

Diaquabis[4-(1*H*-imidazol-2-yl)pyridine- κ N]bis(nitrato- κ O)cadmium

Chuan-Yue Zhang, Tao Wang and Chuan-Ming Jin*

Hubei Key Laboratory of Pollutant Analysis & Reuse Technology, College of Chemistry and Environmental Engineering, Hubei Normal University, Huangshi 435002, People's Republic of China

Correspondence e-mail: jinm1999@yahoo.com

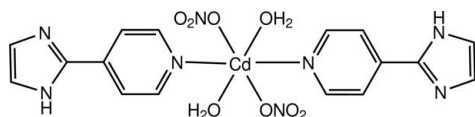
Received 2 December 2012; accepted 14 December 2012

 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.035; wR factor = 0.084; data-to-parameter ratio = 15.7.

In the title compound, $[\text{Cd}(\text{NO}_3)_2(\text{C}_8\text{H}_7\text{N}_3)_2(\text{H}_2\text{O})_2]$, the Cd^{II} cation is situated on an inversion center and is coordinated by the O atoms of two nitrate anions, by the N atoms of two 4-(imidazol-2-yl)pyridine ligands and by two water O atoms in a slightly distorted N_2O_4 octahedral geometry. The dihedral angle between the imidazole and pyridine rings is $1.6(2)^\circ$. In the crystal, molecules are linked by $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{N}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a three-dimensional network.

Related literature

For background to compounds with metal-organic framework (MOF) structures, see: Batten & Robson (1998); Burrows (2011); Jin *et al.* (2010); Tanabe & Cohen (2011). For the use of N,N' -type ligands in MOFs, see: Custelcean (2010); Pschirer *et al.* (2002). For the structural analysis of an imidazole closely related to the ligand, see: Voss *et al.* (2008).



Experimental

Crystal data

$[\text{Cd}(\text{NO}_3)_2(\text{C}_8\text{H}_7\text{N}_3)_2(\text{H}_2\text{O})_2]$
 $M_r = 562.78$
 Monoclinic, $P2_1/n$
 $a = 7.2508(7)$ Å
 $b = 12.1372(12)$ Å
 $c = 12.3509(12)$ Å
 $\beta = 102.278(2)^\circ$

$V = 1062.07(18)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.09$ mm⁻¹
 $T = 298$ K
 $0.16 \times 0.12 \times 0.10$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.845$, $T_{\text{max}} = 0.899$
 6543 measured reflections
 2462 independent reflections
 2272 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.084$
 $S = 1.10$
 2462 reflections
 157 parameters
 3 restraints
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.73$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.47$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N3}-\text{H3}\cdots\text{O3}^{\text{i}}$	0.86	2.10	2.923 (3)	160
$\text{O4}-\text{H4B}\cdots\text{N2}^{\text{ii}}$	0.82 (1)	1.98 (1)	2.796 (3)	174 (4)
$\text{O4}-\text{H4A}\cdots\text{O2}^{\text{iii}}$	0.81 (1)	2.14 (1)	2.946 (4)	174 (4)
$\text{O4}-\text{H4A}\cdots\text{O3}^{\text{iii}}$	0.81 (1)	2.65 (3)	3.197 (3)	126 (3)

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2004); 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.

We gratefully acknowledge financial support by the National Natural Science Foundation of China (21171053) and the Science Foundation of Hubei Provincial Department of Education (Z20102501).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2415).

