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Bis(2-aminopyrazine-κN^1)tetraaquacadmium(II) bis(perchlorate)–2-aminopyrazine (1/4)

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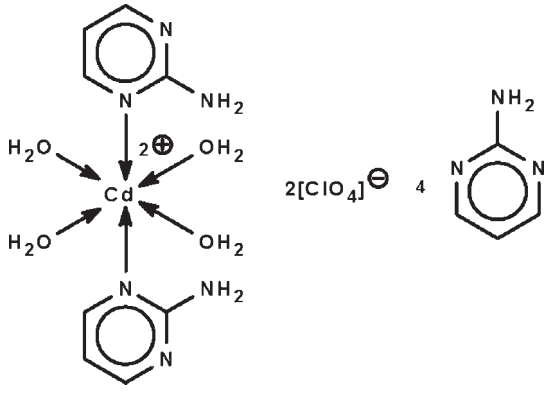
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.072; data-to-parameter ratio = 14.7.

In the title compound, $[Cd(C_4H_5N_3)_2(H_2O)_4](ClO_4)_2\cdot 4C_4H_5N_3$, the Cd^{II} atom (site symmetry $\overline{1}$) is coordinated by two *N*-heterocycles and four water molecules, resulting in a distorted *trans*-CdN_2O_4 octahedral geometry for the metal. In the crystal, the cation, anion and free *N*-heterocycle molecules are linked by N—H···N, N—H···O, O—H···N and O—H···O hydrogen bonds, forming a three-dimensional network.

Related literature

For the cadmium nitrate adduct of 2-aminopyrazine, see: Tai *et al.* (2008).



Experimental

Crystal data

$[Cd(C_4H_5N_3)_2(H_2O)_4](ClO_4)_2\cdot 4C_4H_5N_3$
M_r = 954.02
Monoclinic, $P2_1/c$
a = 8.8912 (2) Å
b = 23.2402 (4) Å
c = 9.3689 (2) Å
β = 96.4263 (7)°
V = 1923.76 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 293 K
0.18 × 0.15 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.871, T_{max} = 0.891
18645 measured reflections
4393 independent reflections
3982 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.072
S = 1.08
4393 reflections
299 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O1*W*	2.282 (1)	Cd1—N1	2.323 (1)
Cd1—O2*W*	2.367 (1)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···N4	0.84 (1)	1.92 (1)	2.758 (2)	171 (3)
O1w—H12···N6^{i}	0.84 (1)	2.24 (1)	3.059 (3)	165 (2)
O2w—H21···N7	0.84 (1)	1.92 (1)	2.756 (2)	178 (3)
O2w—H22···O1	0.84 (1)	1.98 (1)	2.806 (2)	167 (3)
N3—H31···O2w^{ii}	0.85 (1)	2.28 (1)	3.070 (2)	154 (2)
N3—H32···N5^{iii}	0.85 (1)	2.28 (1)	3.127 (2)	175 (2)
N6—H61···N2^{iii}	0.85 (1)	2.23 (1)	3.071 (2)	173 (2)
N6—H62···O2^{i}	0.85 (1)	2.35 (1)	3.140 (2)	155 (2)
N9—H91···O3^{iv}	0.85 (1)	2.20 (1)	3.009 (4)	159 (3)
N9—H92···O4	0.85 (1)	2.41 (2)	3.073 (3)	135 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5230).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tai, X.-S., Feng, Y.-M. & Wang, L.-T. (2008). *Acta Cryst.* E**64**, m537.
Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

Acta Cryst. (2009). E**65**, m1634 [doi:10.1107/S1600536809048387]

Bis(2-aminopyrazine-κN^1)tetraaquacadmium(II) bis(perchlorate)–2-aminopyrazine (1/4)

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S1. Experimental

To an aqueous solution of 2-aminopyrimidine (0.19 g, 2 mmol) was added cadmium perchlorate hydrate (0.662 g, 2 mmol). Colorless prisms of (I) separated from the solution after a few days.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H = 0.93 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C). The amino and water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of N–H = O–H = 0.85±0.01 Å; their U_{iso} values were refined.

