Acta Cryst E STRUCTURE REPORTS

ISSN 1600-5368

Crystal structure of bis(acetato-κO)bis(pyridine-2-carboxamide oxime-$\kappa^2 N,N'$)cadmium ethanol disolvate

Jiyong Liu

Department of Chemistry, Zhejiang University, Hangzhou, Zhejiang 310027, People's Republic of China. *Correspondence e-mail: shawnLau.zj@hotmail.com

Received 8 July 2014
Accepted 5 August 2014

Edited by R. F. Baggio, Comisión Nacional de Energía Atómica, Argentina

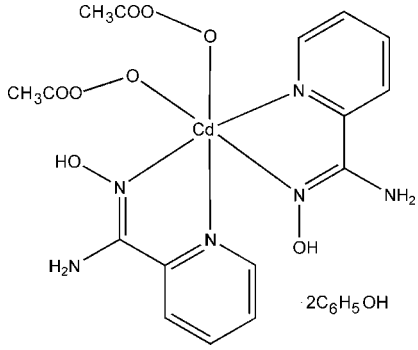
Keywords: crystal structure; Cd^{II} complex; acetate; pyridine-2-carboxamide oxime; N—H···O hydrogen bonding

CCDC reference: 1017896
Supporting information: this article has supporting information at journals.iucr.org/e

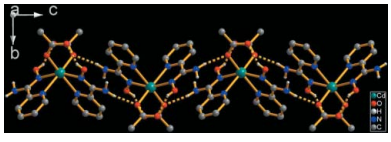
In the title compound, $[Cd(CH_3COO)_2(C_6H_7N_3O)_2]\cdot 2C_2H_5OH$, the Cd^{II} atom, which lies on a twofold rotation axis, is coordinated by two monodentate acetate groups and two *N*,*N*′-chelating pyridine-2-carboxamide oxime ligands, leading to a distorted octahedral coordination sphere. The mononuclear complex molecules are assembled into chains along the *c*-axis direction *via* N—H···O hydrogen-bonding interactions. These chains are further assembled by O—H···O hydrogen bonds involving the ethanol solvent molecules into a three-dimensional supramolecular structure.

1. Chemical context

The monoanions of simple of 2-pyridyl oximes, (py)C(*R*)NOH (*R* = a non-coordinating group, *e.g.* H, Me, Ph *etc.*), are remarkable sources of homo- and heterometallic complexes with novel structures and interesting physical properties (Miyasaka *et al.*, 2003; Stamatatos *et al.*, 2007). A logical extension of such studies is the investigation of the coordination chemistry of analogous organic molecules in which the non-donor *R* group is replaced by a donor group such as pyridine, cyano *etc.* (Alcazar *et al.*, 2013; Escuer *et al.*, 2011). When *R* is an amino group, the resulting ligand is pyridine-2-amidoxime, (py)C(NH_2)NOH, which belongs to the class of amidoximes. The presence of the amine functionality is expected to alter the coordination behaviour of this ligand in comparison with that of the (py)C(*R*)NOH (*R* = a non-coordinating group) ligands. The characteristics that differentiate the amino group are its coordination capability, potential for deprotonation, different electronic properties and hydrogen-bonding effects.



The present work reports the first use of (py)C(NH_2)NOH in Cd^{II} coordination chemistry and describes the synthesis and structure of the mononuclear title compound.



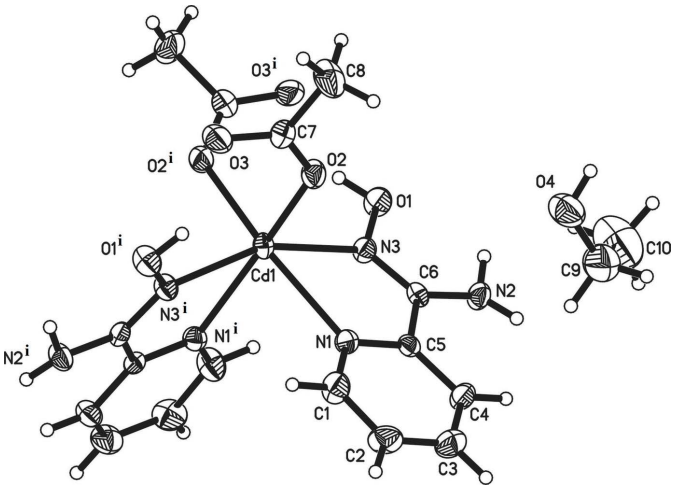


Figure 1
The title compound with displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.]

