °)

Cd1—N6	2.303 (4)	C22—H22A	0.97
Cd1—N5	2.306 (3)	C22—H22B	0.97
Cd1—N4	2.363 (4)	Cd2—N10	2.294 (4)
Cd1—N3	2.397 (4)	Cd2—N12	2.306 (4)
Cd1—N1	2.443 (3)	Cd2—N9	2.346 (4)
Cd1—N2	2.464 (3)	Cd2—N11	2.373 (4)
S1—O1	1.434 (3)	Cd2—N7	2.458 (3)
S1—O2	1.438 (3)	Cd2—N8	2.470 (3)
S1—N2	1.618 (3)	S3—O8	1.440 (3)
S1—C7	1.759 (4)	S3—O7	1.445 (3)
S2A—O5A	1.440 (10)	S3—N8	1.613 (3)
S2A—O4A	1.483 (9)	S3—C29	1.754 (4)
S2A—N1	1.595 (6)	S4—O10	1.426 (3)
S2A—C14	1.740 (6)	S4—O11	1.441 (3)
S2B—O4B	1.21 (4)	S4—N7	1.616 (3)
S2B—O5B	1.47 (5)	S4—C36	1.761 (4)
S2B—N1	1.79 (3)	O9—C23	1.224 (4)
S2B—C14	1.93 (3)	O12—C30	1.227 (5)
O3—C1	1.230 (4)	N7—C30	1.349 (5)
O6—C8	1.224 (4)	N8—C23	1.369 (4)
N1—C8	1.361 (5)	N9—C39	1.430 (7)
N2—C1	1.351 (4)	N9—C40	1.493 (7)
N3—C17	1.435 (6)	N9—H9	0.88 (5)
N3—C18	1.481 (5)	N10—C44	1.443 (6)
N3—H3A	0.99 (6)	N10—H10B	0.80 (5)
N4—C19	1.443 (5)	N10—H10A	0.94 (6)
N4—C20	1.480 (6)	N11—C41	1.451 (6)
N4—H4A	0.96 (5)	N11—C42	1.457 (6)
N5—C22	1.432 (6)	N11—H11A	0.91
N5—H5B	0.98 (5)	N12—C37	1.479 (7)
N5—H5A	0.87 (5)	N12—H12A	0.88 (5)
N6—C15	1.527 (6)	N12—H12B	0.81 (5)
N6—H6A	0.85 (6)	C23—C24	1.499 (5)
N6—H6B	0.98 (4)	C24—C29	1.376 (5)
C1—C2	1.498 (5)	C24—C25	1.384 (5)
C2—C3	1.375 (5)	C25—C26	1.380 (6)

C2—C7	1.383 (5)	C25—H25	0.93
C3—C4	1.371 (6)	C26—C27	1.363 (6)
C3—H3	0.93	C26—H26	0.93
C4—C5	1.366 (6)	C27—C28	1.378 (6)
C4—H4	0.93	C27—H27	0.93
C5—C6	1.380 (5)	C28—C29	1.387 (5)
C5—H5	0.93	C28—H28	0.93
C6—C7	1.365 (5)	C30—C31	1.505 (5)
C6—H6	0.93	C31—C32	1.375 (5)
C8—C9	1.491 (5)	C31—C36	1.377 (5)
C9—C14	1.367 (5)	C32—C33	1.371 (6)
C9—C10	1.370 (6)	C32—H32	0.93
C10—C11	1.394 (6)	C33—C34	1.370 (6)
C10—H10	0.93	C33—H33	0.93
C11—C12	1.368 (6)	C34—C35	1.375 (6)
C11—H11	0.93	C34—H34	0.93
C12—C13	1.368 (6)	C35—C36	1.378 (5)
C12—H12	0.93	C35—H35	0.93
C13—C14	1.382 (5)	C37—C38	1.503 (9)
C13—H13	0.93	C37—H37B	0.97
C15—C16	1.484 (7)	C37—H37A	0.97
C15—H15B	0.97	C38—C39	1.511 (10)
C15—H15A	0.97	C38—H38A	0.97
C16—C17	1.483 (7)	C38—H38B	0.97
C16—H16A	0.97	C39—H39A	0.97
C16—H16B	0.97	C39—H39B	0.97
C17—H17B	0.97	C40—C41	1.486 (8)
