Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaqua(1,10-phenanthroline-κ^2N,N')-cadmium(II) sulfate dihydrate

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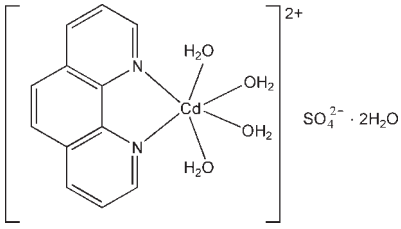
Received 5 July 2010; accepted 14 July 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.033; wR factor = 0.065; data-to-parameter ratio = 13.8.

In the title mononuclear complex, $[Cd(C_{12}H_8N_2)(H_2O)_4]SO_4\cdot 2H_2O$, the coordination geometry around the Cd^{II} atom is a distorted octahedron, with two aqua ligands occupying the axial positions. Intermolecular O—H···O hydrogen bonds lead to the formation of a two-dimensional layer structure parallel to (001). The layers are connected by π–π interactions between the pyridyl and benzene rings of the phenanthroline ligands [centroid–centroid distances = 3.591 (1) and 3.610 (1) Å].

Related literature

For general backgound to supramolecular structures with coordination frameworks, see: Bie *et al.* (2006); Huang *et al.* (2010); Wu *et al.* (2009). For related structures, see: Li *et al.* (2003); Zheng & Lin (2003).



Experimental

Crystal data

$[Cd(C_{12}H_8N_2)(H_2O)_4]SO_4\cdot 2H_2O$
M_r = 496.78
Orthorhombic, *Pbca*
a = 8.8398 (9) Å
b = 18.6996 (19) Å
c = 22.349 (2) Å
V = 3694.3 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.35 mm^{-1}
T = 298 K
0.41 × 0.30 × 0.27 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.622, T_{max} = 0.695
17188 measured reflections
3266 independent reflections
2789 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.065
S = 1.16
3266 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O9^{i}	0.85	1.85	2.682 (4)	167
O1—H1B···O4^{ii}	0.85	2.10	2.952 (4)	176
O2—H2A···O5^{iii}	0.85	1.83	2.682 (3)	178
O2—H2B···O8^{iv}	0.85	1.93	2.757 (4)	165
O3—H3A···O8^{iii}	0.85	1.95	2.787 (4)	170
O3—H3B···O7^{ii}	0.85	1.90	2.746 (4)	170
O4—H4A···O7	0.85	1.84	2.679 (4)	171
O4—H4B···O6^{iv}	0.85	1.87	2.686 (4)	159
O9—H9A···O5^{iii}	0.85	2.00	2.844 (4)	172
O9—H9B···O10^{iv}	0.85	1.92	2.768 (4)	176
O10—H10A···O8	0.85	2.05	2.875 (4)	162
O10—H10B···O6^{v}	0.85	2.06	2.909 (4)	172

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; 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*.

This work was supported by the National Keystone Basic Research Program (973 Program) under grant Nos. 2007CB310408 and 2006CB302901, the Funding Project for Academic Human Resources Development in Institutions of Higher Learning under the Jurisdiction of Beijing Municipality, and the State Key Laboratory of Functional Materials for Informatics, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2328).

References

Bie, H.-Y., Ji, W., Yu, J.-H., Wang, T.-G., Lu, J. & Xu, J.-Q. (2006). *Mater. Lett.* **60**, 2475–2479.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Huang, K.-L., Liu, X., Li, J.-K., Ding, Y.-W., Chen, X., Zhang, M.-X., Xu, X.-B. & Song, X.-J. (2010). *Cryst. Growth Des.* **10**, 1508–1515.
Li, X., Cao, R., Bi, W., Sun, D. & Hong, M. (2003). *Acta Cryst.* E**59**, m230–m231.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wu, J.-Q., Jin, Q.-H., Hu, K.-Y. & Zhang, C.-L. (2009). *Acta Cryst.* E**65**, m1096–m1097.
Zheng, Y.-Q. & Lin, J.-L. (2003). *Z. Anorg. Allg. Chem.* **629**, 185–187.

supporting information

Acta Cryst. (2010). E**66**, m970 [https://doi.org/10.1107/S1600536810028175]

Tetraaqua(1,10-phenanthroline-κ^2N,N')cadmium(II) sulfate dihydrate

Yuan-Yuan Zhang, Qiong-Hua Jin, Wei Yang and Cun-Lin Zhang

S1. Comment

Supramolecular compounds with coordination frameworks have received increasing attention due to their fascinating architectures and potential applications as functional materials of catalysis, magnetism, superconductor, non-linear optical materials and molecular recognition (Bie *et al.*, 2006; Huang *et al.*, 2010; Wu *et al.*, 2009). In this paper, we report the structure of the title compound, a new cadmium(II) complex.

