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Bis(2-aminopyrimidine-κN^1)diaqua-dinitrato-κO;$\kappa^2 O,O'$-cadmium(II) monohydrate

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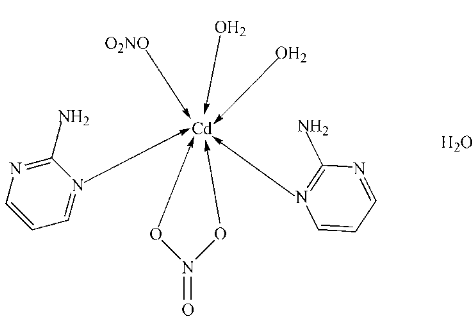
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.030; wR factor = 0.079; data-to-parameter ratio = 16.0.

In the title compound, $[Cd(NO_3)_2(C_4H_5N_3)_2(H_2O)_2]\cdot H_2O$, the Cd atom is seven-coordinated by two 2-aminopyrimidine molecules, two water molecules, one bidentate nitrate anion and one monodentate nitrate anion. A network of N—H···O, N—H···N and O—H···O hydrogen bonds helps to consolidate the crystal structure.

Related literature

For related literature, see: Cui *et al.* (2003).



Experimental

Crystal data

$[Cd(NO_3)_2(C_4H_5N_3)_2(H_2O)_2]\cdot H_2O$	V = 1733.2 (5) Å^3
M_r = 480.69	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 13.451 (2) Å	μ = 1.32 mm^{-1}
b = 7.8692 (14) Å	T = 298 (2) K
c = 16.699 (3) Å	0.57 × 0.47 × 0.34 mm
β = 101.330 (2)°	

Data collection

Bruker SMART CCD diffractometer	9748 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	3771 independent reflections
T_{min} = 0.519, T_{max} = 0.662	3209 reflections with $I > 2\sigma(I)$
	R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029	236 parameters
$wR(F^2)$ = 0.079	H-atom parameters constrained
S = 1.04	$\Delta\rho_{max}$ = 0.83 e Å^{-3}
3771 reflections	$\Delta\rho_{min}$ = −0.99 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O7	2.3009 (19)	Cd1—O4	2.407 (2)
Cd1—O8	2.335 (2)	Cd1—O2	2.512 (2)
Cd1—N1	2.361 (3)	Cd1—O1	2.640 (3)
Cd1—N4	2.399 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O5^{i}	0.86	2.29	3.105 (4)	158
N3—H3B···O7	0.86	2.10	2.945 (4)	167
N6—H6A···N5^{ii}	0.86	2.20	3.054 (4)	170
N6—H6B···O2	0.86	2.19	2.931 (4)	144
N6—H6B···O3^{iii}	0.86	2.52	3.171 (4)	133
O7—H7A···O9^{iv}	0.85	1.94	2.787 (3)	178
O7—H7B···O9^{v}	0.85	1.87	2.724 (3)	178
O8—H8A···O3^{vi}	0.85	1.97	2.820 (3)	176
O8—H8B···O3^{iii}	0.85	2.09	2.936 (3)	176
O9—H9A···O5^{iv}	0.85	2.44	3.255 (3)	162
O9—H9A···O7^{iv}	0.85	2.28	2.787 (3)	119
O9—H9B···O6^{vii}	0.85	1.99	2.809 (4)	161

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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: HB2693).

References

Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cui, Y., Ngo, L. H., White, P. S. & Lin, W. B. (2003). *Inorg. Chem.* **42**, 652–660.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, m537 [doi:10.1107/S1600536808006521]

Bis(2-aminopyrimidine-*κN*[1])diaquadinitrato-*κO*;*κ*[2]*O*,*O*′-cadmium(II) monohydrate

Xi-Shi Tai, Yi-Min Feng and Lin-Tong Wang

S1. Comment

As part of the ongoing studies (Cui *et al.*, 2003) of the coordination chemistry of Cd(II) ion, we now report the synthesis and structure of the title compound, (I), (Fig. 1).

The Cd atom in (I) is seven-coordinate with two N-donor 2-aminopyrimidine molecules, two water molecules and one bidentate NO_3^- and one monodentate NO_3^- ions (Table 1). The coordination polyhedron around Cd is a distorted pengonal bipyramidal with the N atoms in the axial positions [N1—Cd1—N4 = 164.13 (9)°]. The dihedral angle between the aromatic ring planes is 33.76 (17)°.