References

- Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed. Engl.* **37**, 1460–1494.
 Bruker (2004). SAINT-Plus and APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
 Burrows, A. D. (2011). *CrystEngComm*, **13**, 3623–3642.
 Custelcean, R. (2010). *Chem. Soc. Rev.* **39**, 3675–3685.
 Jin, C.-M., Zhu, Z., Chen, Z.-F., Hu, Y.-J. & Meng, X.-G. (2010). *Cryst. Growth Des.* **10**, 2054–2056.
 Pschirer, N. G., Curtin, D. M., Smith, M. D., Bunz, U. H. F. & Zur Loye, H.-C. (2002). *Angew. Chem. Int. Ed. Engl.* **41**, 583–585.
 Sheldrick, G. M. (1996). SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Tanabe, K. K. & Cohen, S. M. (2011). *Chem. Soc. Rev.* **40**, 498–519.
 Voss, M. E., Beer, C. M., Mitchell, S. A., Blomgren, P. A. & Zhichkin, P. E. (2008). *Tetrahedron*, **64**, 645–651.

supporting information

Acta Cryst. (2013). E69, m67 [https://doi.org/10.1107/S1600536812050908]

Diaquabis[4-(1*H*-imidazol-2-yl)pyridine- κ N]bis(nitrato- κ O)cadmium**Chuan-Yue Zhang, Tao Wang and Chuan-Ming Jin****S1. Comment**

The construction of functional metal-organic frameworks is of great interest due to their intriguing network topologies and their potential applications as microporous, magnetism, catalysis, nonlinear optics, molecular separation, toxic materials adsorption and molecular sensors (Batten & Robson, 1998; Burrows, 2011; Jin *et al.*, 2010; Tanabe & Cohen, 2011). The molecular geometry and flexibility of multidentate ligands play key roles in the field of supramolecular self-assembly on metal-organic frameworks. For example, 4, 4'-bipyridine, 1, 2-bis(4-pyridyl)ethane and *trans*-bis(4-pyridyl)ethene as ligands can form a lot of coordination polymers with different structure features (Custelcean, 2010; Pschirer *et al.*, 2002). Our interest is to exploit the coordination chemistry of 2-pyridinyl-imidazole and its derivatives together with their potential application in material science.

In the report, the mono-nuclear cadmium(II) complex, $[\text{Cd}(\text{C}_8\text{H}_7\text{N}_3)_2(\text{NO}_3)_2(\text{H}_2\text{O})_2]$, was obtained *via* the reaction of 4-(1*H*-imidazol-2-yl)-pyridine and cadmium(II) nitrate. Single crystal X-ray diffraction analysis reveals that the cadmium(II) atom is six-coordinated in a slightly distorted octahedral geometry by two pyridine nitrogen atoms, two nitrate anions oxygen atoms and two aqua oxygen atoms forming N_2O_4 donor set (Figure 1). The cadmium atom is situated on an inversion center. Bond distances of Cd(1)—N(1), Cd(1)—O(1) and Cd(1)—O(4) are 2.276 (2), 2.503 (3) and 2.310 (2) Å, respectively. The dihedral angle between the imidazole and pyridine rings is 1.6 (2)°. In the crystal, molecules are linked by N—H \cdots O, O—H \cdots N and O—H \cdots O hydrogen bonds, forming a three-dimensional network (Figure 2).

S2. Experimental

The organic ligand 4-(1*H*-imidazol-2-yl)-pyridine was prepared according to the previously reported literature methods (Voss *et al.*, 2008). $\text{Cd}(\text{NO}_3)_2$ (24 mg, 0.1 mmol) dissolved in 5 ml ethanol and a solution of 4-(1*H*-imidazol-2-yl)-pyridine (29 mg, 0.2 mmol) in another 5 ml of ethanol were mixed, refluxed for 5 h and filtered. The filtrate was left at room temperature. Suitable single crystals for a X-ray diffraction study were obtained after a few days (yield: 73% based on Cd(II) salts).

S3. Refinement

H atoms were positioned geometrically at distances of 0.93 (CH), and 0.86 (NH) from the respective parent atoms, a riding model was used during the refinement process. U_{iso} values were constrained to be 1.2 times U_{eq} of the carrier atom.