2. Structural commentary

The title complex consists of isolated $[Cd(O_2CMe)_2\{(py)C(NH_2)NOH\}_2]$ complex molecules and ethanol solvent molecules. The central Cd^{II} atom is located on a twofold rotation axis (Wyckoff site 4*e*). The Cd^{II} atom is coordinated by two monodentate $MeCO_2^-$ groups and two *N*,*N*′-chelating (py)C(NH_2)NOH ligands (Fig. 1 and Table 1). The (py)C(NH_2)NOH donor atoms are the N atoms of the neutral oxime and the 2-pyridyl groups. The amino N atom of each ligand remains uncoordinating, albeit participating in an extensive intermolecular hydrogen-bonding network. Each of the two coordinating (py)C(NH_2)NOH molecules results in the formation of a five-membered chelate ring including a Cd^{II} atom, in which the chelate angle N1—Cd1—N1 [86.7 (2)°] is noteably larger than comparable angles found in $[Cd(HCO_2)_2(pya)_2]$ (pya = pyridine-2-aldoxime**;** Croitor *et al.*, 2013).

3. Supramolecular features

Table 2 shows the hydrogen-bonding interactions. There are two strong symmetry-related intramolecular hydrogen bonds between the unbound oxime (–O1—H1) group and uncoordinating acetate atom O3. Uncoordinating amino atom N2 acts as a donor for two hydrogen bonds; in one of these, the acceptor is coordinating atom O2 from the acetate group, which leads to the formation of chains running along the *c*-axis direction (Fig. 2). These chains are further linked into a three-dimensional network by hydrogen bonds involving the ethanol solvent molecule (O4), acting as a donor for the uncoordinating carboxylate O atom (O3) and as an acceptor for the remaining amino H atom H2*B* (Table 2 and Fig. 3).

Table 1
Selected bond lengths (Å).

Cd1—O2	2.288 (3)	Cd1—N3	2.315 (3)
Cd1—N1	2.413 (4)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3^{i}	0.85 (1)	1.86 (4)	2.600 (5)	145 (6)
N2—H2*A*···O2^{ii}	0.85 (1)	2.20 (2)	3.040 (5)	169 (5)
N2—H2*B*···O4	0.85 (1)	2.45 (4)	3.113 (6)	136 (5)
O4—H4*A*···O3^{iii}	0.85 (1)	2.09 (3)	2.903 (5)	161 (8)

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

4. Synthesis and crystallization

A stoichiometric amount of (py)C(NH_2)NOH and $Cd(OAc)_2\cdot 3H_2O$ in a 2:1 ratio was dissolved in 20 ml ethanol

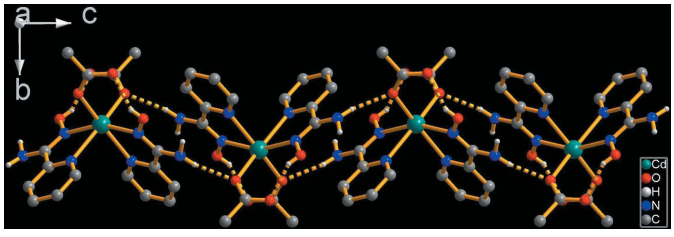


Figure 2
The hydrogen-bonded chain along the *c* axis. Dashed lines represent hydrogen bonds and H atoms bonded to C atoms have been omitted for clarity.