The Cd^{II} atom is six-coordinated by two N atoms from a phenanthroline (phen) ligand, four O atoms from water molecules, forming a $[Cd(phen)(H_2O)_4]^{2+}$ cation. The structure contains a sulfate anion to balance the charge and two uncoordinated molecules (Fig. 1). The complex cations, sulfate anions and water molecules are held together *via* O—H···O hydrogen bonds (Table 1), forming a two-dimensional layer. Interdigitation of phen ligands leads to the formation of a three-dimensional network (Fig.2), stabilized by significant π–π stacking interactions between the pyridyl and benzene rings of the phen ligands [centroid–centroid distances = 3.591 (1) and 3.610 (1) Å].

The Cd—O distances of 2.260 (3)–2.304 (2)Å in the title compound are slightly longer than the reported Cd—O distances of 2.246 (2)–2.325 (3) Å, and Cd—N distances of 2.317 (3)–2.337 (3)Å are shorter than the reported Cd—N distances of 2.318 (3)–2.351 (2)Å (Bie *et al.*, 2006). The cis O—Cd—O angles are in the range of 82.52 (9)–96.46 (11)° and the trans one is 165.28 (9)°. The cis N—Cd—O angles are in the range of 87.35 (10)–105.41 (10)° and the trans ones are 160.98 (12) and 168.48 (11)°. The N—Cd—N angle is 72.09 (11)°. These confirm the distorted octahedral environment around the Cd^{II} atom. It is noticable that in the similar complexes reported, $[Cd(SO_4)(C_{12}H_8N_2)(H_2O)_3]$ (Li *et al.*, 2003), $[Cd(C_{12}H_8N_2)(H_2O)_2(SO_4)]_n$ (Bie *et al.*, 2006) and $[Mn(C_{12}H_8N_2)(H_2O)_2(SO_4)]$ (Zheng & Lin, 2003), the center metals are coordinated to O atom from sulfate, while in the title compound the sulfate acts as a free anion.

S2. Experimental

A mixture of $CdSO_4.8H_2O$ (0.2 mmol), biimidazole (0.1 mmol), H_2O (15 ml) and 1,10-phenanthroline (0.2 mmol) was sealed in a 25 ml Teflon-lined stainless-steel reactor and heated to 160°C for 72 h. After cooling, colorless crystals of the title compound were obtained.

S3. Refinement

C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The water H atoms were located in a difference Fourier map and refined as riding, with O—H = 0.85 Å and U_{iso}(H) = 1.2U_{eq}(O).