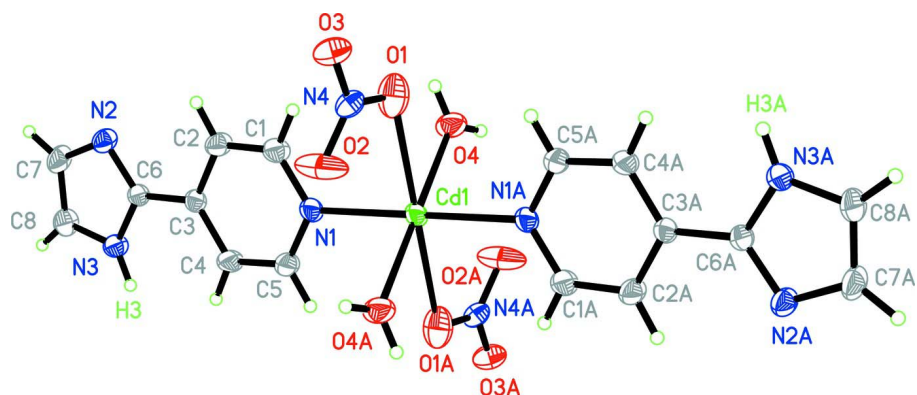


Figure 1

The molecular structure of (I) with atom labels and 30% probability displacement ellipsoids for non-H atoms.

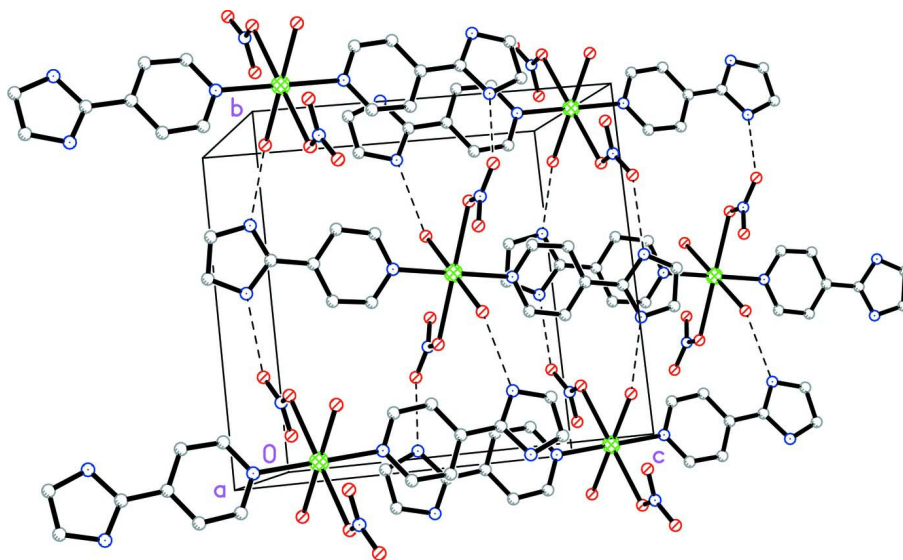


Figure 2

The three-dimensional supramolecular packing architecture of (I) with hydrogen-bonds depicted as dashed lines.

Diaquabis[4-(1*H*-imidazol-2-yl)pyridine- κ N]bis(nitrato- κ O)cadmium

Crystal data

$[\text{Cd}(\text{NO}_3)_2(\text{C}_8\text{H}_7\text{N}_3)_2(\text{H}_2\text{O})_2]$

$M_r = 562.78$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 7.2508$ (7) Å

$b = 12.1372$ (12) Å

$c = 12.3509$ (12) Å

$\beta = 102.278$ (2)°

$V = 1062.07$ (18) Å³

$Z = 2$

$F(000) = 564$

$D_x = 1.760$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4257 reflections

$\theta = 2.4\text{--}28.3^\circ$

$\mu = 1.09$ mm⁻¹

$T = 298$ K

Block, colorless

$0.16 \times 0.12 \times 0.10$ mm

Data collection

Bruker APEXII CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.845$, $T_{\max} = 0.899$