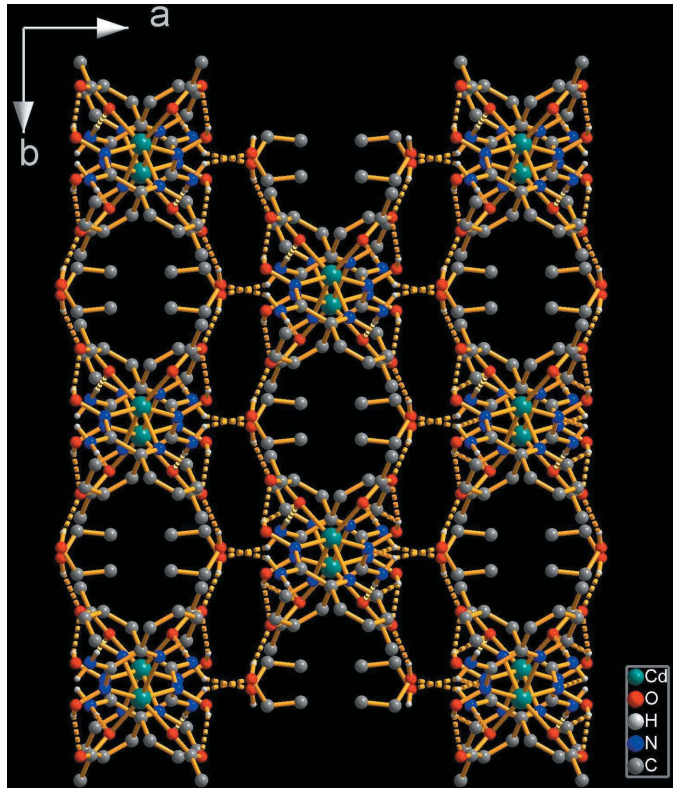


Figure 3
The crystal structure projected along the *c* axis. Dashed lines represent hydrogen bonds and H atoms bonded to C atoms have been omitted for clarity.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Cd(C_2H_3O_2)_2(C_6H_7N_3O)_2]\cdot 2C_2H_6O$
M_r	596.92
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	294
a, *b*, *c* (Å)	15.894 (3), 10.9654 (17), 15.0212 (16)
β (°)	91.746 (12)
V (Å^3)	2616.7 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.89
Crystal size (mm)	0.28 × 0.26 × 0.2
Data collection	
Diffractometer	Agilent Xcalibur, Atlas, Gemini ultra
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min}, T_{max}	0.910, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5661, 2400, 2017
R_{int}	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.125, 1.05
No. of reflections	2400
No. of parameters	173
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.85, −0.48

Computer programs: *CrysAlis PRO* (Agilent, 2011), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

and 10 ml DMF, and the solution left to evaporate slowly to afford colourless block-like crystals after three weeks at room temperature.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms bonded to C atoms were placed in geometrically calculated position and were refined using a riding model, with C—H = 0.93 (aromatic) or 0.96 Å (methyl) and U_{iso}(H) = 1.2U_{eq}($C_{aromatic}$) and 1.5U_{eq}(C_{methyl}). The N- and O-bound H atoms were located in a difference map and the coordinates were refined with N—H = 0.86 (1) Å and U_{iso}(H) = 1.2U_{eq}(N) or 1.5U_{eq}(O).

Acknowledgements

This project was supported by the Expert Project of Key Basic Research of the Ministry of Science and Technology of China (grant No. 2003CCA00800), the Science and Technology Department of Zhejiang Province (grant No. 2006 C21105) and the Education Department of Zhejiang Province.

References

Agilent (2011). *CrysAlis PRO* and *CrysAlis RED*. Agilent Technologies, Yarnton, England.
Alcazar, A., Cordero, B., Esteban, J., Tangoulis, V., Font-Bardia, M., Calvet, T. & Escuer, A. (2013). *Dalton Trans.* **42**, 12334–12345.
Croitor, L., Coropceanu, E. B., Siminel, A. V., Masunov, A. E. & Fonari, M. S. (2013). *Polyhedron*, **60**, 140–150.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Escuer, A., Vlahopoulou, G., Perlepes, S. P. & Mautner, F. A. (2011). *Inorg. Chem.* **50**, 2468–2478.
Miyasaka, H., Nezu, T., Iwahori, F., Furukawa, S., Sugimoto, K., Cleŕac, R., Sugiura, K. & Yamashita, M. (2003). *Inorg. Chem.* **42**, 4501–4503.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stamatatos, T. C., Foguet-Albiol, D., Lee, S. C., Raptopoulou, C. P., Terzis, A., Wernsdorfer, W., Hill, S. O., Perlepes, S. P. & Christou, G. (2007). *J.Am.Chem.Soc.* **129**, 9484–9499.

supporting information

Acta Cryst. (2014). E**70**, 142-144 [doi:10.1107/S1600536814017978]

Crystal structure of bis(acetato-κO)bis(pyridine-2-carboxamide oxime-$\kappa^2 N,N'$)cadmium ethanol disolvate

Jiyong Liu

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: Olex2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: Olex2 (Dolomanov *et al.*, 2009).