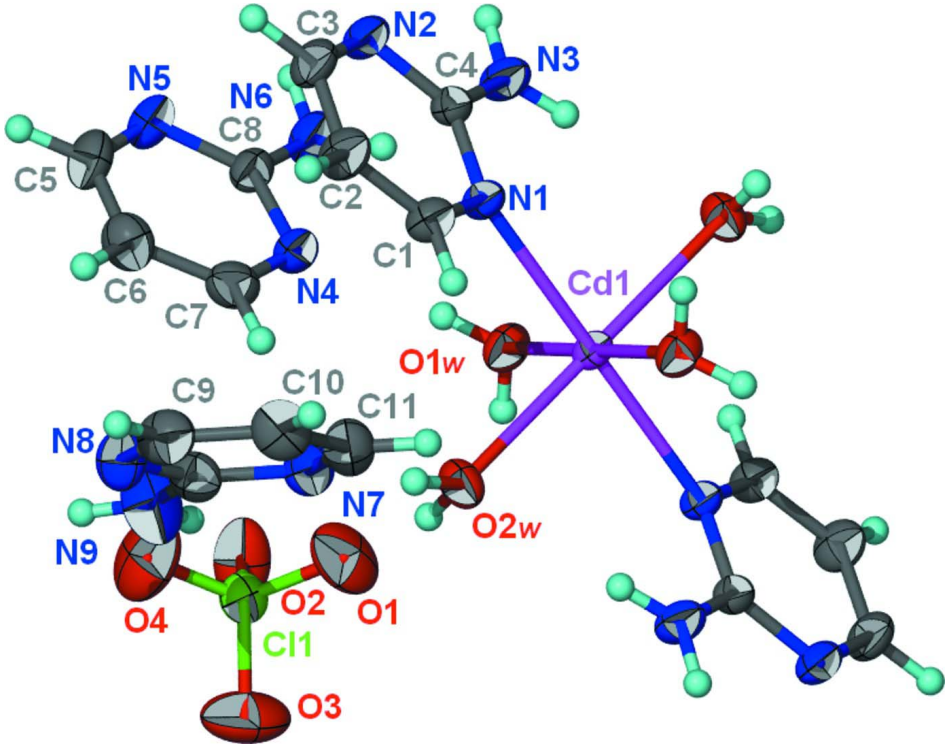

Figure 1

The molecular structure of (I) shown at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. Unlabelled atoms are generated by the symmetry operation (1–x, 1–y, 1–z).

Bis(2-aminopyrazine-κN^1)tetraaquacadmium(II) bis(perchlorate)–2-aminopyrazine (1/4)

Crystal data

$[Cd(C_4H_5N_3)_2(H_2O)_4](ClO_4)_2\cdot 4C_4H_5N_3$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.8912$ (2) Å
$b = 23.2402$ (4) Å
$c = 9.3689$ (2) Å
$\beta = 96.4263$ (7)°
$V = 1923.76$ (7) Å^3
$Z = 2$
$F(000) = 972$
$D_x = 1.647$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 16676 reflections
$\theta = 3.0$–$27.5°$
$\mu = 0.79$ mm^{-1}
$T = 293$ K
Prism, colorless
0.18 × 0.15 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.871$, $T_{max} = 0.891$
18645 measured reflections
4393 independent reflections
3982 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -11\rightarrow 11$
$k = -30\rightarrow 30$
$l = -12\rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.072$
$S = 1.08$
4393 reflections
299 parameters
10 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.6531P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.58$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.5000	0.5000	0.02847 (7)
Cl1	0.09644 (5)	0.653770 (19)	0.68436 (5)	0.04031 (11)
O1	0.2212 (2)	0.61643 (9)	0.6674 (2)	0.0791 (6)
O2	−0.03933 (19)	0.62083 (7)	0.6713 (2)	0.0740 (5)
O3	0.1197 (3)	0.67800 (11)	0.8235 (2)	0.0915 (7)
O4	0.0861 (3)	0.69789 (9)	0.5810 (2)	0.0915 (7)
O1W	0.24457 (16)	0.49525 (6)	0.50677 (16)	0.0390 (3)
H11	0.191 (3)	0.5138 (10)	0.443 (2)	0.058 (7)*
H12	0.214 (3)	0.5019 (9)	0.5870 (18)	0.057 (8)*
O2W	0.50795 (16)	0.59683 (5)	0.57870 (14)	0.0396 (3)
H21	0.534 (3)	0.6274 (7)	0.541 (3)	0.067 (8)*
H22	0.4296 (19)	0.6048 (11)	0.618 (3)	0.064 (8)*