6543 measured reflections
2462 independent reflections
2272 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.046$
 $\theta_{\text{max}} = 28.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$
 $h = -7 \rightarrow 9$
 $k = -15 \rightarrow 15$
 $l = -14 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.084$
 $S = 1.10$
2462 reflections
157 parameters
3 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
 $w = 1/[\sigma^2(F_o^2) + (0.0252P)^2 + 1.0694P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.73 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.47 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	1.0000	0.5000	0.5000	0.03811 (11)
C1	0.8396 (5)	0.6142 (2)	0.2671 (2)	0.0466 (7)
H1	0.8465	0.6754	0.3131	0.056*
C2	0.7823 (5)	0.6301 (2)	0.1550 (2)	0.0456 (7)
H2	0.7498	0.7002	0.1269	0.055*
C3	0.7732 (4)	0.5408 (2)	0.0842 (2)	0.0341 (5)
C4	0.8205 (5)	0.4390 (2)	0.1325 (2)	0.0499 (8)
H4	0.8146	0.3764	0.0885	0.060*
C5	0.8761 (5)	0.4304 (3)	0.2458 (2)	0.0497 (7)
H5	0.9086	0.3612	0.2762	0.060*
C6	0.7176 (4)	0.5554 (2)	-0.0359 (2)	0.0337 (5)
C7	0.6323 (5)	0.6241 (3)	-0.1984 (2)	0.0502 (7)
H7	0.5950	0.6748	-0.2552	0.060*
C8	0.6534 (5)	0.5154 (3)	-0.2132 (3)	0.0506 (8)
H8	0.6350	0.4779	-0.2803	0.061*

N1	0.8860 (4)	0.51635 (18)	0.3142 (2)	0.0396 (5)
N2	0.6733 (4)	0.6497 (2)	-0.08794 (19)	0.0426 (5)
N3	0.7075 (4)	0.4715 (2)	-0.1096 (2)	0.0427 (6)
H3	0.7309	0.4032	-0.0939	0.051*
N4	0.7084 (3)	0.6785 (2)	0.5340 (2)	0.0411 (5)
O1	0.8766 (3)	0.6853 (3)	0.5384 (2)	0.0747 (8)
O2	0.6297 (5)	0.5914 (2)	0.5037 (3)	0.0965 (11)
O3	0.6156 (3)	0.75586 (18)	0.5590 (2)	0.0562 (6)
O4	1.2220 (3)	0.63059 (19)	0.4800 (2)	0.0573 (6)
H4B	1.200 (5)	0.6945 (15)	0.461 (4)	0.086*
H4A	1.334 (2)	0.617 (3)	0.490 (4)	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.05052 (19)	0.03477 (16)	0.02528 (16)	-0.00965 (11)	-0.00034 (11)	0.00115 (10)
C1	0.071 (2)	0.0372 (14)	0.0297 (13)	-0.0023 (14)	0.0073 (13)	-0.0033 (11)
C2	0.069 (2)	0.0356 (14)	0.0303 (14)	0.0046 (14)	0.0079 (13)	0.0017 (11)
C3	0.0388 (13)	0.0346 (12)	0.0279 (12)	-0.0030 (11)	0.0050 (10)	0.0008 (10)
C4	0.081 (2)	0.0318 (14)	0.0306 (14)	-0.0012 (14)	-0.0011 (14)	-0.0041 (11)
C5	0.074 (2)	0.0355 (14)	0.0333 (15)	-0.0032 (14)	-0.0040 (13)	0.0036 (12)
C6	0.0389 (13)	0.0332 (13)	0.0285 (12)	0.0001 (10)	0.0059 (10)	-0.0012 (10)
C7	0.065 (2)	0.0547 (18)	0.0284 (14)	0.0112 (15)	0.0049 (13)	0.0079 (12)
C8	0.069 (2)	0.0556 (19)	0.0252 (14)	0.0020 (15)	0.0045 (13)	-0.0020 (12)
N1	0.0523 (14)	0.0368 (12)	0.0267 (12)	-0.0080 (10)	0.0014 (10)	0.0007 (9)
N2	0.0578 (15)	0.0393 (12)	0.0303 (11)	0.0077 (11)	0.0083 (10)	0.0027 (9)
N3	0.0615 (16)	0.0356 (11)	0.0293 (12)	0.0016 (11)	0.0055 (11)	-0.0029 (9)
N4	0.0460 (13)	0.0387 (13)	0.0408 (13)	0.0056 (10)	0.0142 (10)	0.0112 (10)
O1	0.0446 (13)	0.111 (2)	0.0681 (17)	0.0082 (14)	0.0112 (12)	0.0077 (16)
O2	0.114 (3)	0.0367 (14)	0.151 (3)	-0.0131 (15)	0.055 (2)	-0.0218 (17)
O3	0.0654 (14)	0.0389 (11)	0.0700 (16)	0.0107 (11)	0.0271 (12)	0.0021 (10)
O4	0.0418 (11)	0.0386 (12)	0.0886 (18)	-0.0045 (9)	0.0075 (12)	0.0101 (12)