Bis(acetato-κO)bis(pyridine-2-carboxamide oxime-$\kappa^2 N,N'$)cadmium ethanol disolvate

Crystal data

$[Cd(C_2H_3O_2)_2(C_6H_7N_3O)_2]\cdot 2C_2H_6O$
$M_r = 596.92$
Monoclinic, $C2/c$
$a = 15.894\ (3)$ Å
$b = 10.9654\ (17)$ Å
$c = 15.0212\ (16)$ Å
$\beta = 91.746\ (12)°$
$V = 2616.7\ (7)$ Å^3
$Z = 4$
$F(000) = 1224$
$D_x = 1.515$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1816 reflections
$\theta = 2.9–29.6°$
$\mu = 0.89$ mm^{-1}
$T = 294$ K
Block, colourless
0.28 × 0.26 × 0.2 mm

Data collection

Agilent Xcalibur, Atlas, Gemini ultra diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.3592 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.910$, $T_{max} = 1.000$
5661 measured reflections
2400 independent reflections
2017 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 25.4°$, $\theta_{min} = 3.5°$
$h = -19\rightarrow16$
$k = -13\rightarrow11$
$l = -18\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.125$
$S = 1.05$
2400 reflections
173 parameters
4 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

$w = 1/[\sigma^2(F_o^2) + (0.0689P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.85$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.55546 (4)	0.7500	0.0336 (2)
O1	0.3289 (2)	0.5799 (3)	0.6185 (2)	0.0456 (9)
H1	0.323 (4)	0.623 (5)	0.664 (2)	0.068*
O2	0.5829 (2)	0.6898 (3)	0.67588 (19)	0.0448 (8)
O3	0.6590 (3)	0.7760 (3)	0.7846 (2)	0.0627 (11)
N1	0.5479 (2)	0.3954 (4)	0.6536 (2)	0.0349 (9)
N2	0.3668 (3)	0.4189 (4)	0.5009 (3)	0.0411 (10)
H2A	0.384 (3)	0.381 (4)	0.456 (2)	0.049*
H2B	0.333 (3)	0.478 (3)	0.493 (4)	0.049*
N3	0.4048 (2)	0.5170 (4)	0.6337 (2)	0.0348 (9)
C1	0.6196 (3)	0.3347 (5)	0.6661 (3)	0.0510 (13)
H1A	0.6528	0.3520	0.7166	0.061*
C2	0.6469 (4)	0.2478 (5)	0.6083 (4)	0.0574 (14)
H2	0.6969	0.2059	0.6200	0.069*
C3	0.5988 (3)	0.2237 (5)	0.5326 (4)	0.0548 (14)
H3	0.6165	0.1666	0.4914	0.066*
C4	0.5238 (3)	0.2855 (4)	0.5189 (3)	0.0421 (12)
H4	0.4900	0.2698	0.4686	0.051*
C5	0.4994 (3)	0.3717 (4)	0.5812 (3)	0.0304 (10)
C6	0.4200 (3)	0.4393 (4)	0.5716 (3)	0.0307 (10)
C7	0.6314 (3)	0.7709 (5)	0.7064 (3)	0.0423 (12)
C8	0.6594 (5)	0.8661 (6)	0.6421 (4)	0.077 (2)
H8A	0.6782	0.8273	0.5890	0.115*
H8B	0.7047	0.9125	0.6688	0.115*
H8C	0.6132	0.9194	0.6273	0.115*
O4	0.2093 (3)	0.5194 (5)	0.3968 (3)	0.0762 (13)
H4A	0.207 (6)	0.583 (5)	0.364 (5)	0.114*
C9	0.1674 (7)	0.4180 (8)	0.3623 (6)	0.105 (3)
H9A	0.1766	0.3505	0.4032	0.126*
H9B	0.1927	0.3961	0.3066	0.126*
C10	0.0799 (7)	0.4315 (9)	0.3466 (8)	0.146 (5)
H10A	0.0541	0.4565	0.4006	0.219*

