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Crystal structure of poly[bis(μ -2-amino-4,5-dicyanoimidazolato- $\kappa^2 N^1:N^3$)-*trans*-bis(*N,N'*-dimethylformamide- κO)cadmium]

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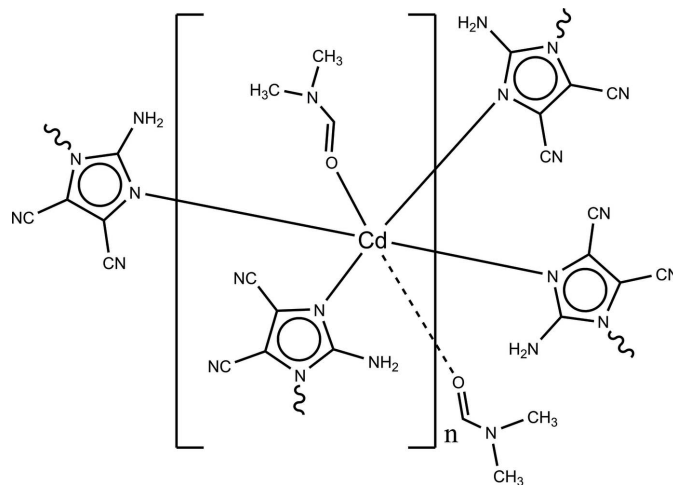
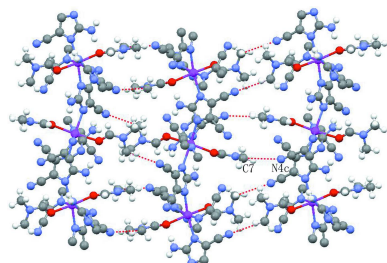
Keywords: crystal structure; 2-amino-4,5-dicyanoimidazole; metal–organic framework; cadmium coordination polymer; hydrogen bonding

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In the title structure, $[\text{Cd}(\text{C}_5\text{H}_2\text{N}_5)_2(\text{C}_3\text{H}_7\text{NO})_2]_n$ or $[\text{Cd}(\text{adci})_2(\text{DMF})_2]_n$, the Cd^{2+} ion is located on a twofold rotation axis and is six-coordinated in a CdN_4O_2 manner by four imidazole N atoms of four symmetry-related 2-amino-4,5-dicyanoimidazolate (adci) anions in the equatorial plane and by two O atoms of symmetry-related *N,N*-dimethylformamide (DMF) ligands in axial positions. The adci^- anions bridge adjacent Cd^{2+} ions [shortest $\text{Cd}\cdots\text{Cd}$ separation = 6.733 (3) Å] into a layered coordination polymer extending parallel to (001). The primary amino group and the non-coordinating cyano groups of adci^- anions are involved in hydrogen-bonding interactions with DMF ligands to stabilize the crystal structure.

1. Chemical context

Porous materials such as metal-organic frameworks (MOFs) combining advantages of both organic and inorganic components have emerged as a unique class of crystalline solid-state materials today due to their potential applications in gas adsorption and separation (Collins & Zhou, 2007), catalysis (Gu *et al.*, 2012) and analytical chemistry (Mondal *et al.*, 2013). As a branch of MOFs, zeolitic imidazolate frameworks (ZIFs), which are topologically related to inorganic zeolites, commonly reveal high thermal and chemical stability (Eddaoudi *et al.*, 2015). Bridging N-donor ligands such as 2-substituted 4,5-dicyanoimidazole (dci) molecules are often used to synthesize ZIFs (Sava *et al.*, 2009; Mondal *et al.*, 2014). In addition, the cyano group of dci can generate carboxylate- (Orcajo *et al.*, 2014) or tetrazole-based (Xiong *et al.*, 2002) ligands by *in-situ* ligand reactions.



