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Diaquabis(nitrato-κ^2O,O')bis(pyrazine-2-carboxamide-κN^4)cadmium–pyrazine-2-carboxamide (1/2)

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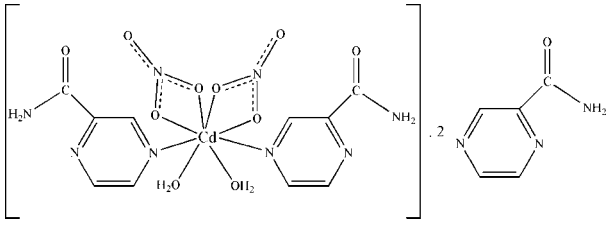
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.069; data-to-parameter ratio = 17.4.

In the title compound, $[Cd(NO_3)_2(C_5H_5N_3O)_2(H_2O)_2]\cdot 2C_5H_5N_3O$, the Cd^{II} cation is located on a twofold rotation axis and is coordinated by two pyrazine-2-carboxamide ligands and two water molecules and chelated by two nitrate anions in a distorted square-antiprismatic geometry. Extensive intermolecular N—H···O, N—H···N, O—H···O and O—H···N hydrogen bonds, as well as weak intermolecular C—H···N and C—H···O interactions occur in the crystal. π–π stacking between between pyrazine rings of coordinating ligands and lattice molecules [centroid–centroid distance = 3.5669 (14) Å] may further stabilize the structure.

Related literature

For related structures, see: Abu-Youssef *et al.* (2006); Azhdari Tehrani *et al.* (2010); Goher & Mautner (2000); Kristiansson (2002); Mir Mohammad Sadegh *et al.* (2010); Munakata *et al.* (1997); Pacigova *et al.* (2008); Shirvan & Haydari Dezfuli (2012*a*,*b*,*c*).



Experimental

Crystal data

$[Cd(NO_3)_2(C_5H_5N_3O)_2(H_2O)_2]\cdot 2C_5H_5N_3O$
M_r = 764.94
Monoclinic, $C2/c$
a = 13.5650 (5) Å
b = 6.7845 (3) Å
c = 31.2031 (11) Å
β = 95.665 (3)°
V = 2857.65 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 298 K
0.22 × 0.21 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.835, T_{max} = 0.865
15388 measured reflections
3850 independent reflections
3099 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.069
S = 1.02
3850 reflections
221 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O3	2.386 (2)	Cd1—O5	2.469 (2)
Cd1—O4	2.529 (2)	Cd1—N2	2.3459 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3D···N6^{i}	0.82 (1)	2.13 (1)	2.937 (3)	169 (4)
O3—H3E···O5^{ii}	0.82 (3)	2.44 (3)	3.215 (4)	158 (3)
O3—H3E···O6^{ii}	0.82 (3)	2.39 (3)	3.130 (3)	150 (3)
N3—H3B···O2	0.86	2.22	3.072 (3)	170
N3—H3C···O2^{iii}	0.86	2.30	2.987 (3)	137
N4—H4A···N5^{iv}	0.86	2.50	3.180 (3)	137
N4—H4B···O1	0.86	1.97	2.832 (3)	179
C6—H6···N1^{iii}	0.93	2.57	3.364 (4)	143
C8—H8···O1^{iv}	0.93	2.57	3.429 (3)	155

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We are grateful to the Islamic Azad University, Omidieh Branch, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5577).

References

Abu-Youssef, M. A. M., Escuer, A. & Langer, V. (2006). *Eur. J. Inorg. Chem.* pp. 3177–3184.
Azhdari Tehrani, A., Mir Mohammad Sadegh, B. & Khavasi, H. R. (2010). *Acta Cryst.* E**66**, m261.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Goher, M. A. S. & Mautner, F. A. (2000). *Polyhedron*, **19**, 601–606.
Kristiansson, O. (2002). *Acta Cryst.* E**58**, m130–m132.
Mir Mohammad Sadegh, B., Azhdari Tehrani, A. & Khavasi, H. R. (2010). *Acta Cryst.* E**66**, m158.
Munakata, M., Wu, L. P., Sowa, T. K., Maekawa, M., Moriwaki, K. & Kitagawa, S. (1997). *Inorg. Chem.* **36**, 5416–5418.