A network of N—H···O, N—H···N and O—H···O hydrogen bonds (Table 2) helps to establish the structure of (I).

S2. Experimental

A solution of 0.5 mmol C d$(NO_3)_2$.4H_2O in 10 ml 95% ethanol was added to a solution of 1.0 mmol 2-aminopyrimidine in 10 ml e thanol at room temperature. The mixture was refluxed for 2 h with stirring, then the resulting precipitate was filtered, washed, and dried *in vacuo* over P_4O_{10} for 48 h. Colourless blocks of (I) were recrystallized from methanol at room temperature.

S3. Refinement

The H atoms were placed geometrically (C—H = 0.93–0.96 Å, O—H = 0.82 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C). Some short H···H contacts arise from this geometrical placement scheme and the positions of the water H atoms should be regarded as less certain.

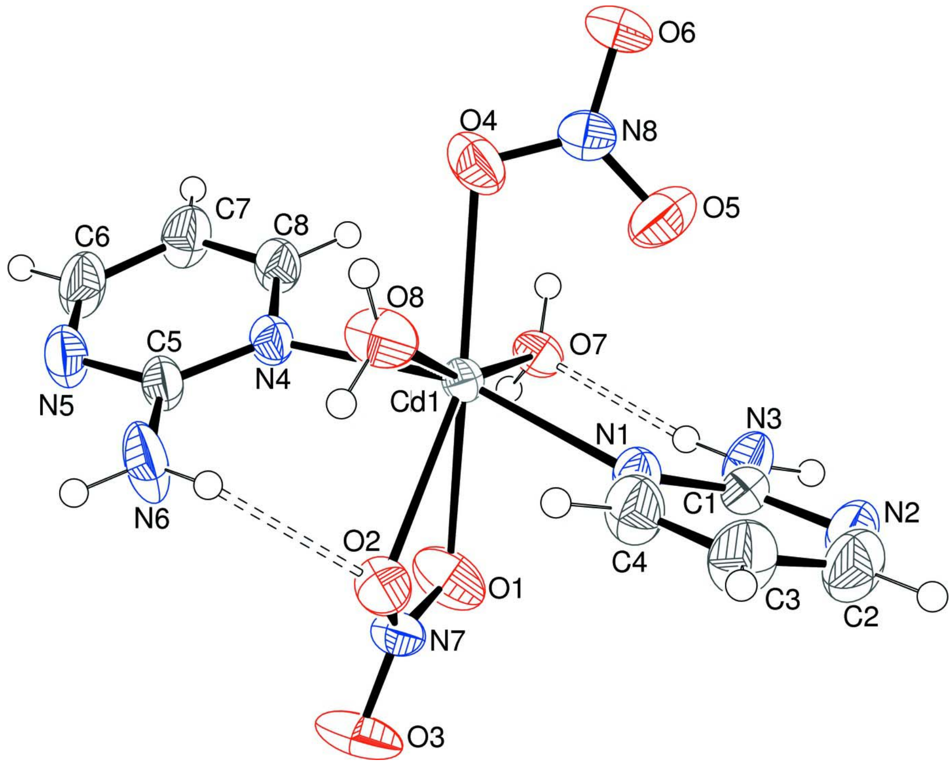

Figure 1

The molecular structure of the complex ion in (I) showing 50% displacement ellipsoids for the non-hydrogen atoms. Hydrogen bonds are indicated by double-dashed lines.

Bis(2-aminopyrimidine-κ*N*[1])diaquadinitrato-κ*O*;κ[2]*O*,*O*′-cadmium(II) monohydrate