C17—H17A	0.97	C40—H40A	0.97
C18—C19	1.472 (6)	C40—H40B	0.97
C18—H18B	0.97	C41—H41A	0.97
C18—H18A	0.97	C41—H41B	0.97
C19—H19B	0.97	C42—C43	1.519 (8)
C19—H19A	0.97	C42—H42B	0.97
C20—C21	1.540 (7)	C42—H42A	0.97
C20—H20B	0.97	C43—C44	1.443 (8)
C20—H20A	0.97	C43—H43A	0.97
C21—C22	1.443 (7)	C43—H43B	0.97
C21—H21B	0.97	C44—H44B	0.97
C21—H21A	0.97	C44—H44A	0.97
N6—Cd1—N5	109.60 (16)	N5—C22—H22A	108.9
N6—Cd1—N4	161.19 (15)	C21—C22—H22A	108.9
N5—Cd1—N4	87.56 (14)	N5—C22—H22B	108.9
N6—Cd1—N3	87.97 (15)	C21—C22—H22B	108.9
N5—Cd1—N3	162.43 (14)	H22A—C22—H22B	107.8
N4—Cd1—N3	74.97 (13)	N10—Cd2—N12	108.84 (18)
N6—Cd1—N1	90.54 (14)	N10—Cd2—N9	160.43 (17)
N5—Cd1—N1	84.02 (13)	N12—Cd2—N9	90.24 (19)
N4—Cd1—N1	99.13 (12)	N10—Cd2—N11	86.14 (15)
N3—Cd1—N1	96.76 (12)	N12—Cd2—N11	163.22 (16)

N6—Cd1—N2	84.27 (14)	N9—Cd2—N11	75.62 (16)
N5—Cd1—N2	84.86 (13)	N10—Cd2—N7	88.55 (14)
N4—Cd1—N2	89.84 (12)	N12—Cd2—N7	81.83 (13)
N3—Cd1—N2	96.72 (12)	N9—Cd2—N7	98.76 (14)
N1—Cd1—N2	165.37 (10)	N11—Cd2—N7	91.31 (12)
O1—S1—O2	115.02 (18)	N10—Cd2—N8	83.72 (13)
O1—S1—N2	110.82 (17)	N12—Cd2—N8	86.66 (12)
O2—S1—N2	110.55 (17)	N9—Cd2—N8	93.35 (13)
O1—S1—C7	111.05 (17)	N11—Cd2—N8	102.90 (11)
O2—S1—C7	111.27 (17)	N7—Cd2—N8	163.28 (10)
N2—S1—C7	96.67 (17)	O8—S3—O7	114.31 (17)
O5A—S2A—O4A	111.9 (5)	O8—S3—N8	110.96 (16)
O5A—S2A—N1	112.0 (5)	O7—S3—N8	111.12 (16)
O4A—S2A—N1	110.5 (3)	O8—S3—C29	110.96 (17)
O5A—S2A—C14	111.3 (5)	O7—S3—C29	110.95 (16)
O4A—S2A—C14	111.9 (4)	N8—S3—C29	97.29 (17)
N1—S2A—C14	98.5 (3)	O10—S4—O11	115.0 (2)
O4B—S2B—O5B	127 (3)	O10—S4—N7	111.23 (18)
O4B—S2B—N1	114 (3)	O11—S4—N7	109.84 (17)
O5B—S2B—N1	106 (3)	O10—S4—C36	111.16 (19)
O4B—S2B—C14	111 (3)	O11—S4—C36	111.40 (18)
O5B—S2B—C14	105 (3)	N7—S4—C36	96.80 (18)
N1—S2B—C14	85.5 (13)	C30—N7—S4	112.0 (3)
C8—N1—S2A	110.0 (3)	C30—N7—Cd2	122.1 (2)
C8—N1—S2B	116.0 (9)	S4—N7—Cd2	125.46 (17)
C8—N1—Cd1	125.0 (2)	C23—N8—S3	111.3 (2)
S2A—N1—Cd1	124.3 (2)	C23—N8—Cd2	127.2 (2)
S2B—N1—Cd1	118.9 (9)	S3—N8—Cd2	121.55 (16)
C1—N2—S1	112.0 (3)	C39—N9—C40	111.6 (5)
C1—N2—Cd1	121.4 (2)	C39—N9—Cd2	116.8 (4)