H10B	0.0563	0.3551	0.3271	0.219*
H10C	0.0698	0.4922	0.3014	0.219*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0343 (3)	0.0403 (3)	0.0260 (3)	0.000	−0.00478 (18)	0.000
O1	0.0355 (19)	0.053 (2)	0.047 (2)	0.0123 (16)	−0.0101 (15)	−0.0073 (16)
O2	0.054 (2)	0.046 (2)	0.0348 (17)	−0.0145 (18)	−0.0026 (14)	−0.0009 (15)
O3	0.089 (3)	0.042 (2)	0.055 (2)	−0.020 (2)	−0.027 (2)	0.0086 (17)
N1	0.036 (2)	0.034 (2)	0.0340 (19)	0.0011 (18)	−0.0032 (16)	−0.0007 (16)
N2	0.043 (2)	0.045 (3)	0.034 (2)	0.005 (2)	−0.0100 (18)	−0.0086 (18)
N3	0.031 (2)	0.040 (2)	0.033 (2)	0.0060 (18)	−0.0039 (15)	−0.0039 (17)
C1	0.039 (3)	0.065 (4)	0.049 (3)	0.013 (3)	−0.012 (2)	−0.008 (3)
C2	0.048 (3)	0.051 (3)	0.073 (4)	0.019 (3)	−0.004 (3)	−0.002 (3)
C3	0.058 (3)	0.048 (3)	0.059 (3)	0.008 (3)	0.008 (3)	−0.009 (3)
C4	0.046 (3)	0.041 (3)	0.039 (2)	0.004 (2)	−0.001 (2)	−0.010 (2)
C5	0.035 (2)	0.028 (2)	0.028 (2)	−0.003 (2)	0.0008 (18)	0.0048 (17)
C6	0.031 (2)	0.035 (2)	0.026 (2)	−0.003 (2)	0.0000 (17)	0.0072 (18)
C7	0.043 (3)	0.046 (3)	0.038 (3)	−0.001 (2)	−0.001 (2)	−0.006 (2)
C8	0.097 (5)	0.075 (5)	0.057 (4)	−0.045 (4)	−0.008 (3)	0.020 (3)
O4	0.081 (3)	0.068 (3)	0.079 (3)	−0.001 (3)	−0.021 (2)	0.015 (2)
C9	0.148 (9)	0.080 (6)	0.086 (6)	−0.003 (6)	−0.029 (6)	0.001 (4)
C10	0.139 (10)	0.150 (11)	0.147 (9)	−0.070 (8)	−0.041 (8)	0.044 (7)

Geometric parameters (Å, º)

Cd1—O2	2.288 (3)	C2—C3	1.376 (8)
Cd1—O2^{i}	2.288 (3)	C3—H3	0.9300
Cd1—N1	2.413 (4)	C3—C4	1.381 (7)
Cd1—N1^{i}	2.413 (4)	C4—H4	0.9300
Cd1—N3^{i}	2.315 (3)	C4—C5	1.394 (6)
Cd1—N3	2.315 (3)	C5—C6	1.468 (6)
O1—H1	0.846 (10)	C7—C8	1.498 (7)
O1—N3	1.404 (5)	C8—H8A	0.9600
O2—C7	1.254 (6)	C8—H8B	0.9600
O3—C7	1.244 (5)	C8—H8C	0.9600
N1—C1	1.328 (6)	O4—H4A	0.851 (10)
N1—C5	1.339 (5)	O4—C9	1.388 (10)
N2—H2A	0.851 (10)	C9—H9A	0.9700
N2—H2B	0.847 (10)	C9—H9B	0.9700
N2—C6	1.355 (6)	C9—C10	1.412 (14)
N3—C6	1.291 (6)	C10—H10A	0.9600
C1—H1A	0.9300	C10—H10B	0.9600
C1—C2	1.368 (7)	C10—H10C	0.9600
C2—H2	0.9300		
O2—Cd1—O2^{i}	99.86 (18)	C2—C3—C4	118.9 (5)

O2—Cd1—N1	88.81 (13)	C4—C3—H3	120.5
O2^{i}—Cd1—N1	163.16 (12)	C3—C4—H4	120.4
O2—Cd1—N1^{i}	163.16 (12)	C3—C4—C5	119.3 (4)
O2^{i}—Cd1—N1^{i}	88.81 (13)	C5—C4—H4	120.4
O2—Cd1—N3^{i}	96.42 (12)	N1—C5—C4	120.8 (4)
O2—Cd1—N3	97.07 (12)	N1—C5—C6	117.0 (4)
O2^{i}—Cd1—N3	96.42 (12)	C4—C5—C6	122.2 (4)
O2^{i}—Cd1—N3^{i}	97.07 (12)	N2—C6—C5	120.5 (4)
N1^{i}—Cd1—N1	86.69 (19)	N3—C6—N2	123.3 (4)
N3—Cd1—N1	68.01 (13)	N3—C6—C5	116.1 (4)
N3—Cd1—N1^{i}	96.27 (13)	O2—C7—C8	116.7 (4)
N3^{i}—Cd1—N1^{i}	68.01 (13)	O3—C7—O2	124.9 (5)
N3^{i}—Cd1—N1	96.27 (13)	O3—C7—C8	118.3 (5)
N3^{i}—Cd1—N3	159.0 (2)	C7—C8—H8A	109.5
N3—O1—H1	106 (4)	C7—C8—H8B	109.5
C7—O2—Cd1	129.4 (3)	C7—C8—H8C	109.5
C1—N1—Cd1	124.4 (3)	H8A—C8—H8B	109.5
C1—N1—C5	119.2 (4)	H8A—C8—H8C	109.5
C5—N1—Cd1	116.4 (3)	H8B—C8—H8C	109.5
H2A—N2—H2B	119 (5)	C9—O4—H4A	116 (6)
C6—N2—H2A	120 (4)	O4—C9—H9A	108.3
C6—N2—H2B	111 (4)	O4—C9—H9B	108.3
O1—N3—Cd1	124.9 (3)	O4—C9—C10	115.9 (9)
C6—N3—Cd1	122.3 (3)	H9A—C9—H9B	107.4
C6—N3—O1	112.6 (3)	C10—C9—H9A	108.3
N1—C1—H1A	118.5	C10—C9—H9B	108.3
N1—C1—C2	123.1 (4)	C9—C10—H10A	109.5
C2—C1—H1A	118.5	C9—C10—H10B	109.5
C1—C2—H2	120.7	C9—C10—H10C	109.5
C1—C2—C3	118.7 (5)	H10A—C10—H10B	109.5
C3—C2—H2	120.7	H10A—C10—H10C	109.5
C2—C3—H3	120.5	H10B—C10—H10C	109.5