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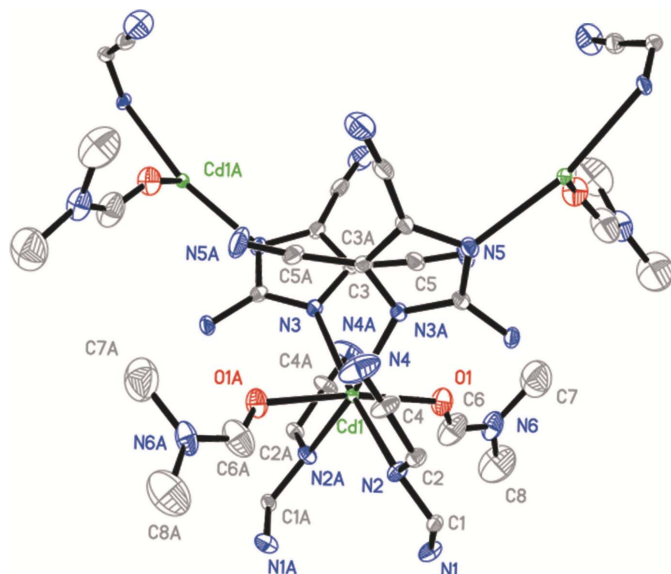


Figure 1

The coordination sphere around Cd^{2+} in the structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms bonded to C and N atoms have been omitted for clarity. [Symmetry code: (A) $2 - x, y, \frac{3}{2} - z$.]

We chose a rigid planar ligand, *viz.* 2-amino-4,5-dicyanoimidazole (adci), and Cd^{2+} that exhibits strong coordination capabilities for imidazoles, to prepare new metal-organic polymers and report here the structure of the title compound, $[\text{Cd}(\text{C}_5\text{H}_2\text{N}_5)_2(\text{C}_3\text{H}_7\text{NO})_2]_n$, or $[\text{Cd}(\text{adci})_2(\text{DMF})_2]_n$ (DMF is dimethylformamide), (I).

2. Structural commentary

Complex (I) is a mononuclear cadmium coordination polymer, in which the central Cd^{2+} ion exhibits a tetragonally distorted octahedral coordination environment (Fig. 1). The asymmetric unit of (I) comprises one Cd^{2+} ion located on a twofold rotation axis, one 2-amino-4,5-dicyanoimidazolate ion and one DMF ligand, both in general positions. The Cd^{2+} ion has an N_4O_2 coordination set defined by four N atoms of four symmetry-related adci^- anions in the equatorial plane and by two oxygen atoms of two symmetry-related DMF ligands in axial positions. The $\text{Cd}-\text{N}$ bond lengths [2.339 (4) and 2.353 (4) Å] and $\text{Cd}-\text{O}$ bond length [2.322 (4) Å] fall in normal ranges (Groom & Allen, 2014). Each adci^- anion bridges two adjacent Cd^{2+} ions in a bis-monodentate mode through two imidazole N atoms whereas the DMF molecules serve as terminal ligands. Thus, four Cd^{2+} ions and four bridging adci^- ligands generate a square motif aligned parallel to (001), as shown in Fig. 2. The $\text{Cd}\cdots\text{Cd}$ distance along the edge of the square is 6.733 (3) Å, which is similar to previously reported structures (Li *et al.*, 2010; Wang *et al.*, 2010).

3. Supramolecular features

Complex (I) possesses various hydrogen-bonding interactions (Table 1). The amino group and the non-coordinating cyano N

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O1}^i$	0.86	2.45	3.187 (6)	144
$\text{C7}-\text{H7C}\cdots\text{N5}^i$	0.96	2.68	3.429 (12)	135
$\text{C7}-\text{H7B}\cdots\text{N4}^{ii}$	0.96	2.65	3.496 (11)	148

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

atoms are involved in hydrogen-bonding interactions with DMF ligands to stabilize the crystal structure. In the 2D metal-organic network, intermolecular $\text{N1}-\text{H1A}\cdots\text{O1}$ hydrogen bonds between the primary amine group of adci^- and the O atoms of an DMF ligand as well as $\text{C7}-\text{H7C}\cdots\text{N5}$ interactions between the methyl C atoms of DMF and the non-coordinating N atoms of the cyano group of an adci^- anion play a crucial role in directing and stabilizing the assembly of the supramolecular structure (Kim *et al.*, 2015; Sava *et al.*, 2009), as shown in Fig. 3a. The layers are packed together by weak $\text{C7}-\text{H7B}\cdots\text{N4}$ interactions, involving the methyl C atom of DMF and another N atom of a cyano group (Fig. 3b). The lengths of these three hydrogen bonds fall in or approach the range (3.2–4.0 Å) of weak hydrogen-bonding interactions (Desiraju, 1996; Steed & Atwood, 2000).