S1—N2—Cd1	126.08 (16)	C40—N9—Cd2	108.8 (3)
C17—N3—C18	112.5 (4)	C39—N9—H9	100 (4)
C17—N3—Cd1	116.5 (3)	C40—N9—H9	117 (4)
C18—N3—Cd1	106.9 (3)	Cd2—N9—H9	102 (4)
C17—N3—H3A	103 (3)	C44—N10—Cd2	120.5 (3)
C18—N3—H3A	107 (3)	C44—N10—H10B	119 (3)
Cd1—N3—H3A	111 (3)	Cd2—N10—H10B	99 (3)
C19—N4—C20	115.1 (4)	C44—N10—H10A	107 (3)
C19—N4—Cd1	109.1 (3)	Cd2—N10—H10A	101 (3)
C20—N4—Cd1	114.1 (3)	H10B—N10—H10A	108 (5)
C19—N4—H4A	107 (3)	C41—N11—C42	114.0 (4)
C20—N4—H4A	107 (3)	C41—N11—Cd2	108.3 (3)
Cd1—N4—H4A	104 (3)	C42—N11—Cd2	118.1 (3)
C22—N5—Cd1	120.4 (3)	C41—N11—H11A	105.1
C22—N5—H5B	109 (3)	C42—N11—H11A	105.0
Cd1—N5—H5B	104 (3)	Cd2—N11—H11A	105.0
C22—N5—H5A	115 (3)	C37—N12—Cd2	114.4 (4)
Cd1—N5—H5A	100 (3)	C37—N12—H12A	119 (4)
H5B—N5—H5A	108 (4)	Cd2—N12—H12A	96 (4)

C15—N6—Cd1	115.2 (3)	C37—N12—H12B	110 (4)
C15—N6—H6A	146 (5)	Cd2—N12—H12B	107 (4)
Cd1—N6—H6A	91 (5)	H12A—N12—H12B	110 (6)
C15—N6—H6B	85 (3)	O9—C23—N8	123.9 (4)
Cd1—N6—H6B	132 (3)	O9—C23—C24	123.6 (4)
H6A—N6—H6B	94 (5)	N8—C23—C24	112.5 (3)
O3—C1—N2	124.1 (4)	C29—C24—C25	120.0 (4)
O3—C1—C2	123.1 (4)	C29—C24—C23	111.6 (3)
N2—C1—C2	112.8 (3)	C25—C24—C23	128.5 (4)
C3—C2—C7	119.8 (4)	C26—C25—C24	118.0 (4)
C3—C2—C1	128.9 (4)	C26—C25—H25	121.0
C7—C2—C1	111.3 (3)	C24—C25—H25	121.0
C4—C3—C2	118.2 (4)	C27—C26—C25	121.4 (4)
C4—C3—H3	120.9	C27—C26—H26	119.3
C2—C3—H3	120.9	C25—C26—H26	119.3
C5—C4—C3	121.8 (4)	C26—C27—C28	121.7 (4)
C5—C4—H4	119.1	C26—C27—H27	119.1
C3—C4—H4	119.1	C28—C27—H27	119.1
C4—C5—C6	120.4 (4)	C27—C28—C29	116.7 (4)
C4—C5—H5	119.8	C27—C28—H28	121.6
C6—C5—H5	119.8	C29—C28—H28	121.6
C7—C6—C5	117.9 (4)	C24—C29—C28	122.1 (4)
C7—C6—H6	121.0	C24—C29—S3	107.3 (3)
C5—C6—H6	121.0	C28—C29—S3	130.5 (3)
C6—C7—C2	121.8 (4)	O12—C30—N7	124.9 (4)
C6—C7—S1	130.9 (3)	O12—C30—C31	122.5 (4)
C2—C7—S1	107.3 (3)	N7—C30—C31	112.6 (3)
O6—C8—N1	123.2 (4)	C32—C31—C36	119.6 (4)
O6—C8—C9	123.5 (4)	C32—C31—C30	129.0 (4)
N1—C8—C9	113.3 (3)	C36—C31—C30	111.4 (3)
C14—C9—C10	120.3 (4)	C33—C32—C31	118.4 (4)
C14—C9—C8	111.4 (4)	C33—C32—H32	120.8
C10—C9—C8	128.3 (4)	C31—C32—H32	120.8