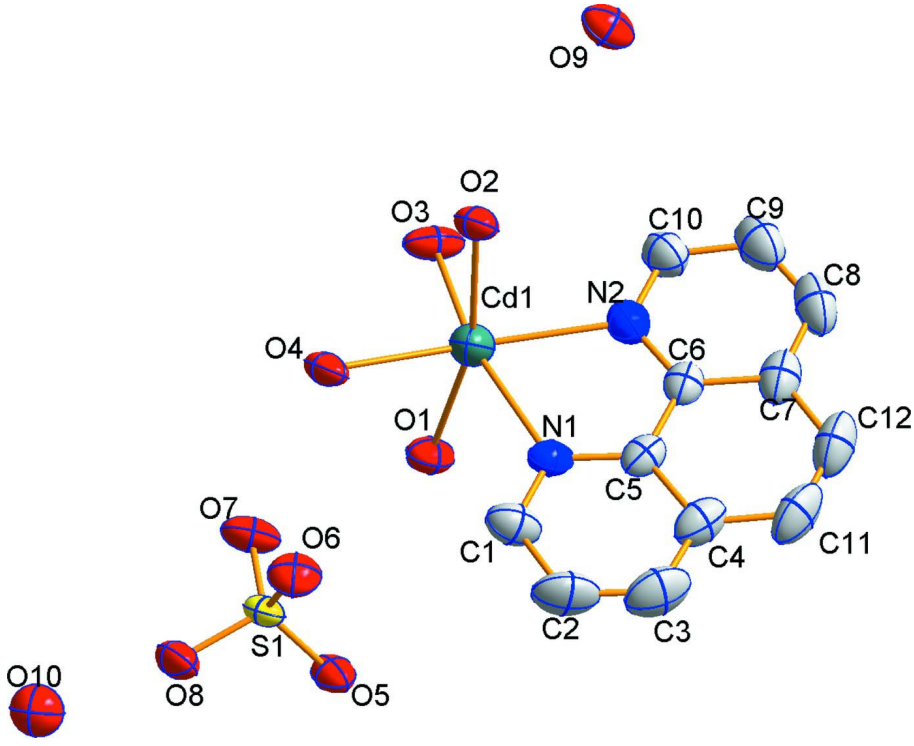


Figure 1

Molecular structure of the title complex. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

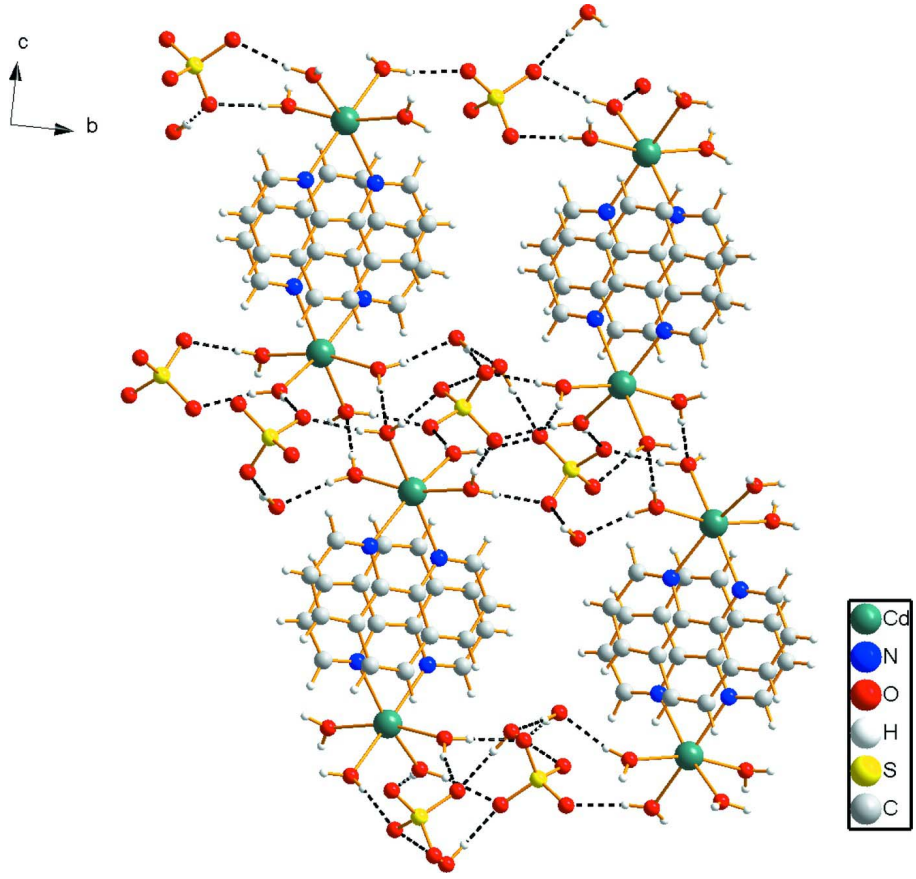


Figure 2

Crystal packing of the title complex. Dashed lines denote hydrogen bonds.