4. Database survey

The cyano groups of the dci ligands exhibit a strong electron-withdrawing effect. Consequently, the formation of anionic species is relatively straightforward (Prasad *et al.*, 1999) and 4,5-dicyanoimidazoles can be used in the preparation of coordination frameworks with different metal ions. However,

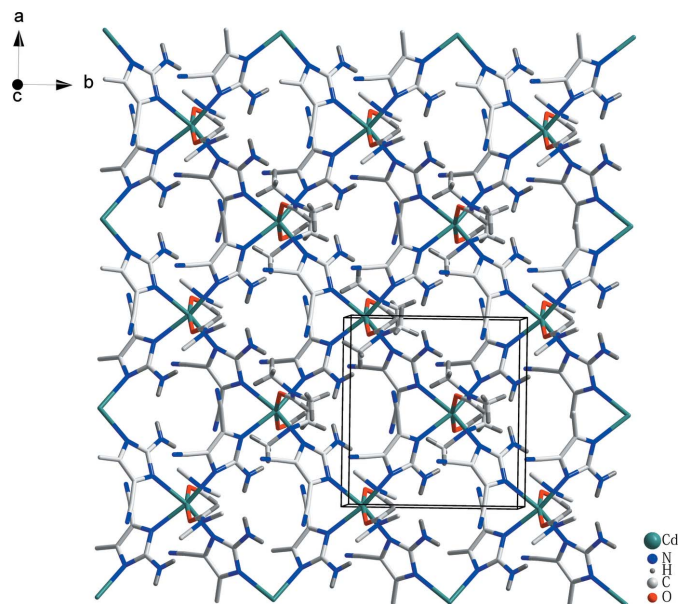


Figure 2

The two-dimensional network in the structure of (I), viewed perpendicular to the *ab* plane. Colour key: Cd steel, N blue, H grey, C light grey and O red.

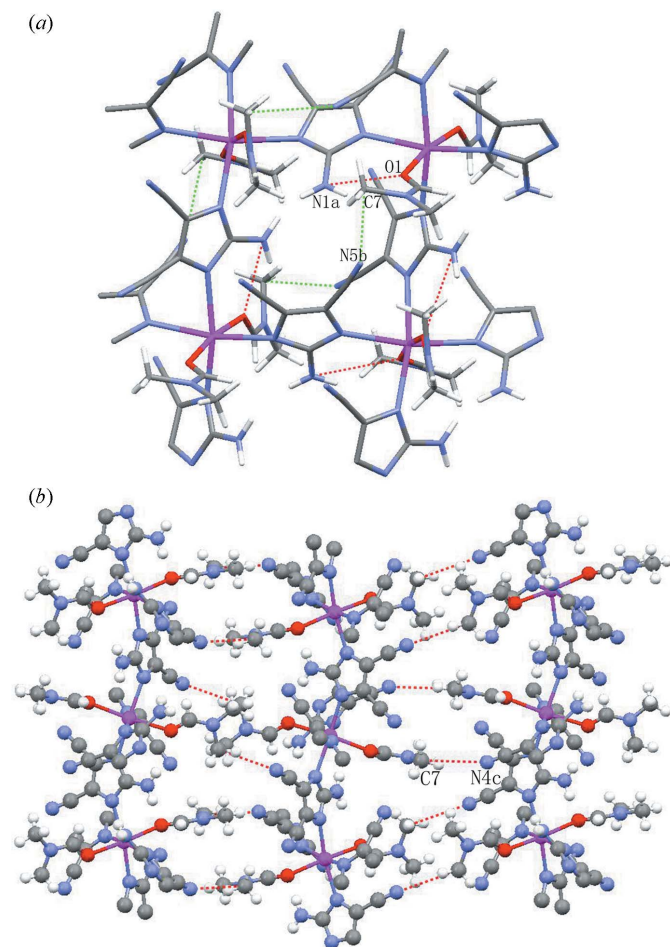


Figure 3
(a) View of two kinds of hydrogen bonds in the layers. Dashed lines represent C—H...N (green) and N—H...O (red) hydrogen bonds, respectively. (b) The crystal packing between the layers in the title structure. C—H...N hydrogen-bonding interactions are drawn as red dashed lines. [Symmetry codes: (a) $\frac{3}{2} - x, -\frac{1}{2} + y, z$; (b) $\frac{3}{2} - x, \frac{1}{2} + y, z$; (c) $x, -y, -\frac{1}{2} + z$].