Geometric parameters (Å, °)

Cd1—N1	2.276 (2)	C5—N1	1.335 (4)
Cd1—N1 ⁱ	2.276 (2)	C5—H5	0.9300
Cd1—O4	2.310 (2)	C6—N2	1.319 (3)
Cd1—O4 ⁱ	2.310 (2)	C6—N3	1.357 (3)
Cd1—O1	2.503 (3)	C7—C8	1.345 (4)
Cd1—O1 ⁱ	2.503 (3)	C7—N2	1.368 (4)
C1—N1	1.333 (4)	C7—H7	0.9300
C1—C2	1.371 (4)	C8—N3	1.364 (4)
C1—H1	0.9300	C8—H8	0.9300
C2—C3	1.386 (4)	N3—H3	0.8600
C2—H2	0.9300	N4—O1	1.211 (3)
C3—C4	1.384 (4)	N4—O2	1.222 (4)
C3—C6	1.463 (3)	N4—O3	1.232 (3)

C4—C5	1.374 (4)	O4—H4B	0.816 (10)
C4—H4	0.9300	O4—H4A	0.814 (10)
N1—Cd1—N1 ⁱ	180.00 (4)	N1—C5—C4	123.4 (3)
N1—Cd1—O4	86.81 (9)	N1—C5—H5	118.3
N1 ⁱ —Cd1—O4	93.19 (9)	C4—C5—H5	118.3
N1—Cd1—O4 ⁱ	93.19 (9)	N2—C6—N3	110.6 (2)
N1 ⁱ —Cd1—O4 ⁱ	86.81 (9)	N2—C6—C3	125.8 (2)
O4—Cd1—O4 ⁱ	180.0	N3—C6—C3	123.6 (2)
N1—Cd1—O1	92.58 (9)	C8—C7—N2	110.6 (3)
N1 ⁱ —Cd1—O1	87.42 (9)	C8—C7—H7	124.7
O4—Cd1—O1	71.89 (9)	N2—C7—H7	124.7
O4 ⁱ —Cd1—O1	108.11 (9)	C7—C8—N3	105.9 (3)
N1—Cd1—O1 ⁱ	87.42 (9)	C7—C8—H8	127.1
N1 ⁱ —Cd1—O1 ⁱ	92.58 (9)	N3—C8—H8	127.1
O4—Cd1—O1 ⁱ	108.11 (9)	C1—N1—C5	116.4 (3)
O4 ⁱ —Cd1—O1 ⁱ	71.89 (9)	C1—N1—Cd1	121.42 (18)
O1—Cd1—O1 ⁱ	180.00 (7)	C5—N1—Cd1	121.97 (19)
N1—C1—C2	124.1 (3)	C6—N2—C7	105.5 (2)
N1—C1—H1	118.0	C6—N3—C8	107.4 (3)
C2—C1—H1	118.0	C6—N3—H3	126.3
C1—C2—C3	119.4 (3)	C8—N3—H3	126.3
C1—C2—H2	120.3	O1—N4—O2	118.2 (3)
C3—C2—H2	120.3	O1—N4—O3	122.4 (3)
C4—C3—C2	116.9 (2)	O2—N4—O3	119.4 (3)
C4—C3—C6	122.3 (3)	N4—O1—Cd1	109.1 (2)