Pacigova, S., Gyepes, R., Tatiersky, J. & Sivak, M. (2008). *Dalton Trans*. pp. 121–130.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shirvan, S. A. & Haydari Dezfuli, S. (2012*a*). *Acta Cryst.* E**68**, m527.
Shirvan, S. A. & Haydari Dezfuli, S. (2012*b*). *Acta Cryst.* E**68**, m627–m628.
Shirvan, S. A. & Haydari Dezfuli, S. (2012*c*). *Acta Cryst.* E**68**, m546.

supporting information

Acta Cryst. (2012). E**68**, m1008–m1009 [https://doi.org/10.1107/S1600536812028577]

Diaquabis(nitrato-κ^2O,O')bis(pyrazine-2-carboxamide-κN^4)cadmium–pyrazine-2-carboxamide (1/2)

Sadif A. Shirvan and Sara Haydari Dezfuli

S1. Comment

Pyrazine-2-carboxamide (pzc), is a good ligand, and a few complexes with pzc have been prepared, such as that of mercury (Azhdari Tehrani *et al.*, 2010; Mir Mohammad Sadegh *et al.*, 2010), vanadium (Pacigova *et al.*, 2008), manganese (Abu-Youssef *et al.*, 2006), copper (Kristiansson, 2002; Munakata *et al.*, 1997; Goher & Mautner, 2000) and zinc (Shirvan & Haydari Dezfuli, 2012*a*,*b*,*c*). Here, we report the synthesis and structure of the title compound.

The asymmetric unit of the title compound, (Fig. 1), contains one half of Cd^{II} atom, one coordinated pyrazine-2-carboxamide ligand, one water molecule, one nitrate anion and one none coordinated pyrazine-2-carboxamide. The Cd^{II} atom is eight-coordinated by two N atoms from two pyrazine-2-carboxamide ligands, two O atoms from two water molecules and four O atoms from two nitrate anions. The Cd—O and Cd—N bond lengths and angles are collected in Table 1.

In the crystal structure, intra and intermolecular N—H···O, N—H···N, O—H···O, C—H···N and C—H···O hydrogen bonds (Table 2) and π-π contacts (Fig. 2) between the pyrazine rings, *Cg*1—*Cg*2^{i} [symmetry cods: (i) 1-*X*,-Y,1-*Z*, where *Cg*1 and *Cg*2 are centroids of the rings (N1/C2—C3/N2/C1/C4) and (N5/C7—C8/N6/C6/C9), respectively] may stabilize the structure, with centroid-centroid distance of 3.5669 (14) Å.

S2. Experimental

A solution of pyrazine-2-carboxamide (0.50 g, 4.0 mmol) in methanol (10 ml) was added to a solution of $Cd(NO_3)_2.4H_2O$ (0.31 g, 1.0 mmol) in methanol (10 ml) and the resulting colorless solution was stirred for 15 min at room temperature. This solution was left to evaporate slowly at room temperature. After one week, colorless block crystals of the title compound were isolated (yield 0.56 g, 73.2%).

S3. Refinement

H atoms were positioned geometrically with C—H = 0.93 and N—H = 0.86 Å, and constrained to ride on their parent atoms, $U_{iso}(H) = 1.2U_{eq}(N,C)$.