reports on systems with 2-amino-4,5-dicyanoimidazole, a novel rigid planar ligand with five potential coordination sites, are rather scarce. A search in the Cambridge Structural Database (Version 5.27, May 2014; Groom & Allen, 2014) for 4,5-dicyanoimidazole revealed eleven complexes with 2-substituted 4,5-imidazoledicarbonitrile ligands. An unprecedented SHG-active silver-containing MOF with a rare 10³ topology has been reported (Yang *et al.*, 2013), as well as the synthesis and fluorescent properties of a 3D heterometallic polymeric complex $\{[\text{K}[\text{Cd}(\text{dci})_2(\text{H}_2\text{O})_6]\text{Cl}]\}_n$ (Li *et al.*, 2010), and of $\{[\text{Zn}_2(\text{IMDN})_4(\text{H}_2\text{O})_3] \cdot 3\text{H}_2\text{O}_3\}_n$ and $[\text{Co}(\text{IMDN})_2(\text{H}_2\text{O})_2]_n$ (Hu *et al.*, 2013) (IMDN is 2*H*-imidazole-4,5-dicarbonitrile) with chain structures. However, the coordination modes of the imidazoles in these complexes are different.

5. Synthesis and crystallization

Compound (I) was synthesized as follows: adci (0.0266 g, 0.2 mmol) and HNO₃ (0.2 ml, 3.5 *M* in DMF) were mixed in

Table 2
Experimental details.

Crystal data	
Chemical formula	$[\text{Cd}(\text{C}_5\text{H}_2\text{N}_5)_2(\text{C}_3\text{H}_7\text{NO})_2]$
M_r	522.83
Crystal system, space group	Orthorhombic, <i>Pbcn</i>
Temperature (K)	296
a, b, c (Å)	9.8438 (2), 9.1897 (2), 22.8948 (4)
V (Å ³)	2071.10 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.10
Crystal size (mm)	0.18 × 0.12 × 0.10
Data collection	
Diffractometer	Bruker SMART APEX CCD area detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2008)
$T_{\min}, T_{\max}$	0.854, 0.896
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9497, 2386, 1741
R_{int}	0.022
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.042, 0.159, 1.07
No. of reflections	2353
No. of parameters	143
No. of restraints	96
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.71, -0.66

Computer programs: *SMART* and *SAINT* (Bruker, 2008), *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2006) and *DIAMOND* (Brandenburg, 2006).

2 ml DMF. After stirring for 0.5 h, Cd(NO₃)₂·4H₂O (0.0308 g, 0.1 mmol) in 6 ml methanol was added dropwise. The mixture was further stirred for another hour and then filtrated. The filtrate was kept at ambient temperature. After about three weeks, yellow block-shaped crystals of (I) suitable for single X-ray diffraction were obtained. Yield: 0.0224 g (43% based on Cd). FT-IR (KBr, cm⁻¹): 3436, 3346, 2930, 2217, 1658, 1525, 1486, 1444, 1385, 1328, 1305, 1115, 675.

6. Refinement

Crystal data, data collection and refinement details are summarized in Table 2. Hydrogen atoms of the organic ligands were placed in idealized positions, with $d(\text{C}-\text{H}) = 0.93$ Å for *sp*²-bound H atoms and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, and $d(\text{C}-\text{H}) = 0.96$ Å for methyl H atoms and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. H atoms of the amino group were located from a difference map and were refined with $d(\text{N}-\text{H}) = 0.86$ Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

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Crystal structure of poly[bis(μ -2-amino-4,5-dicyanoimidazolato- $\kappa^2 N^1:N^3$)-trans-bis(N,N' -dimethylformamide- κO)cadmium]

Jin-Li Zhu, Guo -Qing Jiang, Xiao-Qing Guo, Yan-Feng Tang and Miao Wang

Computing details

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.* (2006) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Poly[bis(μ -2-amino-4,5-dicyanoimidazolato- $\kappa^2 N^1:N^3$)-trans-bis(N,N' -dimethylformamide- κO)cadmium]