C9—C10—C11	117.7 (4)	C34—C33—C32	121.2 (4)
C9—C10—H10	121.1	C34—C33—H33	119.4
C11—C10—H10	121.1	C32—C33—H33	119.4
C12—C11—C10	121.1 (4)	C33—C34—C35	121.6 (4)
C12—C11—H11	119.5	C33—C34—H34	119.2
C10—C11—H11	119.5	C35—C34—H34	119.2
C11—C12—C13	121.5 (4)	C34—C35—C36	116.5 (4)
C11—C12—H12	119.3	C34—C35—H35	121.8
C13—C12—H12	119.3	C36—C35—H35	121.8
C12—C13—C14	116.9 (4)	C31—C36—C35	122.7 (4)
C12—C13—H13	121.6	C31—C36—S4	107.1 (3)
C14—C13—H13	121.6	C35—C36—S4	130.2 (3)
C9—C14—C13	122.6 (4)	N12—C37—C38	114.5 (5)
C9—C14—S2A	106.5 (3)	N12—C37—H37B	108.6
C13—C14—S2A	130.8 (4)	C38—C37—H37B	108.6
C9—C14—S2B	112.1 (9)	N12—C37—H37A	108.6

C13—C14—S2B	124.8 (10)	C38—C37—H37A	108.6
C16—C15—N6	115.8 (4)	H37B—C37—H37A	107.6
C16—C15—H15B	108.3	C37—C38—C39	118.1 (6)
N6—C15—H15B	108.3	C37—C38—H38A	107.8
C16—C15—H15A	108.3	C39—C38—H38A	107.8
N6—C15—H15A	108.3	C37—C38—H38B	107.8
H15B—C15—H15A	107.4	C39—C38—H38B	107.8
C17—C16—C15	118.0 (4)	H38A—C38—H38B	107.1
C17—C16—H16A	107.8	N9—C39—C38	113.0 (5)
C15—C16—H16A	107.8	N9—C39—H39A	109.0
C17—C16—H16B	107.8	C38—C39—H39A	109.0
C15—C16—H16B	107.8	N9—C39—H39B	109.0
H16A—C16—H16B	107.2	C38—C39—H39B	109.0
N3—C17—C16	115.3 (4)	H39A—C39—H39B	107.8
N3—C17—H17B	108.5	C41—C40—N9	111.3 (4)
C16—C17—H17B	108.5	C41—C40—H40A	109.4
N3—C17—H17A	108.5	N9—C40—H40A	109.4
C16—C17—H17A	108.5	C41—C40—H40B	109.4
H17B—C17—H17A	107.5	N9—C40—H40B	109.4
C19—C18—N3	112.7 (3)	H40A—C40—H40B	108.0
C19—C18—H18B	109.0	N11—C41—C40	112.5 (4)
N3—C18—H18B	109.0	N11—C41—H41A	109.1
C19—C18—H18A	109.0	C40—C41—H41A	109.1
N3—C18—H18A	109.0	N11—C41—H41B	109.1
H18B—C18—H18A	107.8	C40—C41—H41B	109.1
N4—C19—C18	111.4 (4)	H41A—C41—H41B	107.8
N4—C19—H19B	109.3	N11—C42—C43	114.5 (4)
C18—C19—H19B	109.3	N11—C42—H42B	108.6
N4—C19—H19A	109.3	C43—C42—H42B	108.6
C18—C19—H19A	109.3	N11—C42—H42A	108.6
H19B—C19—H19A	108.0	C43—C42—H42A	108.6
N4—C20—C21	110.7 (4)	H42B—C42—H42A	107.6
N4—C20—H20B	109.5	C44—C43—C42	116.7 (5)
C21—C20—H20B	109.5	C44—C43—H43A	108.1
N4—C20—H20A	109.5	C42—C43—H43A	108.1
C21—C20—H20A	109.5	C44—C43—H43B	108.1