C2—C3—C6	120.8 (2)	Cd1—O4—H4B	126 (3)
C5—C4—C3	119.9 (3)	Cd1—O4—H4A	123 (3)
C5—C4—H4	120.0	H4B—O4—H4A	111 (2)
C3—C4—H4	120.0		
N1—C1—C2—C3	-0.9 (5)	O1 ⁱ —Cd1—N1—C1	-161.4 (3)
C1—C2—C3—C4	1.1 (5)	N1 ⁱ —Cd1—N1—C5	-114 (15)
C1—C2—C3—C6	-178.3 (3)	O4—Cd1—N1—C5	121.5 (3)
C2—C3—C4—C5	-1.0 (5)	O4 ⁱ —Cd1—N1—C5	-58.5 (3)
C6—C3—C4—C5	178.4 (3)	O1—Cd1—N1—C5	-166.8 (3)
C3—C4—C5—N1	0.7 (6)	O1 ⁱ —Cd1—N1—C5	13.2 (3)
C4—C3—C6—N2	-179.0 (3)	N3—C6—N2—C7	0.5 (3)
C2—C3—C6—N2	0.4 (4)	C3—C6—N2—C7	179.7 (3)
C4—C3—C6—N3	0.1 (4)	C8—C7—N2—C6	-0.6 (4)
C2—C3—C6—N3	179.4 (3)	N2—C6—N3—C8	-0.2 (4)
N2—C7—C8—N3	0.5 (4)	C3—C6—N3—C8	-179.4 (3)
C2—C1—N1—C5	0.6 (5)	C7—C8—N3—C6	-0.2 (4)
C2—C1—N1—Cd1	175.5 (3)	O2—N4—O1—Cd1	-6.3 (4)
C4—C5—N1—C1	-0.5 (5)	O3—N4—O1—Cd1	173.7 (2)
C4—C5—N1—Cd1	-175.3 (3)	N1—Cd1—O1—N4	77.8 (2)
N1 ⁱ —Cd1—N1—C1	72 (15)	N1 ⁱ —Cd1—O1—N4	-102.2 (2)
O4—Cd1—N1—C1	-53.1 (3)	O4—Cd1—O1—N4	163.6 (2)

O4 ⁱ —Cd1—N1—C1	126.9 (3)	O4 ⁱ —Cd1—O1—N4	-16.4 (2)
O1—Cd1—N1—C1	18.6 (3)	O1 ⁱ —Cd1—O1—N4	29 (12)

Symmetry code: (i) $-x+2, -y+1, -z+1$.

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N3—H3...O3 ⁱⁱ	0.86	2.10	2.923 (3)	160
O4—H4B...N2 ⁱⁱⁱ	0.82 (1)	1.98 (1)	2.796 (3)	174 (4)
O4—H4A...O2 ^{iv}	0.81 (1)	2.14 (1)	2.946 (4)	174 (4)
O4—H4A...O3 ^{iv}	0.81 (1)	2.65 (3)	3.197 (3)	126 (3)

Symmetry codes: (ii) $-x+3/2, y-1/2, -z+1/2$; (iii) $x+1/2, -y+3/2, z+1/2$; (iv) $x+1, y, z$.