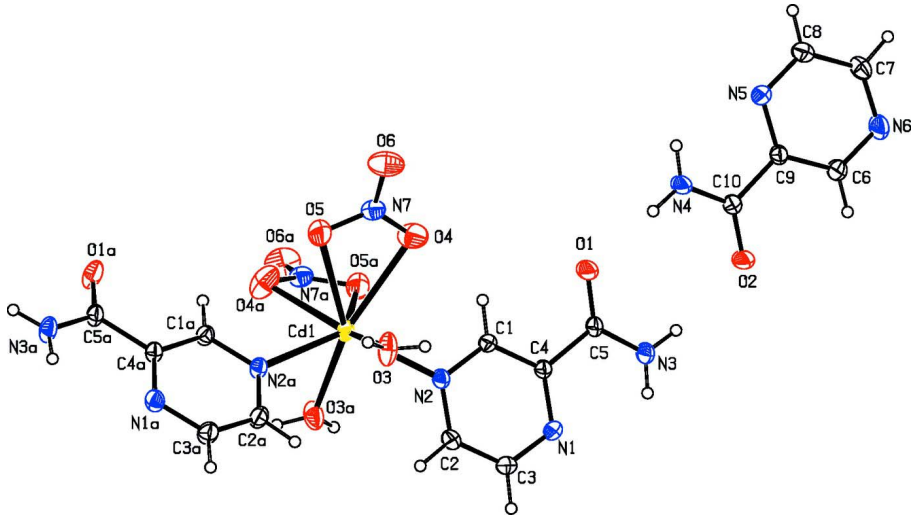


Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (*a*) 1 - *x*,*y*,3/2 - *z*].

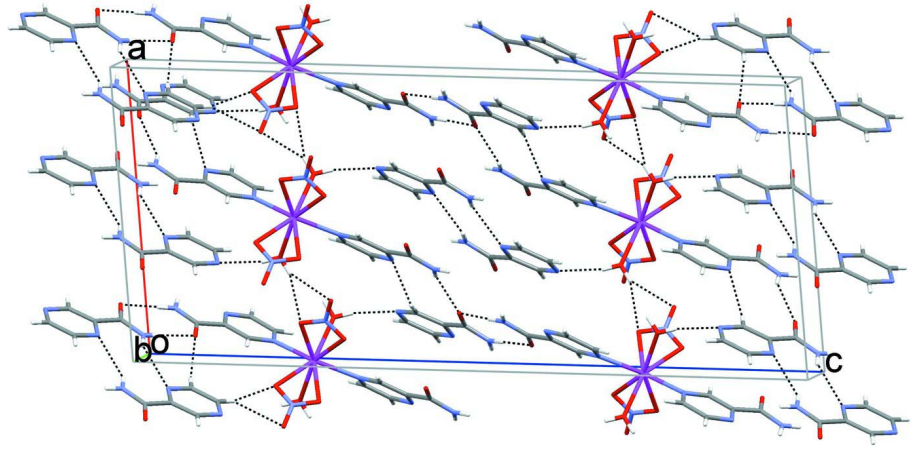


Figure 2

Unit-cell packing diagram for title molecule. Hydrogen bonds are shown as dashed lines.

Diaquabis(nitrato-κ^2O,O')bis(pyrazine-2- carboxamide-κN^4)cadmium–pyrazine-2-carboxamide (1/2)

Crystal data

$[Cd(NO_3)_2(C_5H_5N_3O)_2(H_2O)_2]\cdot 2C_5H_5N_3O$
$M_r = 764.94$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 13.5650\ (5)$ Å
$b = 6.7845\ (3)$ Å
$c = 31.2031\ (11)$ Å
$\beta = 95.665\ (3)°$
$V = 2857.65\ (19)$ Å^3
$Z = 4$
$F(000) = 1544$
$D_x = 1.778$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 15388 reflections
$\theta = 2.6–29.2°$
$\mu = 0.85$ mm^{-1}
$T = 298$ K
Block, colorless
0.22 × 0.21 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.835, T_{max} = 0.865
15388 measured reflections
3850 independent reflections
3099 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 29.2°, θ_{min} = 2.6°
h = −15→18
k = −9→9
l = −42→42