Crystal data

$[Cd(NO_3)_2(C_4H_5N_3)_2(H_2O)_2]\cdot H_2O$
$M_r = 480.69$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.451$ (2) Å
$b = 7.8692$ (14) Å
$c = 16.699$ (3) Å
$\beta = 101.330$ (2)°
$V = 1733.2$ (5) Å^3
$Z = 4$
$F(000) = 960$
$D_x = 1.842$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6206 reflections
$\theta = 2.6$–28.2°
$\mu = 1.32$ mm^{-1}
$T = 298$ K
Block, colourless
0.57 × 0.47 × 0.34 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.519$, $T_{max} = 0.662$
9748 measured reflections
3771 independent reflections
3209 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.5°$
$h = -16\rightarrow17$
$k = -10\rightarrow9$
$l = -21\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.079$
$S = 1.04$
3771 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
$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2 + 0.7065P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.83$ e Å^{-3}
$\Delta\rho_{min} = -0.99$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0486 (12)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.247663 (13)	0.03671 (3)	0.205049 (12)	0.02590 (11)
N1	0.26466 (19)	−0.0114 (4)	0.06883 (17)	0.0349 (6)
N2	0.2023 (2)	−0.0805 (4)	−0.07156 (17)	0.0471 (7)
N3	0.10954 (19)	−0.1429 (4)	0.02583 (17)	0.0441 (7)
H3A	0.0637	−0.1851	−0.0122	0.053*
H3B	0.1010	−0.1433	0.0755	0.053*
N4	0.26970 (18)	0.0332 (3)	0.35116 (16)	0.0326 (6)
N5	0.3562 (2)	0.0073 (4)	0.49009 (17)	0.0452 (7)
N6	0.4438 (2)	−0.0069 (5)	0.38605 (19)	0.0649 (11)
H6A	0.4983	−0.0206	0.4223	0.078*
H6B	0.4468	−0.0050	0.3351	0.078*
N7	0.36446 (17)	−0.2853 (3)	0.22553 (16)	0.0343 (6)
N8	0.10409 (17)	0.3297 (3)	0.14881 (17)	0.0349 (6)
O1	0.27101 (15)	−0.2961 (4)	0.21618 (17)	0.0569 (7)
O2	0.40409 (16)	−0.1442 (3)	0.21968 (15)	0.0416 (5)
O3	0.41920 (17)	−0.4123 (3)	0.2418 (2)	0.0610 (8)
O4	0.16425 (16)	0.3041 (3)	0.21572 (16)	0.0496 (6)
O5	0.0921 (2)	0.2158 (3)	0.09573 (16)	0.0580 (7)
O6	0.0575 (2)	0.4627 (3)	0.13678 (18)	0.0554 (7)
O7	0.09014 (14)	−0.0842 (3)	0.19628 (13)	0.0323 (5)
H7A	0.0430	−0.0155	0.2014	0.039*
H7B	0.0838	−0.1732	0.2236	0.039*
O8	0.37736 (15)	0.2381 (3)	0.21821 (16)	0.0471 (6)