H20B—C20—H20A	108.1	C42—C43—H43B	108.1
C22—C21—C20	116.4 (5)	H43A—C43—H43B	107.3
C22—C21—H21B	108.2	N10—C44—C43	113.6 (5)
C20—C21—H21B	108.2	N10—C44—H44B	108.8
C22—C21—H21A	108.2	C43—C44—H44B	108.8
C20—C21—H21A	108.2	N10—C44—H44A	108.8
H21B—C21—H21A	107.3	C43—C44—H44A	108.8
N5—C22—C21	113.2 (5)	H44B—C44—H44A	107.7
O5A—S2A—N1—C8	121.1 (6)	O5B—S2B—C14—S2A	−159 (7)
O4A—S2A—N1—C8	−113.4 (4)	N1—S2B—C14—S2A	−53 (4)
C14—S2A—N1—C8	4.0 (4)	Cd1—N6—C15—C16	54.7 (6)
O5A—S2A—N1—S2B	2(5)	N6—C15—C16—C17	−74.5 (6)
O4A—S2A—N1—S2B	127 (5)	C18—N3—C17—C16	−177.8 (4)

C14—S2A—N1—S2B	−115 (5)	Cd1—N3—C17—C16	−53.8 (5)
O5A—S2A—N1—Cd1	−68.2 (6)	C15—C16—C17—N3	74.1 (6)
O4A—S2A—N1—Cd1	57.3 (4)	C17—N3—C18—C19	169.4 (4)
C14—S2A—N1—Cd1	174.6 (2)	Cd1—N3—C18—C19	40.2 (4)
O4B—S2B—N1—C8	−122 (2)	C20—N4—C19—C18	173.3 (4)
O5B—S2B—N1—C8	93 (3)	Cd1—N4—C19—C18	43.6 (4)
C14—S2B—N1—C8	−12.0 (17)	N3—C18—C19—N4	−59.0 (5)
O4B—S2B—N1—S2A	−57 (5)	C19—N4—C20—C21	175.0 (4)
O5B—S2B—N1—S2A	159 (7)	Cd1—N4—C20—C21	−57.9 (5)
C14—S2B—N1—S2A	54 (4)	N4—C20—C21—C22	84.0 (6)
O4B—S2B—N1—Cd1	61 (3)	Cd1—N5—C22—C21	49.9 (6)
O5B—S2B—N1—Cd1	−84 (3)	C20—C21—C22—N5	−77.2 (6)
C14—S2B—N1—Cd1	171.2 (4)	O10—S4—N7—C30	114.6 (3)
N6—Cd1—N1—C8	115.0 (3)	O11—S4—N7—C30	−117.0 (3)
N5—Cd1—N1—C8	−135.3 (3)	C36—S4—N7—C30	−1.3 (3)
N4—Cd1—N1—C8	−48.8 (3)	O10—S4—N7—Cd2	−73.4 (2)
N3—Cd1—N1—C8	27.0 (3)	O11—S4—N7—Cd2	55.0 (3)
N2—Cd1—N1—C8	−176.0 (4)	C36—S4—N7—Cd2	170.7 (2)
N6—Cd1—N1—S2A	−54.3 (3)	N10—Cd2—N7—C30	60.3 (3)
N5—Cd1—N1—S2A	55.4 (3)	N12—Cd2—N7—C30	−49.0 (3)
N4—Cd1—N1—S2A	141.9 (3)	N9—Cd2—N7—C30	−137.9 (3)
N3—Cd1—N1—S2A	−142.3 (3)	N11—Cd2—N7—C30	146.4 (3)
N2—Cd1—N1—S2A	14.7 (6)	N8—Cd2—N7—C30	−2.0 (6)
N6—Cd1—N1—S2B	−68.5 (14)	N10—Cd2—N7—S4	−111.0 (2)
N5—Cd1—N1—S2B	41.2 (14)	N12—Cd2—N7—S4	139.8 (3)
N4—Cd1—N1—S2B	127.7 (14)	N9—Cd2—N7—S4	50.8 (2)
N3—Cd1—N1—S2B	−156.5 (14)	N11—Cd2—N7—S4	−24.8 (2)
N2—Cd1—N1—S2B	0.5 (15)	N8—Cd2—N7—S4	−173.3 (3)
O1—S1—N2—C1	−115.3 (3)	O8—S3—N8—C23	−117.9 (3)
O2—S1—N2—C1	116.0 (3)	O7—S3—N8—C23	113.7 (3)
C7—S1—N2—C1	0.3 (3)	C29—S3—N8—C23	−2.1 (3)