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.069
S = 1.02
3850 reflections
221 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 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}
C1	0.56965 (17)	0.2539 (3)	0.65471 (7)	0.0297 (5)
H1	0.5493	0.1230	0.6550	0.036*
C2	0.5882 (2)	0.5543 (3)	0.68646 (8)	0.0360 (6)
H2	0.5799	0.6396	0.7092	0.043*
C3	0.6311 (2)	0.6240 (4)	0.65109 (8)	0.0388 (6)
H3	0.6524	0.7543	0.6510	0.047*
C4	0.61084 (17)	0.3260 (3)	0.61922 (7)	0.0271 (5)
C5	0.61752 (18)	0.1922 (3)	0.58134 (7)	0.0309 (5)
C6	0.6697 (2)	−0.3057 (4)	0.40570 (8)	0.0409 (6)
H6	0.6978	−0.1827	0.4018	0.049*
C7	0.6301 (2)	−0.6120 (4)	0.38209 (9)	0.0407 (6)
H7	0.6307	−0.7109	0.3615	0.049*
C8	0.5894 (2)	−0.6511 (4)	0.41992 (9)	0.0401 (6)
H8	0.5617	−0.7745	0.4237	0.048*
C9	0.63094 (18)	−0.3443 (3)	0.44398 (7)	0.0294 (5)

C10	0.63336 (19)	−0.1919 (3)	0.47903 (8)	0.0323 (5)
N1	0.64298 (17)	0.5111 (3)	0.61710 (7)	0.0349 (5)
N2	0.55839 (15)	0.3686 (3)	0.68886 (6)	0.0288 (4)
N3	0.66404 (16)	0.2610 (3)	0.54907 (6)	0.0400 (5)
H3B	0.6688	0.1894	0.5266	0.048*
H3C	0.6895	0.3772	0.5506	0.048*
N4	0.58381 (19)	−0.2357 (3)	0.51183 (7)	0.0473 (6)
H4B	0.5827	−0.1543	0.5329	0.057*
H4A	0.5525	−0.3458	0.5122	0.057*
N5	0.58844 (17)	−0.5180 (3)	0.45120 (7)	0.0357 (5)
N6	0.66844 (19)	−0.4378 (4)	0.37415 (7)	0.0457 (6)
N7	0.35495 (17)	−0.0688 (3)	0.72058 (7)	0.0381 (5)
O1	0.57917 (17)	0.0284 (3)	0.58187 (6)	0.0502 (5)
O2	0.68015 (15)	−0.0373 (3)	0.47604 (6)	0.0452 (5)
O3	0.35625 (17)	0.3987 (4)	0.72005 (7)	0.0526 (5)
H3D	0.341 (3)	0.410 (5)	0.6940 (4)	0.068 (11)*
H3E	0.3053 (18)	0.407 (6)	0.7322 (12)	0.085 (14)*
O4	0.41705 (19)	−0.0161 (3)	0.69628 (8)	0.0698 (7)
O5	0.3670 (2)	−0.0147 (3)	0.75901 (7)	0.0651 (7)
O6	0.28421 (17)	−0.1698 (3)	0.70757 (9)	0.0702 (7)
Cd1	0.5000	0.22584 (4)	0.7500	0.03053 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0371 (12)	0.0264 (11)	0.0269 (10)	−0.0051 (9)	0.0093 (9)	−0.0015 (9)
C2	0.0477 (16)	0.0323 (12)	0.0292 (13)	−0.0037 (11)	0.0087 (11)	−0.0067 (9)
C3	0.0531 (17)	0.0288 (12)	0.0356 (14)	−0.0102 (11)	0.0106 (12)	−0.0035 (10)
C4	0.0290 (12)	0.0297 (11)	0.0230 (11)	−0.0047 (9)	0.0042 (9)	−0.0015 (8)
C5	0.0366 (13)	0.0343 (12)	0.0228 (11)	−0.0046 (10)	0.0078 (10)	−0.0024 (9)
C6	0.0480 (16)	0.0442 (14)	0.0325 (13)	−0.0153 (12)	0.0143 (12)	−0.0046 (11)
C7	0.0437 (16)	0.0435 (14)	0.0354 (14)	0.0006 (12)	0.0059 (12)	−0.0118 (11)
C8	0.0485 (16)	0.0320 (12)	0.0404 (15)	−0.0047 (11)	0.0071 (13)	−0.0063 (10)
C9	0.0299 (12)	0.0347 (11)	0.0238 (11)	−0.0058 (9)	0.0042 (10)	−0.0018 (9)
C10	0.0366 (13)	0.0333 (12)	0.0275 (12)	−0.0060 (10)	0.0047 (10)	−0.0025 (9)
N1	0.0441 (13)	0.0321 (10)	0.0298 (11)	−0.0089 (9)	0.0102 (10)	0.0020 (8)
N2	0.0314 (11)	0.0322 (10)	0.0237 (10)	−0.0026 (8)	0.0072 (8)	−0.0028 (7)
N3	0.0525 (13)	0.0427 (12)	0.0274 (9)	−0.0133 (10)	0.0171 (9)	−0.0060 (9)
N4	0.0688 (15)	0.0409 (12)	0.0364 (11)	−0.0256 (11)	0.0254 (11)	−0.0140 (10)
N5	0.0453 (13)	0.0313 (10)	0.0318 (11)	−0.0063 (9)	0.0096 (10)	−0.0002 (8)
N6	0.0517 (15)	0.0558 (14)	0.0316 (12)	−0.0092 (11)	0.0136 (11)	−0.0071 (10)
N7	0.0377 (13)	0.0308 (11)	0.0468 (14)	−0.0010 (9)	0.0088 (11)	−0.0010 (9)
O1	0.0752 (15)	0.0408 (10)	0.0390 (11)	−0.0237 (10)	0.0281 (10)	−0.0141 (8)
O2	0.0569 (13)	0.0402 (10)	0.0411 (11)	−0.0225 (9)	0.0175 (10)	−0.0087 (8)
O3	0.0475 (14)	0.0815 (15)	0.0305 (11)	0.0188 (11)	0.0128 (10)	0.0083 (10)
O4	0.0758 (17)	0.0646 (14)	0.0773 (17)	−0.0271 (12)	0.0495 (14)	−0.0193 (12)
O5	0.107 (2)	0.0472 (12)	0.0426 (13)	−0.0008 (12)	0.0159 (13)	−0.0011 (9)
O6	0.0452 (13)	0.0619 (14)	0.103 (2)	−0.0182 (11)	0.0033 (13)	−0.0088 (13)