N1	0.46982 (16)	0.52799 (6)	0.26042 (14)	0.0307 (3)
N2	0.33224 (18)	0.53698 (7)	0.02729 (15)	0.0390 (3)
N3	0.29425 (19)	0.45974 (7)	0.17037 (16)	0.0410 (3)
H31	0.322 (3)	0.4384 (8)	0.2423 (18)	0.052 (6)*
H32	0.235 (2)	0.4467 (9)	0.1011 (18)	0.047 (6)*
N4	0.09370 (18)	0.56440 (7)	0.29843 (16)	0.0388 (3)
N5	−0.08831 (18)	0.58548 (7)	0.09866 (17)	0.0442 (4)
N6	−0.0911 (2)	0.49855 (7)	0.2172 (2)	0.0469 (4)
H61	−0.151 (2)	0.4875 (10)	0.1456 (19)	0.048 (6)*
H62	−0.031 (2)	0.4731 (8)	0.256 (3)	0.055 (7)*
N7	0.5948 (2)	0.69581 (7)	0.44802 (18)	0.0450 (4)
N8	0.5465 (2)	0.78730 (7)	0.3350 (2)	0.0517 (4)
N9	0.3655 (3)	0.74176 (11)	0.4486 (3)	0.0756 (7)
H91	0.304 (3)	0.7695 (9)	0.432 (3)	0.077 (9)*
H92	0.329 (3)	0.7163 (10)	0.500 (3)	0.079 (9)*
C1	0.5453 (2)	0.57603 (8)	0.23394 (18)	0.0374 (4)
H1	0.6196	0.5892	0.3041	0.045*
C2	0.5189 (2)	0.60663 (8)	0.1092 (2)	0.0445 (4)
H2	0.5728	0.6398	0.0927	0.053*
C3	0.4069 (2)	0.58525 (9)	0.00885 (19)	0.0436 (4)
H3	0.3827	0.6058	−0.0758	0.052*
C4	0.3672 (2)	0.50879 (7)	0.15276 (18)	0.0314 (3)
C5	−0.0272 (3)	0.63751 (9)	0.0928 (2)	0.0507 (5)
H5	−0.0691	0.6630	0.0228	0.061*
C6	0.0952 (3)	0.65560 (9)	0.1854 (2)	0.0514 (5)
H6	0.1368	0.6921	0.1791	0.062*
C7	0.1519 (2)	0.61674 (9)	0.2871 (2)	0.0456 (4)
H7	0.2347	0.6274	0.3512	0.055*
C8	−0.02538 (19)	0.55082 (8)	0.20305 (18)	0.0351 (3)
C9	0.6867 (3)	0.78674 (9)	0.3004 (2)	0.0515 (5)
H9	0.7190	0.8176	0.2485	0.062*
C10	0.7873 (3)	0.74272 (10)	0.3375 (3)	0.0541 (5)
H10	0.8859	0.7435	0.3134	0.065*
C11	0.7340 (2)	0.69784 (9)	0.4116 (2)	0.0506 (5)
H11A	0.7989	0.6673	0.4377	0.061*
C12	0.5058 (2)	0.74143 (8)	0.4095 (2)	0.0443 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03046 (10)	0.03085 (10)	0.02343 (9)	−0.00094 (6)	0.00002 (6)	0.00250 (5)
Cl1	0.0351 (2)	0.0404 (2)	0.0463 (2)	0.00001 (17)	0.00821 (17)	0.00029 (18)
O1	0.0470 (9)	0.0858 (13)	0.1065 (15)	0.0166 (9)	0.0179 (9)	−0.0229 (11)
O2	0.0410 (8)	0.0577 (10)	0.1204 (16)	−0.0111 (7)	−0.0042 (9)	0.0201 (10)
O3	0.0815 (14)	0.1346 (19)	0.0612 (11)	−0.0055 (13)	0.0194 (10)	−0.0369 (12)
O4	0.1003 (16)	0.0766 (13)	0.0950 (15)	−0.0187 (11)	−0.0007 (12)	0.0428 (11)
O1W	0.0313 (6)	0.0494 (8)	0.0356 (7)	0.0028 (5)	0.0013 (5)	0.0050 (5)
O2W	0.0476 (7)	0.0292 (6)	0.0440 (7)	0.0020 (5)	0.0133 (6)	0.0006 (5)