Tetraaqua(1,10-phenanthroline-κ^2N,N')cadmium(II) sulfate dihydrate

Crystal data

$[Cd(C_{12}H_8N_2)(H_2O)_4]SO_4\cdot 2H_2O$
$M_r = 496.78$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 8.8398$ (9) Å
$b = 18.6996$ (19) Å
$c = 22.349$ (2) Å
$V = 3694.3$ (6) Å^3
$Z = 8$
$F(000) = 2000.0$
$D_x = 1.786$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8439 reflections
$\theta = 2.2$–$28.1°$
$\mu = 1.35$ mm^{-1}
$T = 298$ K
Block, yellow
0.41 × 0.30 × 0.27 mm

Data collection

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.622$, $T_{max} = 0.695$
17188 measured reflections
3266 independent reflections
2789 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -10\rightarrow7$
$k = -22\rightarrow22$
$l = -22\rightarrow26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.065$
$S = 1.16$
3266 reflections
236 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
$w = 1/[\sigma^2(F_o^2) + (0.0047P)^2 + 7.3452P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00446 (16)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.63465 (3)	0.587420 (13)	0.411381 (11)	0.03164 (12)
N1	0.7363 (4)	0.52699 (16)	0.33033 (14)	0.0367 (7)
N2	0.5467 (4)	0.64254 (17)	0.32424 (14)	0.0379 (8)
O1	0.4794 (3)	0.49034 (13)	0.42568 (12)	0.0433 (7)
H1A	0.5121	0.4505	0.4127	0.052*
H1B	0.4110	0.4828	0.4516	0.052*
O2	0.7916 (3)	0.68309 (13)	0.42330 (11)	0.0392 (6)
H2A	0.7508	0.7241	0.4202	0.047*
H2B	0.8638	0.6858	0.4483	0.047*
O3	0.4697 (3)	0.64814 (14)	0.46954 (13)	0.0505 (8)
H3A	0.4856	0.6921	0.4769	0.061*
H3B	0.3776	0.6393	0.4775	0.061*
O4	0.7684 (3)	0.53557 (13)	0.48847 (12)	0.0433 (7)
H4A	0.7885	0.4911	0.4880	0.052*
H4B	0.8429	0.5579	0.5037	0.052*
O5	0.8325 (3)	0.31356 (13)	0.41435 (12)	0.0445 (7)
O6	1.0491 (3)	0.38259 (15)	0.44410 (13)	0.0500 (8)
O7	0.8156 (3)	0.39447 (14)	0.49742 (14)	0.0517 (8)
O8	0.9605 (3)	0.28672 (13)	0.50624 (13)	0.0489 (8)
O9	0.9479 (3)	0.86732 (14)	0.37107 (13)	0.0499 (8)
H9A	0.8684	0.8471	0.3842	0.060*
H9B	1.0241	0.8436	0.3830	0.060*
O10	0.7963 (3)	0.20834 (17)	0.59585 (14)	0.0601 (8)
H10A	0.8254	0.2339	0.5666	0.072*
H10B	0.7303	0.1791	0.5829	0.072*
S1	0.91417 (11)	0.34438 (4)	0.46528 (4)	0.0313 (2)
C1	0.8259 (5)	0.4706 (2)	0.3331 (2)	0.0528 (12)
H1	0.8577	0.4545	0.3704	0.063*
C2	0.8748 (6)	0.4343 (3)	0.2817 (3)	0.0679 (15)
H2	0.9362	0.3941	0.2850	0.082*
C3	0.8315 (6)	0.4584 (3)	0.2274 (3)	0.0711 (16)
H3	0.8640	0.4348	0.1931	0.085*