Cd1	0.03867 (15)	0.03185 (13)	0.02309 (12)	0.000	0.01321 (10)	0.000

Geometric parameters (Å, º)

Cd1—O3	2.386 (2)	N3—H3C	0.8600
Cd1—O4	2.529 (2)	N4—C10	1.313 (3)
Cd1—O5	2.469 (2)	N5—C8	1.331 (3)
Cd1—N2	2.3459 (19)	N5—C9	1.341 (3)
Cd1—O3^{i}	2.386 (2)	N6—C7	1.324 (4)
Cd1—O4^{i}	2.529 (2)	N6—C6	1.330 (4)
Cd1—O5^{i}	2.469 (2)	N4—H4B	0.8600
Cd1—N2^{i}	2.3459 (19)	N4—H4A	0.8600
O1—C5	1.228 (3)	C1—C4	1.378 (3)
O4—N7	1.240 (3)	C2—C3	1.381 (4)
O5—N7	1.249 (3)	C4—C5	1.500 (3)
O6—N7	1.216 (3)	C1—H1	0.9300
O3—H3D	0.822 (14)	C2—H2	0.9300
O3—H3E	0.82 (3)	C3—H3	0.9300
O2—C10	1.234 (3)	C6—C9	1.377 (3)
N1—C3	1.331 (3)	C7—C8	1.377 (4)
N1—C4	1.333 (3)	C9—C10	1.503 (3)
N2—C2	1.328 (3)	C6—H6	0.9300
N2—C1	1.340 (3)	C7—H7	0.9300
N3—C5	1.325 (3)	C8—H8	0.9300
N3—H3B	0.8600		