H8A	0.3866	0.3445	0.2246	0.056*
H8B	0.4348	0.1893	0.2293	0.056*
O9	0.06716 (14)	0.8659 (3)	0.78566 (13)	0.0373 (5)
H9A	0.0160	0.8574	0.8083	0.045*
H9B	0.0501	0.9217	0.7415	0.045*
C1	0.1937 (2)	−0.0771 (4)	0.00777 (19)	0.0346 (7)
C2	0.2866 (3)	−0.0177 (5)	−0.0896 (2)	0.0549 (10)
H2	0.2937	−0.0173	−0.1439	0.066*
C3	0.3639 (3)	0.0467 (5)	−0.0314 (3)	0.0543 (10)
H3	0.4234	0.0880	−0.0448	0.065*
C4	0.3488 (2)	0.0470 (5)	0.0473 (2)	0.0473 (9)
H4	0.3999	0.0902	0.0880	0.057*
C5	0.3540 (2)	0.0118 (4)	0.40915 (19)	0.0347 (7)
C6	0.2691 (3)	0.0261 (5)	0.5134 (2)	0.0506 (9)
H6	0.2684	0.0218	0.5690	0.061*
C7	0.1779 (2)	0.0521 (5)	0.4590 (2)	0.0476 (9)
H7	0.1172	0.0670	0.4768	0.057*
C8	0.1826 (2)	0.0548 (4)	0.3780 (2)	0.0390 (8)
H8	0.1231	0.0721	0.3399	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02132 (13)	0.02807 (15)	0.02691 (14)	0.00027 (7)	0.00130 (8)	−0.00120 (8)
N1	0.0284 (12)	0.0439 (15)	0.0309 (14)	−0.0010 (11)	0.0027 (10)	−0.0027 (12)
N2	0.0498 (16)	0.0603 (19)	0.0316 (15)	−0.0003 (14)	0.0091 (12)	−0.0078 (15)
N3	0.0411 (14)	0.0565 (19)	0.0344 (14)	−0.0135 (13)	0.0068 (11)	−0.0118 (14)
N4	0.0259 (11)	0.0400 (15)	0.0300 (13)	0.0013 (10)	0.0007 (10)	−0.0027 (11)
N5	0.0373 (14)	0.068 (2)	0.0273 (14)	0.0051 (13)	−0.0008 (11)	−0.0018 (14)
N6	0.0285 (14)	0.135 (3)	0.0289 (15)	0.0179 (16)	−0.0006 (12)	0.0009 (18)
N7	0.0295 (12)	0.0305 (14)	0.0426 (15)	0.0048 (10)	0.0067 (10)	−0.0004 (12)
N8	0.0287 (11)	0.0337 (14)	0.0438 (15)	0.0006 (11)	0.0109 (11)	0.0013 (12)
O1	0.0241 (10)	0.0641 (18)	0.083 (2)	0.0028 (11)	0.0109 (11)	0.0149 (15)
O2	0.0442 (11)	0.0270 (12)	0.0487 (14)	−0.0064 (9)	−0.0025 (10)	0.0000 (10)
O3	0.0417 (13)	0.0315 (13)	0.112 (3)	0.0132 (11)	0.0204 (14)	0.0121 (15)
O4	0.0369 (11)	0.0470 (14)	0.0571 (15)	0.0023 (10)	−0.0096 (10)	0.0069 (12)
O5	0.0936 (19)	0.0413 (14)	0.0451 (15)	−0.0025 (13)	0.0288 (14)	−0.0077 (12)
O6	0.0562 (15)	0.0451 (15)	0.0617 (18)	0.0282 (12)	0.0039 (13)	0.0021 (13)
O7	0.0255 (9)	0.0335 (11)	0.0384 (11)	0.0016 (8)	0.0069 (8)	0.0045 (10)
O8	0.0296 (10)	0.0326 (12)	0.0763 (18)	−0.0078 (9)	0.0038 (10)	−0.0030 (12)
O9	0.0358 (10)	0.0433 (13)	0.0343 (11)	0.0034 (9)	0.0103 (9)	0.0027 (10)
C1	0.0370 (15)	0.0350 (17)	0.0305 (15)	0.0058 (12)	0.0033 (12)	−0.0055 (13)
C2	0.059 (2)	0.073 (3)	0.0362 (19)	0.0019 (19)	0.0197 (17)	−0.0019 (19)
C3	0.0426 (19)	0.076 (3)	0.048 (2)	−0.0033 (17)	0.0194 (16)	−0.001 (2)
C4	0.0312 (16)	0.066 (3)	0.044 (2)	−0.0030 (15)	0.0043 (14)	−0.0048 (18)
C5	0.0278 (14)	0.0475 (18)	0.0265 (15)	0.0022 (13)	−0.0005 (12)	−0.0014 (14)
C6	0.050 (2)	0.076 (3)	0.0254 (16)	−0.0004 (18)	0.0075 (15)	−0.0066 (17)
C7	0.0344 (16)	0.072 (3)	0.0373 (18)	−0.0029 (15)	0.0101 (14)	−0.0116 (18)

C8	0.0235 (14)	0.055 (2)	0.0368 (17)	0.0013 (13)	0.0023 (12)	−0.0070 (15)

Geometric parameters (Å, º)