O1—S1—N2—Cd1	73.5 (2)	O8—S3—N8—Cd2	61.9 (2)
O2—S1—N2—Cd1	−55.2 (2)	O7—S3—N8—Cd2	−66.5 (2)
C7—S1—N2—Cd1	−170.9 (2)	C29—S3—N8—Cd2	177.71 (18)
N6—Cd1—N2—C1	49.5 (3)	N10—Cd2—N8—C23	119.6 (3)
N5—Cd1—N2—C1	−60.9 (3)	N12—Cd2—N8—C23	−131.1 (3)
N4—Cd1—N2—C1	−148.4 (3)	N9—Cd2—N8—C23	−41.0 (3)
N3—Cd1—N2—C1	136.7 (3)	N11—Cd2—N8—C23	35.0 (3)
N1—Cd1—N2—C1	−20.3 (6)	N7—Cd2—N8—C23	−177.5 (3)
N6—Cd1—N2—S1	−140.2 (2)	N10—Cd2—N8—S3	−60.2 (2)
N5—Cd1—N2—S1	109.5 (2)	N12—Cd2—N8—S3	49.2 (2)
N4—Cd1—N2—S1	22.0 (2)	N9—Cd2—N8—S3	139.2 (2)
N3—Cd1—N2—S1	−52.9 (2)	N11—Cd2—N8—S3	−144.80 (19)
N1—Cd1—N2—S1	150.1 (4)	N7—Cd2—N8—S3	2.7 (5)
N6—Cd1—N3—C17	33.0 (3)	N10—Cd2—N9—C39	162.1 (5)
N5—Cd1—N3—C17	−145.2 (4)	N12—Cd2—N9—C39	−30.6 (4)
N4—Cd1—N3—C17	−139.0 (4)	N11—Cd2—N9—C39	140.3 (4)
N1—Cd1—N3—C17	123.3 (3)	N7—Cd2—N9—C39	51.2 (4)
N2—Cd1—N3—C17	−51.0 (3)	N8—Cd2—N9—C39	−117.2 (4)

N6—Cd1—N3—C18	159.8 (3)	N10—Cd2—N9—C40	34.7 (7)
N5—Cd1—N3—C18	−18.4 (6)	N12—Cd2—N9—C40	−158.0 (3)
N4—Cd1—N3—C18	−12.2 (3)	N11—Cd2—N9—C40	12.9 (3)
N1—Cd1—N3—C18	−109.9 (3)	N7—Cd2—N9—C40	−76.3 (3)
N2—Cd1—N3—C18	75.8 (3)	N8—Cd2—N9—C40	115.3 (3)
N6—Cd1—N4—C19	−41.6 (6)	N12—Cd2—N10—C44	−159.1 (4)
N5—Cd1—N4—C19	162.1 (3)	N9—Cd2—N10—C44	7.5 (7)
N3—Cd1—N4—C19	−16.1 (3)	N11—Cd2—N10—C44	28.6 (4)
N1—Cd1—N4—C19	78.5 (3)	N7—Cd2—N10—C44	120.0 (4)
N2—Cd1—N4—C19	−113.1 (3)	N8—Cd2—N10—C44	−74.8 (4)
N6—Cd1—N4—C20	−171.8 (4)	N10—Cd2—N11—C41	−157.9 (3)
N5—Cd1—N4—C20	31.8 (3)	N12—Cd2—N11—C41	48.2 (7)
N3—Cd1—N4—C20	−146.3 (3)	N9—Cd2—N11—C41	14.9 (3)
N1—Cd1—N4—C20	−51.7 (3)	N7—Cd2—N11—C41	113.6 (3)
N2—Cd1—N4—C20	116.7 (3)	N8—Cd2—N11—C41	−75.3 (3)
N6—Cd1—N5—C22	160.2 (4)	N10—Cd2—N11—C42	−26.4 (4)
N4—Cd1—N5—C22	−27.7 (4)	N12—Cd2—N11—C42	179.7 (5)
N3—Cd1—N5—C22	−21.7 (7)	N9—Cd2—N11—C42	146.4 (4)
N1—Cd1—N5—C22	71.8 (4)	N7—Cd2—N11—C42	−114.9 (4)
N2—Cd1—N5—C22	−117.7 (4)	N8—Cd2—N11—C42	56.2 (4)
N5—Cd1—N6—C15	147.4 (4)	N10—Cd2—N12—C37	−154.4 (4)
N4—Cd1—N6—C15	−7.4 (7)	N9—Cd2—N12—C37	30.0 (4)
N3—Cd1—N6—C15	−32.0 (4)	N11—Cd2—N12—C37	−2.2 (8)
N1—Cd1—N6—C15	−128.8 (4)	N7—Cd2—N12—C37	−68.8 (4)