C4	0.7386 (5)	0.5184 (3)	0.22216 (19)	0.0513 (12)
C5	0.6928 (4)	0.5516 (2)	0.27550 (16)	0.0370 (9)
C6	0.5959 (4)	0.6128 (2)	0.27248 (16)	0.0361 (9)
C7	0.5517 (5)	0.6411 (3)	0.21632 (18)	0.0500 (12)
C8	0.4601 (6)	0.7016 (3)	0.2162 (2)	0.0628 (14)
H8	0.4307	0.7218	0.1800	0.075*
C9	0.4140 (6)	0.7310 (3)	0.2677 (2)	0.0643 (14)
H9	0.3534	0.7716	0.2676	0.077*
C10	0.4585 (5)	0.6996 (2)	0.3217 (2)	0.0508 (11)
H10	0.4246	0.7197	0.3574	0.061*
C11	0.6927 (6)	0.5484 (3)	0.1662 (2)	0.0679 (15)
H11	0.7245	0.5269	0.1308	0.081*
C12	0.6042 (6)	0.6069 (3)	0.1636 (2)	0.0663 (15)
H12	0.5770	0.6254	0.1265	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03948 (18)	0.02569 (15)	0.02976 (16)	0.00082 (12)	0.00038 (12)	−0.00058 (12)
N1	0.0370 (18)	0.0301 (17)	0.0429 (19)	−0.0027 (15)	0.0088 (15)	−0.0022 (14)
N2	0.040 (2)	0.0347 (18)	0.0389 (18)	−0.0004 (15)	−0.0040 (16)	0.0039 (14)
O1	0.0472 (17)	0.0317 (14)	0.0510 (17)	−0.0061 (13)	0.0075 (14)	−0.0014 (12)
O2	0.0394 (15)	0.0253 (13)	0.0530 (17)	0.0024 (12)	−0.0097 (13)	−0.0017 (12)
O3	0.0479 (18)	0.0342 (15)	0.069 (2)	−0.0064 (13)	0.0238 (15)	−0.0175 (14)
O4	0.0484 (17)	0.0236 (13)	0.0579 (17)	0.0007 (12)	−0.0196 (14)	0.0005 (12)
O5	0.0478 (17)	0.0312 (14)	0.0545 (17)	−0.0085 (13)	−0.0188 (14)	0.0023 (13)
O6	0.0409 (17)	0.0461 (17)	0.0632 (19)	−0.0136 (14)	0.0002 (15)	−0.0023 (14)
O7	0.0480 (18)	0.0301 (15)	0.077 (2)	0.0033 (13)	0.0094 (16)	−0.0063 (14)
O8	0.0584 (19)	0.0302 (15)	0.0580 (18)	0.0041 (13)	−0.0206 (15)	0.0032 (13)
O9	0.0431 (17)	0.0403 (16)	0.066 (2)	0.0016 (14)	0.0109 (15)	0.0069 (14)
O10	0.0499 (19)	0.061 (2)	0.070 (2)	0.0017 (16)	−0.0032 (17)	−0.0018 (16)
S1	0.0291 (5)	0.0196 (4)	0.0451 (5)	−0.0003 (4)	−0.0060 (4)	−0.0012 (4)
C1	0.050 (3)	0.041 (2)	0.067 (3)	0.003 (2)	0.015 (2)	0.000 (2)
C2	0.062 (3)	0.052 (3)	0.090 (4)	0.009 (3)	0.026 (3)	−0.018 (3)
C3	0.067 (4)	0.077 (4)	0.069 (4)	−0.006 (3)	0.026 (3)	−0.027 (3)
C4	0.046 (3)	0.062 (3)	0.046 (3)	−0.015 (2)	0.016 (2)	−0.013 (2)
C5	0.032 (2)	0.045 (2)	0.035 (2)	−0.0137 (18)	0.0064 (17)	−0.0060 (17)
C6	0.032 (2)	0.043 (2)	0.034 (2)	−0.0137 (18)	0.0001 (17)	0.0022 (17)
C7	0.044 (3)	0.068 (3)	0.038 (2)	−0.023 (2)	−0.004 (2)	0.007 (2)
C8	0.056 (3)	0.073 (3)	0.060 (3)	−0.014 (3)	−0.019 (3)	0.026 (3)
C9	0.061 (3)	0.058 (3)	0.074 (4)	−0.003 (3)	−0.020 (3)	0.015 (3)
C10	0.051 (3)	0.045 (3)	0.056 (3)	0.003 (2)	−0.008 (2)	0.004 (2)
C11	0.066 (3)	0.101 (4)	0.036 (3)	−0.019 (3)	0.013 (2)	−0.013 (3)
C12	0.062 (3)	0.101 (4)	0.036 (3)	−0.020 (3)	−0.001 (2)	0.007 (3)

Geometric parameters (Å, º)