N1	0.0335 (7)	0.0336 (7)	0.0243 (6)	−0.0003 (5)	0.0007 (5)	0.0016 (5)
N2	0.0413 (8)	0.0463 (8)	0.0276 (6)	0.0034 (6)	−0.0034 (6)	0.0030 (6)
N3	0.0487 (9)	0.0396 (8)	0.0320 (7)	−0.0089 (7)	−0.0069 (7)	0.0004 (6)
N4	0.0375 (8)	0.0432 (8)	0.0338 (7)	0.0055 (6)	−0.0039 (6)	−0.0007 (6)
N5	0.0398 (8)	0.0505 (9)	0.0401 (8)	0.0005 (7)	−0.0047 (6)	0.0119 (7)
N6	0.0480 (10)	0.0432 (9)	0.0463 (10)	−0.0037 (7)	−0.0091 (8)	0.0079 (7)
N7	0.0522 (10)	0.0364 (8)	0.0461 (9)	−0.0054 (7)	0.0046 (7)	0.0029 (7)
N8	0.0538 (10)	0.0419 (9)	0.0593 (10)	−0.0003 (8)	0.0061 (8)	0.0089 (8)
N9	0.0579 (13)	0.0616 (14)	0.113 (2)	0.0022 (11)	0.0351 (13)	0.0136 (13)
C1	0.0378 (9)	0.0410 (9)	0.0325 (8)	−0.0051 (7)	0.0009 (7)	0.0019 (7)
C2	0.0506 (11)	0.0431 (10)	0.0397 (9)	−0.0076 (8)	0.0054 (8)	0.0101 (8)
C3	0.0505 (11)	0.0491 (10)	0.0307 (8)	0.0048 (8)	0.0027 (7)	0.0111 (7)
C4	0.0327 (8)	0.0350 (8)	0.0264 (7)	0.0046 (6)	0.0022 (6)	−0.0012 (6)
C5	0.0529 (12)	0.0493 (11)	0.0491 (11)	0.0058 (9)	0.0018 (9)	0.0169 (9)
C6	0.0549 (12)	0.0396 (10)	0.0602 (12)	−0.0035 (9)	0.0084 (10)	0.0019 (9)
C7	0.0423 (10)	0.0480 (10)	0.0455 (10)	−0.0015 (8)	0.0006 (8)	−0.0093 (8)
C8	0.0323 (8)	0.0416 (9)	0.0311 (8)	0.0040 (7)	0.0022 (6)	0.0019 (7)
C9	0.0599 (13)	0.0458 (10)	0.0491 (11)	−0.0110 (9)	0.0079 (9)	0.0050 (9)
C10	0.0427 (11)	0.0554 (12)	0.0649 (13)	−0.0085 (9)	0.0098 (10)	−0.0018 (10)
C11	0.0462 (11)	0.0441 (10)	0.0597 (12)	0.0000 (8)	−0.0018 (9)	−0.0013 (9)
C12	0.0478 (10)	0.0378 (9)	0.0475 (10)	−0.0050 (8)	0.0061 (8)	−0.0028 (8)

Geometric parameters (Å, º)