N2—Cd1—N6—C15	64.9 (4)	N8—Cd2—N12—C37	123.4 (4)
S1—N2—C1—O3	179.9 (3)	S3—N8—C23—O9	−178.5 (3)
Cd1—N2—C1—O3	−8.5 (5)	Cd2—N8—C23—O9	1.7 (5)
S1—N2—C1—C2	−0.2 (4)	S3—N8—C23—C24	0.9 (4)
Cd1—N2—C1—C2	171.4 (2)	Cd2—N8—C23—C24	−179.0 (2)
O3—C1—C2—C3	−0.8 (6)	O9—C23—C24—C29	−179.4 (4)
N2—C1—C2—C3	179.3 (4)	N8—C23—C24—C29	1.3 (4)
O3—C1—C2—C7	180.0 (4)	O9—C23—C24—C25	2.4 (6)
N2—C1—C2—C7	0.0 (4)	N8—C23—C24—C25	−176.9 (4)
C7—C2—C3—C4	−1.1 (6)	C29—C24—C25—C26	0.4 (6)
C1—C2—C3—C4	179.7 (4)	C23—C24—C25—C26	178.6 (4)
C2—C3—C4—C5	0.6 (7)	C24—C25—C26—C27	1.3 (7)
C3—C4—C5—C6	0.2 (7)	C25—C26—C27—C28	−1.5 (8)
C4—C5—C6—C7	−0.4 (7)	C26—C27—C28—C29	0.0 (7)
C5—C6—C7—C2	−0.2 (6)	C25—C24—C29—C28	−2.0 (6)
C5—C6—C7—S1	180.0 (3)	C23—C24—C29—C28	179.6 (3)
C3—C2—C7—C6	0.9 (6)	C25—C24—C29—S3	175.8 (3)
C1—C2—C7—C6	−179.8 (4)	C23—C24—C29—S3	−2.6 (4)
C3—C2—C7—S1	−179.2 (3)	C27—C28—C29—C24	1.7 (6)
C1—C2—C7—S1	0.1 (4)	C27—C28—C29—S3	−175.5 (3)
O1—S1—C7—C6	−65.0 (4)	O8—S3—C29—C24	118.6 (3)
O2—S1—C7—C6	64.5 (4)	O7—S3—C29—C24	−113.2 (3)
N2—S1—C7—C6	179.7 (4)	N8—S3—C29—C24	2.8 (3)
O1—S1—C7—C2	115.2 (3)	O8—S3—C29—C28	−63.9 (4)
O2—S1—C7—C2	−115.4 (3)	O7—S3—C29—C28	64.3 (4)

N2—S1—C7—C2	−0.2 (3)	N8—S3—C29—C28	−179.7 (4)
S2A—N1—C8—O6	177.7 (4)	S4—N7—C30—O12	179.7 (4)
S2B—N1—C8—O6	−169.5 (14)	Cd2—N7—C30—O12	7.3 (6)
Cd1—N1—C8—O6	7.1 (6)	S4—N7—C30—C31	0.4 (4)
S2A—N1—C8—C9	−2.4 (5)	Cd2—N7—C30—C31	−171.9 (2)
S2B—N1—C8—C9	10.4 (15)	O12—C30—C31—C32	0.5 (7)
Cd1—N1—C8—C9	−173.0 (2)	N7—C30—C31—C32	179.8 (4)
O6—C8—C9—C14	179.0 (4)	O12—C30—C31—C36	−178.3 (4)
N1—C8—C9—C14	−0.9 (5)	N7—C30—C31—C36	1.0 (5)
O6—C8—C9—C10	−2.3 (7)	C36—C31—C32—C33	0.9 (7)
N1—C8—C9—C10	177.8 (4)	C30—C31—C32—C33	−177.7 (4)
C14—C9—C10—C11	0.3 (6)	C31—C32—C33—C34	0.3 (8)
C8—C9—C10—C11	−178.3 (4)	C32—C33—C34—C35	−1.6 (8)
C9—C10—C11—C12	−1.6 (7)	C33—C34—C35—C36	1.5 (7)
C10—C11—C12—C13	1.6 (7)	C32—C31—C36—C35	−1.0 (6)
C11—C12—C13—C14	−0.3 (7)	C30—C31—C36—C35	177.9 (4)
C10—C9—C14—C13	1.1 (6)	C32—C31—C36—S4	179.3 (3)
C8—C9—C14—C13	179.9 (4)	C30—C31—C36—S4	−1.8 (4)
C10—C9—C14—S2A	−175.4 (4)	C34—C35—C36—C31	−0.3 (7)