Cd1—O7	2.3009 (19)	N7—O3	1.239 (3)
Cd1—O8	2.335 (2)	N7—O2	1.244 (3)
Cd1—N1	2.361 (3)	N8—O6	1.216 (3)
Cd1—N4	2.399 (3)	N8—O5	1.249 (3)
Cd1—O4	2.407 (2)	N8—O4	1.260 (3)
Cd1—O2	2.512 (2)	O7—H7A	0.8500
Cd1—O1	2.640 (3)	O7—H7B	0.8500
N1—C4	1.335 (4)	O8—H8A	0.8500
N1—C1	1.355 (4)	O8—H8B	0.8501
N2—C2	1.324 (5)	O9—H9A	0.8500
N2—C1	1.353 (4)	O9—H9B	0.8500
N3—C1	1.332 (4)	C2—C3	1.373 (6)
N3—H3A	0.8600	C2—H2	0.9300
N3—H3B	0.8600	C3—C4	1.370 (5)
N4—C8	1.345 (4)	C3—H3	0.9300
N4—C5	1.349 (4)	C4—H4	0.9300
N5—C6	1.315 (4)	C6—C7	1.390 (5)
N5—C5	1.346 (4)	C6—H6	0.9300
N6—C5	1.347 (4)	C7—C8	1.366 (5)
N6—H6A	0.8600	C7—H7	0.9300
N6—H6B	0.8600	C8—H8	0.9300
N7—O1	1.239 (3)		
O7—Cd1—O8	161.47 (8)	O6—N8—O5	120.7 (3)
O7—Cd1—N1	97.74 (8)	O6—N8—O4	120.3 (3)
O8—Cd1—N1	89.28 (9)	O5—N8—O4	119.0 (3)
O7—Cd1—N4	89.33 (8)	N7—O1—Cd1	92.53 (19)
O8—Cd1—N4	88.35 (9)	N7—O2—Cd1	98.61 (16)
N1—Cd1—N4	164.13 (9)	N8—O4—Cd1	107.6 (2)
O7—Cd1—O4	85.94 (8)	Cd1—O7—H7A	115.3
O8—Cd1—O4	75.54 (8)	Cd1—O7—H7B	119.7
N1—Cd1—O4	110.25 (9)	H7A—O7—H7B	108.3
N4—Cd1—O4	84.32 (9)	Cd1—O8—H8A	140.2
O7—Cd1—O2	121.01 (7)	Cd1—O8—H8B	110.1
O8—Cd1—O2	77.26 (8)	H8A—O8—H8B	108.3
N1—Cd1—O2	76.42 (8)	H9A—O9—H9B	108.8
N4—Cd1—O2	87.76 (8)	N3—C1—N2	117.0 (3)
O4—Cd1—O2	151.84 (7)	N3—C1—N1	118.8 (3)
O7—Cd1—O1	71.92 (7)	N2—C1—N1	124.2 (3)
O8—Cd1—O1	126.19 (7)	N2—C2—C3	122.7 (4)
N1—Cd1—O1	82.89 (9)	N2—C2—H2	118.6
N4—Cd1—O1	85.87 (9)	C3—C2—H2	118.6
O4—Cd1—O1	155.85 (7)	C4—C3—C2	116.4 (3)
O2—Cd1—O1	49.10 (6)	C4—C3—H3	121.8

C4—N1—C1	116.0 (3)	C2—C3—H3	121.8
C4—N1—Cd1	116.9 (2)	N1—C4—C3	123.4 (3)
C1—N1—Cd1	126.8 (2)	N1—C4—H4	118.3
C2—N2—C1	117.2 (3)	C3—C4—H4	118.3
C1—N3—H3A	120.0	N5—C5—N6	116.1 (3)
C1—N3—H3B	120.0	N5—C5—N4	125.0 (3)
H3A—N3—H3B	120.0	N6—C5—N4	118.9 (3)
C8—N4—C5	116.1 (3)	N5—C6—C7	123.1 (3)
C8—N4—Cd1	113.3 (2)	N5—C6—H6	118.4
C5—N4—Cd1	130.5 (2)	C7—C6—H6	118.4
C6—N5—C5	116.7 (3)	C8—C7—C6	116.3 (3)
C5—N6—H6A	120.0	C8—C7—H7	121.9
C5—N6—H6B	120.0	C6—C7—H7	121.9
H6A—N6—H6B	120.0	N4—C8—C7	122.8 (3)
O1—N7—O3	121.1 (3)	N4—C8—H8	118.6
O1—N7—O2	119.4 (3)	C7—C8—H8	118.6
O3—N7—O2	119.5 (2)		