Cd1—O3	2.260 (3)	O9—H9B	0.8500
Cd1—O2	2.280 (2)	O10—H10A	0.8500
Cd1—O1	2.298 (3)	O10—H10B	0.8500
Cd1—O4	2.304 (2)	C1—C2	1.403 (6)
Cd1—N1	2.317 (3)	C1—H1	0.9300
Cd1—N2	2.337 (3)	C2—C3	1.350 (7)
N1—C1	1.320 (5)	C2—H2	0.9300
N1—C5	1.364 (5)	C3—C4	1.396 (7)
N2—C10	1.323 (5)	C3—H3	0.9300
N2—C6	1.355 (5)	C4—C5	1.403 (5)
O1—H1A	0.8500	C4—C11	1.429 (7)
O1—H1B	0.8499	C5—C6	1.432 (6)
O2—H2A	0.8499	C6—C7	1.417 (5)
O2—H2B	0.8500	C7—C8	1.392 (7)
O3—H3A	0.8500	C7—C12	1.418 (7)
O3—H3B	0.8500	C8—C9	1.340 (7)
O4—H4A	0.8500	C8—H8	0.9300
O4—H4B	0.8500	C9—C10	1.398 (6)
O5—S1	1.466 (3)	C9—H9	0.9300
O6—S1	1.469 (3)	C10—H10	0.9300
O7—S1	1.467 (3)	C11—C12	1.347 (7)
O8—S1	1.473 (3)	C11—H11	0.9300
O9—H9A	0.8500	C12—H12	0.9300
O3—Cd1—O2	86.06 (9)	O7—S1—O8	109.16 (18)
O3—Cd1—O1	86.08 (10)	O6—S1—O8	109.31 (18)
O2—Cd1—O1	165.28 (9)	N1—C1—C2	122.2 (5)
O3—Cd1—O4	96.46 (11)	N1—C1—H1	118.9
O2—Cd1—O4	86.02 (9)	C2—C1—H1	118.9
O1—Cd1—O4	82.52 (9)	C3—C2—C1	119.1 (5)
O3—Cd1—N1	160.98 (12)	C3—C2—H2	120.4
O2—Cd1—N1	103.77 (10)	C1—C2—H2	120.4
O1—Cd1—N1	87.42 (10)	C2—C3—C4	120.8 (5)
O4—Cd1—N1	100.39 (10)	C2—C3—H3	119.6
O3—Cd1—N2	92.46 (11)	C4—C3—H3	119.6
O2—Cd1—N2	87.35 (10)	C3—C4—C5	116.9 (4)
O1—Cd1—N2	105.41 (10)	C3—C4—C11	123.8 (5)
O4—Cd1—N2	168.48 (11)	C5—C4—C11	119.3 (5)
N1—Cd1—N2	72.09 (11)	N1—C5—C4	122.2 (4)
C1—N1—C5	118.7 (4)	N1—C5—C6	118.7 (3)
C1—N1—Cd1	125.8 (3)	C4—C5—C6	119.0 (4)
C5—N1—Cd1	115.4 (2)	N2—C6—C7	120.9 (4)
C10—N2—C6	119.0 (3)	N2—C6—C5	118.7 (3)
C10—N2—Cd1	126.0 (3)	C7—C6—C5	120.4 (4)
C6—N2—Cd1	115.0 (2)	C8—C7—C6	117.8 (4)
Cd1—O1—H1A	116.2	C8—C7—C12	123.7 (5)

Cd1—O1—H1B	130.6	C6—C7—C12	118.5 (5)
H1A—O1—H1B	109.3	C9—C8—C7	120.5 (4)
Cd1—O2—H2A	116.1	C9—C8—H8	119.7
Cd1—O2—H2B	125.5	C7—C8—H8	119.7
H2A—O2—H2B	108.6	C8—C9—C10	119.0 (5)
Cd1—O3—H3A	119.4	C8—C9—H9	120.5
Cd1—O3—H3B	129.9	C10—C9—H9	120.5
H3A—O3—H3B	107.8	N2—C10—C9	122.7 (5)
Cd1—O4—H4A	120.7	N2—C10—H10	118.6
Cd1—O4—H4B	119.3	C9—C10—H10	118.6
H4A—O4—H4B	108.8	C12—C11—C4	121.4 (5)
H9A—O9—H9B	108.3	C12—C11—H11	119.3
H10A—O10—H10B	107.9	C4—C11—H11	119.3
O5—S1—O7	109.79 (17)	C11—C12—C7	121.3 (5)
O5—S1—O6	109.95 (17)	C11—C12—H12	119.3
O7—S1—O6	109.24 (17)	C7—C12—H12	119.3
O5—S1—O8	109.38 (15)		