Cd1—O2—C7—O3	17.9 (8)	N1—Cd1—N3—O1	−178.6 (4)
Cd1—O2—C7—C8	−164.0 (4)	N1—Cd1—N3—C6	−3.7 (3)
Cd1—N1—C1—C2	−177.2 (4)	N1^{i}—Cd1—N3—C6	−87.6 (4)
Cd1—N1—C5—C4	176.5 (3)	N1—C1—C2—C3	1.3 (9)
Cd1—N1—C5—C6	−4.1 (5)	N1—C5—C6—N2	−178.9 (4)
Cd1—N3—C6—N2	−177.2 (3)	N1—C5—C6—N3	0.9 (6)
Cd1—N3—C6—C5	3.0 (5)	N3—Cd1—O2—C7	157.2 (4)
O1—N3—C6—N2	−1.7 (6)	N3^{i}—Cd1—O2—C7	−38.9 (4)
O1—N3—C6—C5	178.5 (3)	N3^{i}—Cd1—N1—C1	−13.3 (4)
O2^{i}—Cd1—O2—C7	59.4 (4)	N3—Cd1—N1—C1	−178.9 (4)
O2^{i}—Cd1—N1—C1	−155.5 (4)	N3^{i}—Cd1—N1—C5	169.5 (3)
O2—Cd1—N1—C1	83.0 (4)	N3—Cd1—N1—C5	3.9 (3)
O2—Cd1—N1—C5	−94.2 (3)	N3^{i}—Cd1—N3—O1	137.7 (3)
O2^{i}—Cd1—N1—C5	27.3 (6)	N3^{i}—Cd1—N3—C6	−47.4 (3)
O2^{i}—Cd1—N3—O1	8.1 (4)	C1—N1—C5—C4	−0.8 (7)

O2—Cd1—N3—O1	−92.8 (3)	C1—N1—C5—C6	178.6 (4)
O2^{i}—Cd1—N3—C6	−177.1 (4)	C1—C2—C3—C4	−1.7 (9)
O2—Cd1—N3—C6	82.1 (4)	C2—C3—C4—C5	0.9 (8)
N1—Cd1—O2—C7	−135.1 (4)	C3—C4—C5—N1	0.4 (7)
N1^{i}—Cd1—O2—C7	−60.6 (6)	C3—C4—C5—C6	−179.0 (4)
N1^{i}—Cd1—N1—C1	−80.8 (4)	C4—C5—C6—N2	0.5 (6)
N1^{i}—Cd1—N1—C5	102.1 (3)	C4—C5—C6—N3	−179.7 (4)
N1^{i}—Cd1—N3—O1	97.6 (3)	C5—N1—C1—C2	−0.1 (8)

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*
O1—H1···O3^{i}	0.85 (1)	1.86 (4)	2.600 (5)	145 (6)
N2—H2*A*···O2^{ii}	0.85 (1)	2.20 (2)	3.040 (5)	169 (5)
N2—H2*B*···O4	0.85 (1)	2.45 (4)	3.113 (6)	136 (5)
O4—H4*A*···O3^{iii}	0.85 (1)	2.09 (3)	2.903 (5)	161 (8)

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