Crystal data

[Cd(C₅H₂N₅)₂(C₃H₇NO)₂]

$M_r = 522.83$

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

$a = 9.8438$ (2) Å

$b = 9.1897$ (2) Å

$c = 22.8948$ (4) Å

$V = 2071.10$ (7) Å³

$Z = 4$

$F(000) = 1048$

$D_x = 1.677$ Mg m⁻³

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

$\theta = 3.5$ – 27.5°

$\mu = 1.10$ mm⁻¹

$T = 296$ K

Block, yellow

$0.18 \times 0.12 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ϕ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2008)

$T_{\min} = 0.854$, $T_{\max} = 0.896$

9497 measured reflections

2386 independent reflections

1741 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 4.1^\circ$

$h = -12 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -29 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.159$

$S = 1.07$

2353 reflections

143 parameters

96 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

$w = 1/[\sigma^2(F_o^2) + (0.0999P)^2 + 4.109P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.71$ e Å⁻³

$\Delta\rho_{\min} = -0.65$ 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 ($\text{\AA}^2$)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	1.0000	0.11224 (5)	0.7500	0.0180 (2)
N1	0.8425 (4)	0.4650 (5)	0.71416 (18)	0.0327 (10)
H1A	0.8043	0.5387	0.6978	0.039*
H1B	0.9243	0.4416	0.7050	0.039*
N2	0.8289 (4)	0.2699 (4)	0.78205 (17)	0.0269 (9)
C4	0.7391 (6)	0.1135 (5)	0.8626 (2)	0.0360 (12)
O1	0.9090 (4)	0.1297 (4)	0.65667 (17)	0.0449 (10)
N3	1.1454 (4)	−0.0840 (4)	0.72898 (18)	0.0224 (8)
C1	0.7732 (6)	0.3852 (5)	0.75474 (18)	0.0235 (10)
C2	0.7281 (5)	0.2249 (5)	0.81951 (18)	0.0258 (9)
C3	1.1166 (4)	−0.1874 (5)	0.6876 (2)	0.0234 (9)
N6	0.9069 (5)	0.1975 (7)	0.5616 (2)	0.0516 (13)
N5	0.8982 (5)	−0.2271 (6)	0.6291 (3)	0.0571 (15)
N4	0.7418 (7)	0.0315 (6)	0.9000 (2)	0.0651 (17)
C5	0.9921 (5)	−0.2038 (6)	0.6565 (2)	0.0308 (11)
C6	0.9373 (9)	0.2022 (10)	0.6174 (3)	0.0700 (18)
H6	0.9931	0.2801	0.6272	0.084*
C8	0.9492 (13)	0.3011 (17)	0.5189 (5)	0.122 (3)
H8A	0.9115	0.3947	0.5282	0.183*
H8B	0.9178	0.2711	0.4811	0.183*
H8C	1.0465	0.3073	0.5187	0.183*
C7	0.8193 (12)	0.0771 (13)	0.5425 (5)	0.113 (3)
H7A	0.8668	−0.0134	0.5472	0.169*
H7B	0.7959	0.0902	0.5022	0.169*
H7C	0.7381	0.0758	0.5657	0.169*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0143 (3)	0.0181 (3)	0.0217 (3)	0.000	0.00059 (15)	0.000
N1	0.023 (2)	0.032 (2)	0.043 (2)	0.0050 (18)	0.0117 (18)	0.0122 (19)
N2	0.0247 (19)	0.029 (2)	0.027 (2)	0.0072 (17)	0.0029 (15)	0.0036 (16)
C4	0.043 (3)	0.033 (3)	0.032 (2)	0.017 (2)	0.010 (2)	0.0043 (19)
O1	0.048 (2)	0.060 (2)	0.0270 (18)	0.0003 (19)	−0.0062 (17)	0.0052 (16)
N3	0.0155 (18)	0.024 (2)	0.0272 (18)	0.0032 (16)	0.0015 (16)	−0.0037 (17)
C1	0.022 (2)	0.024 (2)	0.024 (2)	0.0054 (17)	−0.0030 (16)	−0.0004 (16)