O3—Cd1—O4	76.50 (8)	O5—N7—O6	120.7 (3)
O3—Cd1—O5	77.96 (8)	H3B—N3—H3C	120.00
O3—Cd1—N2	78.87 (7)	C5—N3—H3B	120.00
O3—Cd1—O3^{i}	121.11 (9)	C5—N3—H3C	120.00
O3—Cd1—O4^{i}	150.64 (8)	C8—N5—C9	116.0 (2)
O3—Cd1—O5^{i}	149.14 (8)	C6—N6—C7	116.1 (2)
O3—Cd1—N2^{i}	77.71 (7)	C10—N4—H4B	120.00
O4—Cd1—O5	50.53 (8)	C10—N4—H4A	120.00
O4—Cd1—N2	83.85 (7)	H4A—N4—H4B	120.00
O3^{i}—Cd1—O4	150.64 (8)	N2—C1—C4	121.31 (19)
O4—Cd1—O4^{i}	99.08 (7)	N2—C2—C3	121.7 (2)
O4—Cd1—O5^{i}	77.17 (8)	N1—C3—C2	122.2 (2)
O4—Cd1—N2^{i}	130.02 (8)	C1—C4—C5	118.62 (19)
O5—Cd1—N2	132.42 (7)	N1—C4—C5	119.0 (2)
O3^{i}—Cd1—O5	149.14 (8)	N1—C4—C1	122.3 (2)
O4^{i}—Cd1—O5	77.17 (8)	N3—C5—C4	117.13 (19)
O5—Cd1—O5^{i}	97.26 (8)	O1—C5—C4	118.6 (2)
O5—Cd1—N2^{i}	82.60 (7)	O1—C5—N3	124.3 (2)
O3^{i}—Cd1—N2	77.71 (7)	C4—C1—H1	119.00
O4^{i}—Cd1—N2	130.02 (8)	N2—C1—H1	119.00
O5^{i}—Cd1—N2	82.60 (7)	C3—C2—H2	119.00
N2—Cd1—N2^{i}	131.23 (7)	N2—C2—H2	119.00

O3^{i}—Cd1—O4^{i}	76.50 (8)	C2—C3—H3	119.00
O3^{i}—Cd1—O5^{i}	77.96 (8)	N1—C3—H3	119.00
O3^{i}—Cd1—N2^{i}	78.87 (7)	N6—C6—C9	122.4 (2)
O4^{i}—Cd1—O5^{i}	50.53 (8)	N6—C7—C8	122.0 (3)
O4^{i}—Cd1—N2^{i}	83.85 (7)	N5—C8—C7	122.1 (2)
O5^{i}—Cd1—N2^{i}	132.42 (7)	C6—C9—C10	121.2 (2)
Cd1—O4—N7	93.81 (16)	N5—C9—C6	121.4 (2)
Cd1—O5—N7	96.47 (16)	N5—C9—C10	117.5 (2)
H3D—O3—H3E	108 (4)	O2—C10—N4	123.9 (2)
Cd1—O3—H3D	123 (3)	O2—C10—C9	120.3 (2)
Cd1—O3—H3E	123 (3)	N4—C10—C9	115.8 (2)
C3—N1—C4	115.9 (2)	N6—C6—H6	119.00
C1—N2—C2	116.5 (2)	C9—C6—H6	119.00
Cd1—N2—C1	118.75 (15)	N6—C7—H7	119.00
Cd1—N2—C2	124.53 (16)	C8—C7—H7	119.00
O4—N7—O6	121.3 (2)	N5—C8—H8	119.00
O4—N7—O5	118.0 (2)	C7—C8—H8	119.00