C8—C9—C14—S2A	3.4 (5)	C34—C35—C36—S4	179.4 (4)
C10—C9—C14—S2B	173.1 (13)	O10—S4—C36—C31	−114.1 (3)
C8—C9—C14—S2B	−8.0 (13)	O11—S4—C36—C31	116.3 (3)
C12—C13—C14—C9	−1.1 (6)	N7—S4—C36—C31	1.8 (3)
C12—C13—C14—S2A	174.5 (4)	O10—S4—C36—C35	66.2 (4)
C12—C13—C14—S2B	−172.1 (14)	O11—S4—C36—C35	−63.4 (4)
O5A—S2A—C14—C9	−122.1 (6)	N7—S4—C36—C35	−177.9 (4)
O4A—S2A—C14—C9	111.9 (4)	Cd2—N12—C37—C38	−53.5 (7)
N1—S2A—C14—C9	−4.4 (4)	N12—C37—C38—C39	78.4 (8)
O5A—S2A—C14—C13	61.8 (7)	C40—N9—C39—C38	177.9 (5)
O4A—S2A—C14—C13	−64.2 (6)	Cd2—N9—C39—C38	51.9 (6)
N1—S2A—C14—C13	179.5 (4)	C37—C38—C39—N9	−76.5 (7)
O5A—S2A—C14—S2B	−3(5)	C39—N9—C40—C41	−169.8 (4)
O4A—S2A—C14—S2B	−129 (5)	Cd2—N9—C40—C41	−39.5 (5)
N1—S2A—C14—S2B	115 (5)	C42—N11—C41—C40	−175.7 (4)
O4B—S2B—C14—C9	125 (2)	Cd2—N11—C41—C40	−42.0 (5)
O5B—S2B—C14—C9	−94 (3)	N9—C40—C41—N11	57.0 (6)
N1—S2B—C14—C9	11.2 (16)	C41—N11—C42—C43	177.9 (5)
O4B—S2B—C14—C13	−63 (3)	Cd2—N11—C42—C43	49.1 (6)
O5B—S2B—C14—C13	78 (3)	N11—C42—C43—C44	−74.9 (7)
N1—S2B—C14—C13	−176.9 (5)	Cd2—N10—C44—C43	−54.6 (6)
O4B—S2B—C14—S2A	60 (6)	C42—C43—C44—N10	76.7 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5A···O9^{i}	0.87 (5)	2.26 (5)	3.011 (5)	144 (4)
N9—H9···O3^{ii}	0.88 (5)	2.34 (6)	3.142 (5)	151 (5)
N3—H3A···O12	0.99 (6)	2.29 (6)	3.198 (5)	152 (5)
N4—H4A···O2	0.96 (5)	2.17 (5)	3.095 (5)	161 (4)

N5—H5B···O5A	0.98 (5)	2.39 (5)	3.151 (10)	134 (4)
N12—H12A···O12	0.88 (5)	2.20 (5)	2.960 (6)	144 (5)
N12—H12B···O7	0.81 (5)	2.35 (5)	3.094 (5)	152 (5)
N10—H10B···O6	0.80 (5)	2.22 (5)	2.901 (5)	143 (4)
N10—H10A···O8	0.94 (6)	2.22 (6)	3.076 (5)	151 (5)
N6—H6B···O1W	0.98 (4)	2.21 (5)	3.047 (12)	142 (4)

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

Fig. 1

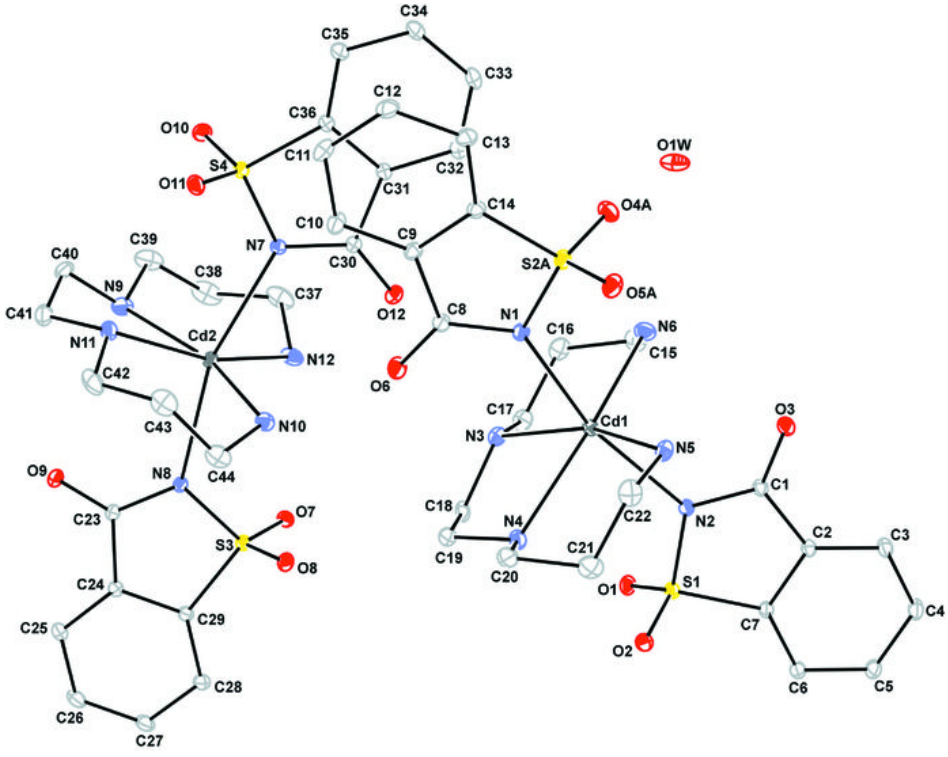
C34
C35
C33
C12
C36
O10
C13
C11
O1W
S4
C32
O11
C31
C14
O4A
C10
C9
N7
C30
S2A
C40
C39
O5A
N9
C38
C37
C41
O12
C8
N1
N11
Cd2
C16
N6
N12
C15
O6
C42
C17
O3
C43
N10
Cd1
N3
N5
O9
N8
C44
C1
C18
C22
N2
O7
C23
N4
C2
C3
S3
C21
C19
C20
O1
S1
O8
C24
C29
C4
C25
C7
O2
C28
C6
C5
C26
C27

Fig. 2