C2	0.029 (2)	0.026 (2)	0.023 (2)	0.0059 (19)	0.0019 (18)	0.0001 (17)
C3	0.021 (2)	0.021 (2)	0.028 (2)	−0.0009 (17)	0.0007 (18)	−0.0001 (17)
N6	0.052 (3)	0.076 (3)	0.027 (2)	0.014 (3)	−0.006 (2)	0.005 (2)
N5	0.036 (3)	0.069 (4)	0.067 (4)	−0.004 (3)	−0.019 (3)	−0.021 (3)
N4	0.100 (5)	0.054 (3)	0.041 (3)	0.030 (3)	0.022 (3)	0.018 (2)
C5	0.029 (3)	0.028 (3)	0.035 (3)	−0.0021 (19)	0.001 (2)	−0.008 (2)
C6	0.072 (4)	0.084 (4)	0.054 (3)	0.025 (4)	0.004 (3)	0.007 (3)
C8	0.143 (7)	0.138 (8)	0.085 (6)	0.023 (7)	0.016 (6)	0.036 (6)
C7	0.116 (7)	0.130 (7)	0.092 (6)	0.023 (6)	−0.024 (5)	−0.032 (6)

Geometric parameters (Å, °)

Cd1—O1 ⁱ	2.322 (4)	C1—N3 ⁱⁱⁱ	1.342 (7)
Cd1—O1	2.322 (4)	C2—C3 ⁱⁱⁱ	1.371 (6)
Cd1—N2 ⁱ	2.339 (4)	C3—C2 ⁱⁱ	1.371 (6)
Cd1—N2	2.339 (4)	C3—C5	1.426 (6)
Cd1—N3 ⁱ	2.353 (4)	N6—C6	1.311 (9)
Cd1—N3	2.353 (4)	N6—C8	1.427 (13)
N1—C1	1.366 (6)	N6—C7	1.469 (12)
N1—H1A	0.8600	N5—C5	1.136 (7)
N1—H1B	0.8600	C6—H6	0.9300
N2—C1	1.347 (6)	C8—H8A	0.9600
N2—C2	1.375 (6)	C8—H8B	0.9600
C4—N4	1.141 (6)	C8—H8C	0.9600
C4—C2	1.426 (6)	C7—H7A	0.9600
O1—C6	1.154 (8)	C7—H7B	0.9600
N3—C1 ⁱⁱ	1.342 (7)	C7—H7C	0.9600
N3—C3	1.371 (6)		
O1 ⁱ —Cd1—O1	172.1 (2)	N3 ⁱⁱⁱ —C1—N1	123.0 (4)
O1 ⁱ —Cd1—N2 ⁱ	88.18 (14)	N2—C1—N1	122.3 (5)
O1—Cd1—N2 ⁱ	86.91 (14)	C3 ⁱⁱⁱ —C2—N2	109.1 (4)
O1 ⁱ —Cd1—N2	86.91 (14)	C3 ⁱⁱⁱ —C2—C4	124.4 (4)
O1—Cd1—N2	88.18 (14)	N2—C2—C4	126.3 (4)
N2 ⁱ —Cd1—N2	103.5 (2)	C2 ⁱⁱ —C3—N3	108.9 (4)
O1 ⁱ —Cd1—N3 ⁱ	95.71 (15)	C2 ⁱⁱ —C3—C5	124.5 (4)
O1—Cd1—N3 ⁱ	90.38 (15)	N3—C3—C5	126.6 (4)
N2 ⁱ —Cd1—N3 ⁱ	167.68 (14)	C6—N6—C8	125.3 (9)
N2—Cd1—N3 ⁱ	88.42 (14)	C6—N6—C7	116.6 (8)
O1 ⁱ —Cd1—N3	90.38 (15)	C8—N6—C7	118.0 (8)
O1—Cd1—N3	95.71 (15)	N5—C5—C3	173.8 (6)
N2 ⁱ —Cd1—N3	88.42 (13)	O1—C6—N6	133.3 (9)
N2—Cd1—N3	167.68 (15)	O1—C6—H6	113.4
N3 ⁱ —Cd1—N3	79.89 (19)	N6—C6—H6	113.4
C1—N1—H1A	120.0	N6—C8—H8A	109.5
C1—N1—H1B	120.0	N6—C8—H8B	109.5
H1A—N1—H1B	120.0	H8A—C8—H8B	109.5
C1—N2—C2	103.4 (4)	N6—C8—H8C	109.5