Cd1—O1W	2.282 (1)	N6—C8	1.361 (2)
Cd1—O2W	2.367 (1)	N6—H61	0.85 (1)
Cd1—O1W^{i}	2.282 (1)	N6—H62	0.85 (1)
Cd1—N1^{i}	2.323 (1)	N7—C11	1.321 (3)
Cd1—N1	2.323 (1)	N7—C12	1.348 (3)
Cd1—O2W^{i}	2.367 (1)	N8—C9	1.323 (3)
Cl1—O4	1.406 (2)	N8—C12	1.345 (3)
Cl1—O3	1.414 (2)	N9—C12	1.338 (3)
Cl1—O2	1.423 (2)	N9—H91	0.85 (1)
Cl1—O1	1.431 (2)	N9—H92	0.85 (1)
O1W—H11	0.84 (1)	C1—C2	1.366 (2)
O1W—H12	0.84 (1)	C1—H1	0.9300
O2W—H21	0.84 (1)	C2—C3	1.383 (3)
O2W—H22	0.84 (1)	C2—H2	0.9300
N1—C1	1.340 (2)	C3—H3	0.9300
N1—C4	1.358 (2)	C5—C6	1.380 (3)
N2—C3	1.324 (3)	C5—H5	0.9300
N2—C4	1.351 (2)	C6—C7	1.367 (3)
N3—C4	1.331 (2)	C6—H6	0.9300
N3—H31	0.85 (1)	C7—H7	0.9300
N3—H32	0.85 (1)	C9—C10	1.378 (3)
N4—C7	1.331 (3)	C9—H9	0.9300
N4—C8	1.344 (2)	C10—C11	1.367 (3)
N5—C5	1.329 (3)	C10—H10	0.9300

N5—C8	1.340 (2)	C11—H11A	0.9300
O1W—Cd1—O1W^{i}	180.0	C9—N8—C12	115.77 (18)
O1W—Cd1—N1^{i}	88.13 (5)	C12—N9—H91	124 (2)
O1W^{i}—Cd1—N1^{i}	91.87 (5)	C12—N9—H92	125 (2)
O1W—Cd1—N1	91.87 (5)	H91—N9—H92	111 (3)
O1W^{i}—Cd1—N1	88.13 (5)	N1—C1—C2	123.39 (16)
N1^{i}—Cd1—N1	180.0	N1—C1—H1	118.3
O1W—Cd1—O2W^{i}	88.14 (5)	C2—C1—H1	118.3
O1W^{i}—Cd1—O2W^{i}	91.86 (5)	C1—C2—C3	115.88 (17)
N1^{i}—Cd1—O2W^{i}	91.78 (5)	C1—C2—H2	122.1
N1—Cd1—O2W^{i}	88.22 (5)	C3—C2—H2	122.1
O1W—Cd1—O2W	91.86 (5)	N2—C3—C2	123.28 (16)
O1W^{i}—Cd1—O2W	88.14 (5)	N2—C3—H3	118.4
N1^{i}—Cd1—O2W	88.22 (5)	C2—C3—H3	118.4
N1—Cd1—O2W	91.78 (5)	N3—C4—N2	117.09 (16)
O2W^{i}—Cd1—O2W	180.0	N3—C4—N1	119.05 (15)
O4—Cl1—O3	109.65 (15)	N2—C4—N1	123.85 (16)
O4—Cl1—O2	110.08 (12)	N5—C5—C6	123.28 (18)
O3—Cl1—O2	109.20 (14)	N5—C5—H5	118.4
O4—Cl1—O1	110.95 (15)	C6—C5—H5	118.4
O3—Cl1—O1	107.97 (14)	C7—C6—C5	116.11 (19)
O2—Cl1—O1	108.96 (12)	C7—C6—H6	121.9
Cd1—O1W—H11	116.4 (19)	C5—C6—H6	121.9
Cd1—O1W—H12	116 (2)	N4—C7—C6	122.90 (18)
H11—O1W—H12	109 (3)	N4—C7—H7	118.5
Cd1—O2W—H21	132.5 (19)	C6—C7—H7	118.5
Cd1—O2W—H22	110.3 (18)	N5—C8—N4	125.27 (17)
H21—O2W—H22	106 (3)	N5—C8—N6	117.33 (16)
C1—N1—C4	116.43 (14)	N4—C8—N6	117.34 (16)
C1—N1—Cd1	113.95 (10)	N8—C9—C10	123.3 (2)
C4—N1—Cd1	128.40 (11)	N8—C9—H9	118.4
C3—N2—C4	117.02 (15)	C10—C9—H9	118.4
C4—N3—H31	119.6 (16)	C11—C10—C9	116.3 (2)
C4—N3—H32	119.0 (15)	C11—C10—H10	121.9
H31—N3—H32	120 (2)	C9—C10—H10	121.9
C7—N4—C8	116.48 (16)	N7—C11—C10	123.1 (2)
C5—N5—C8	115.96 (16)	N7—C11—H11A	118.4
C8—N6—H61	115.5 (17)	C10—C11—H11A	118.4
C8—N6—H62	114.2 (18)	N9—C12—N8	116.8 (2)
H61—N6—H62	116 (2)	N9—C12—N7	117.91 (19)
C11—N7—C12	116.22 (17)	N8—C12—N7	125.3 (2)
O1W—Cd1—N1—C1	127.25 (12)	Cd1—N1—C4—N2	162.47 (13)
O1W^{i}—Cd1—N1—C1	−52.75 (12)	C8—N5—C5—C6	1.1 (3)
O2W^{i}—Cd1—N1—C1	−144.67 (12)	N5—C5—C6—C7	−0.5 (3)
O2W—Cd1—N1—C1	35.33 (12)	C8—N4—C7—C6	0.4 (3)
O1W—Cd1—N1—C4	−39.56 (14)	C5—C6—C7—N4	−0.3 (3)