O3—Cd1—O4—N7	−79.22 (16)	Cd1—O4—N7—O6	169.2 (2)
O5—Cd1—O4—N7	6.18 (14)	Cd1—O5—N7—O4	11.0 (2)
N2—Cd1—O4—N7	−159.21 (16)	Cd1—O5—N7—O6	−168.8 (2)
O3^{i}—Cd1—O4—N7	149.72 (17)	C4—N1—C3—C2	0.0 (4)
O4^{i}—Cd1—O4—N7	71.16 (16)	C3—N1—C4—C1	−1.3 (4)
O5^{i}—Cd1—O4—N7	117.01 (16)	C3—N1—C4—C5	177.3 (2)
N2^{i}—Cd1—O4—N7	−18.40 (19)	Cd1—N2—C2—C3	173.36 (19)
O3—Cd1—O5—N7	76.16 (16)	C1—N2—C2—C3	−1.7 (4)
O4—Cd1—O5—N7	−6.16 (14)	Cd1—N2—C1—C4	−174.91 (17)
N2—Cd1—O5—N7	13.7 (2)	C2—N2—C1—C4	0.5 (3)
O3^{i}—Cd1—O5—N7	−151.55 (16)	C8—N5—C9—C10	−178.6 (2)
O4^{i}—Cd1—O5—N7	−119.56 (17)	C9—N5—C8—C7	−1.0 (4)
O5^{i}—Cd1—O5—N7	−72.90 (16)	C8—N5—C9—C6	2.3 (4)
N2^{i}—Cd1—O5—N7	155.10 (17)	C6—N6—C7—C8	3.1 (4)
O3—Cd1—N2—C1	−104.80 (18)	C7—N6—C6—C9	−1.9 (4)
O4—Cd1—N2—C1	−27.40 (17)	N2—C1—C4—C5	−177.5 (2)
O5—Cd1—N2—C1	−42.7 (2)	N2—C1—C4—N1	1.1 (4)
O3^{i}—Cd1—N2—C1	129.63 (18)	N2—C2—C3—N1	1.6 (4)
O4^{i}—Cd1—N2—C1	69.30 (19)	N1—C4—C5—N3	6.2 (3)
O5^{i}—Cd1—N2—C1	50.41 (17)	C1—C4—C5—O1	5.6 (3)
N2^{i}—Cd1—N2—C1	−167.35 (15)	N1—C4—C5—O1	−173.1 (2)
O3—Cd1—N2—C2	80.2 (2)	C1—C4—C5—N3	−175.1 (2)
O4—Cd1—N2—C2	157.6 (2)	N6—C6—C9—N5	−0.9 (4)
O5—Cd1—N2—C2	142.32 (19)	N6—C6—C9—C10	−179.9 (2)
O3^{i}—Cd1—N2—C2	−45.4 (2)	N6—C7—C8—N5	−1.8 (4)
O4^{i}—Cd1—N2—C2	−105.7 (2)	N5—C9—C10—O2	172.7 (2)
O5^{i}—Cd1—N2—C2	−124.6 (2)	N5—C9—C10—N4	−7.1 (3)

N2^{i}—Cd1—N2—C2	17.7 (2)	C6—C9—C10—O2	−8.2 (4)
Cd1—O4—N7—O5	−10.7 (2)	C6—C9—C10—N4	172.0 (2)

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*
O3—H3*D*···N6^{ii}	0.82 (1)	2.13 (1)	2.937 (3)	169 (4)
O3—H3*E*···O5^{iii}	0.82 (3)	2.44 (3)	3.215 (4)	158 (3)
O3—H3*E*···O6^{iii}	0.82 (3)	2.39 (3)	3.130 (3)	150 (3)
N3—H3*B*···O2	0.86	2.22	3.072 (3)	170
N3—H3*C*···O2^{iv}	0.86	2.30	2.987 (3)	137
N4—H4*A*···N5^{v}	0.86	2.50	3.180 (3)	137
N4—H4*B*···O1	0.86	1.97	2.832 (3)	179
C6—H6···N1^{iv}	0.93	2.57	3.364 (4)	143
C8—H8···O1^{v}	0.93	2.57	3.429 (3)	155

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