C1—N2—Cd1	129.4 (3)	H8A—C8—H8C	109.5
C2—N2—Cd1	122.0 (3)	H8B—C8—H8C	109.5
N4—C4—C2	174.4 (6)	N6—C7—H7A	109.5
C6—O1—Cd1	131.7 (6)	N6—C7—H7B	109.5
C1 ⁱⁱ —N3—C3	103.9 (4)	H7A—C7—H7B	109.5
C1 ⁱⁱ —N3—Cd1	132.5 (3)	N6—C7—H7C	109.5
C3—N3—Cd1	123.1 (3)	H7A—C7—H7C	109.5
N3 ⁱⁱⁱ —C1—N2	114.7 (4)	H7B—C7—H7C	109.5
O1 ⁱ —Cd1—N2—C1	136.9 (5)	N2 ⁱ —Cd1—N3—C3	−116.7 (4)
O1—Cd1—N2—C1	−36.8 (5)	N2—Cd1—N3—C3	78.0 (8)
N2 ⁱ —Cd1—N2—C1	49.6 (4)	N3 ⁱ —Cd1—N3—C3	59.4 (3)
N3 ⁱ —Cd1—N2—C1	−127.3 (5)	C2—N2—C1—N3 ⁱⁱⁱ	−0.9 (5)
N3—Cd1—N2—C1	−145.5 (6)	Cd1—N2—C1—N3 ⁱⁱⁱ	153.2 (3)
O1 ⁱ —Cd1—N2—C2	−73.1 (4)	C2—N2—C1—N1	178.5 (4)
O1—Cd1—N2—C2	113.1 (4)	Cd1—N2—C1—N1	−27.4 (7)
N2 ⁱ —Cd1—N2—C2	−160.5 (4)	C1—N2—C2—C3 ⁱⁱⁱ	1.1 (5)
N3 ⁱ —Cd1—N2—C2	22.7 (3)	Cd1—N2—C2—C3 ⁱⁱⁱ	−155.5 (3)
N3—Cd1—N2—C2	4.4 (9)	C1—N2—C2—C4	−174.0 (5)
O1 ⁱ —Cd1—O1—C6	44.5 (6)	Cd1—N2—C2—C4	29.4 (6)
N2 ⁱ —Cd1—O1—C6	−7.3 (6)	N4—C4—C2—C3 ⁱⁱⁱ	−35 (8)
N2—Cd1—O1—C6	96.3 (6)	N4—C4—C2—N2	140 (7)
N3 ⁱ —Cd1—O1—C6	−175.3 (6)	C1 ⁱⁱ —N3—C3—C2 ⁱⁱ	−0.4 (5)
N3—Cd1—O1—C6	−95.4 (6)	Cd1—N3—C3—C2 ⁱⁱ	172.2 (3)
O1 ⁱ —Cd1—N3—C1 ⁱⁱ	−34.6 (4)	C1 ⁱⁱ —N3—C3—C5	179.5 (5)
O1—Cd1—N3—C1 ⁱⁱ	140.3 (4)	Cd1—N3—C3—C5	−7.9 (7)
N2 ⁱ —Cd1—N3—C1 ⁱⁱ	53.5 (4)	C2 ⁱⁱ —C3—C5—N5	−1 (6)
N2—Cd1—N3—C1 ⁱⁱ	−111.8 (7)	N3—C3—C5—N5	179 (100)
N3 ⁱ —Cd1—N3—C1 ⁱⁱ	−130.4 (5)	Cd1—O1—C6—N6	164.9 (6)
O1 ⁱ —Cd1—N3—C3	155.1 (4)	C8—N6—C6—O1	178.2 (9)
O1—Cd1—N3—C3	−30.0 (4)	C7—N6—C6—O1	−0.2 (13)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ O1 ^{iv}	0.86	2.45	3.187 (6)	144
C7—H7C $\cdots$ N5 ^{iv}	0.96	2.68	3.429 (12)	135
C7—H7B $\cdots$ N4 ^v	0.96	2.65	3.496 (11)	148

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