O1W^{i}—Cd1—N1—C4	140.44 (14)	C5—N5—C8—N4	−1.1 (3)
O2W^{i}—Cd1—N1—C4	48.52 (14)	C5—N5—C8—N6	176.16 (19)
O2W—Cd1—N1—C4	−131.48 (14)	C7—N4—C8—N5	0.3 (3)
C4—N1—C1—C2	2.8 (3)	C7—N4—C8—N6	−176.88 (18)
Cd1—N1—C1—C2	−165.63 (16)	C12—N8—C9—C10	−0.3 (3)
N1—C1—C2—C3	0.3 (3)	N8—C9—C10—C11	1.1 (3)
C4—N2—C3—C2	1.5 (3)	C12—N7—C11—C10	−0.8 (3)
C1—C2—C3—N2	−2.6 (3)	C9—C10—C11—N7	−0.4 (3)
C3—N2—C4—N3	−178.82 (18)	C9—N8—C12—N9	178.4 (2)
C3—N2—C4—N1	2.0 (3)	C9—N8—C12—N7	−1.1 (3)
C1—N1—C4—N3	176.72 (17)	C11—N7—C12—N9	−177.8 (2)
Cd1—N1—C4—N3	−16.7 (2)	C11—N7—C12—N8	1.7 (3)
C1—N1—C4—N2	−4.1 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···N4	0.84 (1)	1.92 (1)	2.758 (2)	171 (3)
O1w—H12···N6^{ii}	0.84 (1)	2.24 (1)	3.059 (3)	165 (2)
O2w—H21···N7	0.84 (1)	1.92 (1)	2.756 (2)	178 (3)
O2w—H22···O1	0.84 (1)	1.98 (1)	2.806 (2)	167 (3)
N3—H31···O2w^{i}	0.85 (1)	2.28 (1)	3.070 (2)	154 (2)
N3—H32···N5^{iii}	0.85 (1)	2.28 (1)	3.127 (2)	175 (2)
N6—H61···N2^{iii}	0.85 (1)	2.23 (1)	3.071 (2)	173 (2)
N6—H62···O2^{ii}	0.85 (1)	2.35 (1)	3.140 (2)	155 (2)
N9—H91···O3^{iv}	0.85 (1)	2.20 (1)	3.009 (4)	159 (3)
N9—H92···O4	0.85 (1)	2.41 (2)	3.073 (3)	135 (3)

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