O7—Cd1—N1—C4	178.2 (2)	O8—Cd1—O2—N7	172.1 (2)
O8—Cd1—N1—C4	15.4 (3)	N1—Cd1—O2—N7	−95.49 (19)
N4—Cd1—N1—C4	−66.0 (5)	N4—Cd1—O2—N7	83.32 (19)
O4—Cd1—N1—C4	89.7 (3)	O4—Cd1—O2—N7	156.87 (19)
O2—Cd1—N1—C4	−61.7 (2)	O1—Cd1—O2—N7	−3.15 (17)
O1—Cd1—N1—C4	−111.3 (2)	O6—N8—O4—Cd1	−175.1 (2)
O7—Cd1—N1—C1	5.2 (3)	O5—N8—O4—Cd1	5.9 (3)
O8—Cd1—N1—C1	−157.6 (3)	O7—Cd1—O4—N8	−65.67 (19)
N4—Cd1—N1—C1	121.0 (3)	O8—Cd1—O4—N8	114.8 (2)
O4—Cd1—N1—C1	−83.3 (3)	N1—Cd1—O4—N8	31.1 (2)
O2—Cd1—N1—C1	125.4 (3)	N4—Cd1—O4—N8	−155.4 (2)
O1—Cd1—N1—C1	75.8 (3)	O2—Cd1—O4—N8	130.22 (19)
O7—Cd1—N4—C8	−32.6 (2)	O1—Cd1—O4—N8	−88.9 (3)
O8—Cd1—N4—C8	129.0 (2)	C2—N2—C1—N3	−178.9 (3)
N1—Cd1—N4—C8	−149.4 (3)	C2—N2—C1—N1	1.2 (5)
O4—Cd1—N4—C8	53.4 (2)	C4—N1—C1—N3	177.6 (3)
O2—Cd1—N4—C8	−153.7 (2)	Cd1—N1—C1—N3	−9.4 (4)
O1—Cd1—N4—C8	−104.5 (2)	C4—N1—C1—N2	−2.4 (5)
O7—Cd1—N4—C5	146.7 (3)	Cd1—N1—C1—N2	170.6 (2)
O8—Cd1—N4—C5	−51.7 (3)	C1—N2—C2—C3	0.9 (6)
N1—Cd1—N4—C5	29.8 (5)	N2—C2—C3—C4	−1.5 (6)
O4—Cd1—N4—C5	−127.3 (3)	C1—N1—C4—C3	1.7 (5)
O2—Cd1—N4—C5	25.6 (3)	Cd1—N1—C4—C3	−172.0 (3)
O1—Cd1—N4—C5	74.7 (3)	C2—C3—C4—N1	0.1 (6)
O3—N7—O1—Cd1	173.5 (3)	C6—N5—C5—N6	179.7 (4)
O2—N7—O1—Cd1	−5.5 (3)	C6—N5—C5—N4	−0.3 (5)
O7—Cd1—O1—N7	−178.1 (2)	C8—N4—C5—N5	1.3 (5)
O8—Cd1—O1—N7	−2.6 (2)	Cd1—N4—C5—N5	−177.9 (2)
N1—Cd1—O1—N7	81.30 (19)	C8—N4—C5—N6	−178.6 (3)
N4—Cd1—O1—N7	−87.48 (19)	Cd1—N4—C5—N6	2.1 (5)

O4—Cd1—O1—N7	−153.7 (2)	C5—N5—C6—C7	−1.0 (6)
O2—Cd1—O1—N7	3.13 (17)	N5—C6—C7—C8	1.0 (6)
O1—N7—O2—Cd1	5.8 (3)	C5—N4—C8—C7	−1.2 (5)
O3—N7—O2—Cd1	−173.2 (3)	Cd1—N4—C8—C7	178.1 (3)
O7—Cd1—O2—N7	−4.5 (2)	C6—C7—C8—N4	0.1 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O5^{i}	0.86	2.29	3.105 (4)	158
N3—H3*B*···O7	0.86	2.10	2.945 (4)	167
N6—H6*A*···N5^{ii}	0.86	2.20	3.054 (4)	170
N6—H6*B*···O2	0.86	2.19	2.931 (4)	144
N6—H6*B*···O3^{iii}	0.86	2.52	3.171 (4)	133
O7—H7*A*···O9^{iv}	0.85	1.94	2.787 (3)	178
O7—H7*B*···O9^{v}	0.85	1.87	2.724 (3)	178
O8—H8*A*···O3^{vi}	0.85	1.97	2.820 (3)	176
O8—H8*B*···O3^{iii}	0.85	2.09	2.936 (3)	176
O9—H9*A*···O5^{iv}	0.85	2.44	3.255 (3)	162
O9—H9*A*···O7^{iv}	0.85	2.28	2.787 (3)	119
O9—H9*B*···O6^{vii}	0.85	1.99	2.809 (4)	161

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