O3—Cd1—N1—C1	−141.9 (4)	Cd1—N1—C5—C6	2.5 (4)
O2—Cd1—N1—C1	98.5 (3)	C3—C4—C5—N1	0.1 (6)
O1—Cd1—N1—C1	−71.8 (3)	C11—C4—C5—N1	−178.0 (4)
O4—Cd1—N1—C1	10.1 (3)	C3—C4—C5—C6	−179.2 (4)
N2—Cd1—N1—C1	−178.9 (3)	C11—C4—C5—C6	2.7 (6)
O3—Cd1—N1—C5	35.5 (5)	C10—N2—C6—C7	−1.2 (6)
O2—Cd1—N1—C5	−84.1 (3)	Cd1—N2—C6—C7	−179.7 (3)
O1—Cd1—N1—C5	105.6 (3)	C10—N2—C6—C5	179.2 (3)
O4—Cd1—N1—C5	−172.5 (2)	Cd1—N2—C6—C5	0.7 (4)
N2—Cd1—N1—C5	−1.5 (2)	N1—C5—C6—N2	−2.2 (5)
O3—Cd1—N2—C10	13.4 (3)	C4—C5—C6—N2	177.1 (4)
O2—Cd1—N2—C10	−72.6 (3)	N1—C5—C6—C7	178.2 (3)
O1—Cd1—N2—C10	100.0 (3)	C4—C5—C6—C7	−2.5 (5)
O4—Cd1—N2—C10	−127.4 (5)	N2—C6—C7—C8	1.9 (6)
N1—Cd1—N2—C10	−178.0 (4)	C5—C6—C7—C8	−178.6 (4)
O3—Cd1—N2—C6	−168.3 (3)	N2—C6—C7—C12	−178.8 (4)
O2—Cd1—N2—C6	105.8 (3)	C5—C6—C7—C12	0.7 (6)
O1—Cd1—N2—C6	−81.6 (3)	C6—C7—C8—C9	−1.0 (7)
O4—Cd1—N2—C6	50.9 (6)	C12—C7—C8—C9	179.7 (5)
N1—Cd1—N2—C6	0.4 (2)	C7—C8—C9—C10	−0.4 (7)
C5—N1—C1—C2	−1.6 (6)	C6—N2—C10—C9	−0.3 (6)
Cd1—N1—C1—C2	175.7 (3)	Cd1—N2—C10—C9	178.0 (3)
N1—C1—C2—C3	1.4 (8)	C8—C9—C10—N2	1.2 (7)
C1—C2—C3—C4	−0.4 (8)	C3—C4—C11—C12	−179.2 (5)
C2—C3—C4—C5	−0.3 (7)	C5—C4—C11—C12	−1.2 (7)
C2—C3—C4—C11	177.8 (5)	C4—C11—C12—C7	−0.6 (8)
C1—N1—C5—C4	0.8 (6)	C8—C7—C12—C11	−180.0 (5)
Cd1—N1—C5—C4	−176.8 (3)	C6—C7—C12—C11	0.8 (7)
C1—N1—C5—C6	−179.9 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O9^{i}	0.85	1.85	2.682 (4)	167
O1—H1*B*···O4^{ii}	0.85	2.10	2.952 (4)	176
O2—H2*A*···O5^{iii}	0.85	1.83	2.682 (3)	178
O2—H2*B*···O8^{iv}	0.85	1.93	2.757 (4)	165
O3—H3*A*···O8^{iii}	0.85	1.95	2.787 (4)	170
O3—H3*B*···O7^{ii}	0.85	1.90	2.746 (4)	170
O4—H4*A*···O7	0.85	1.84	2.679 (4)	171
O4—H4*B*···O6^{iv}	0.85	1.87	2.686 (4)	159
O9—H9*A*···O5^{iii}	0.85	2.00	2.844 (4)	172
O9—H9*B*···O10^{iv}	0.85	1.92	2.768 (4)	176
O10—H10*A*···O8	0.85	2.05	2.875 (4)	162
O10—H10*B*···O6^{v}	0.85	2.06	2.909 (4)	172

Symmetry codes: (i) −*x*+3/2, *y*−1/2, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+3/2, *y*+1/2, *z*; (iv) −*x*+2, −*y*+1, −*z*+1; (v) *x*−1/2, −*y*+1/2, −*z*+1.