

# Crystal structure of *trans*-diaquabis(4-cyano-benzoato- $\kappa$ O)bis(*N,N*-diethylnicotinamide- $\kappa$ N)-cadmium

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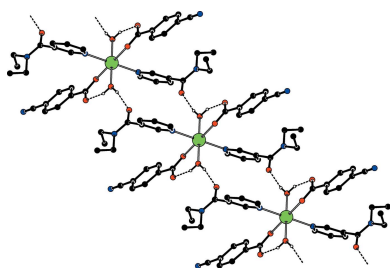
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The mononuclear title cadmium complex,  $[\text{Cd}(\text{C}_{10}\text{H}_{14}\text{N}_2\text{O})_2(\text{C}_8\text{H}_4\text{NO}_2)_2(\text{H}_2\text{O})_2]$ , is centrosymmetric and contains two water molecules, two 4-cyanobenzoate (CB) ligands and two diethylnicotinamide (DENA) ligands. All the ligands are coordinated to the  $\text{Cd}^{\text{II}}$  atom in a monodentate mode. The four nearest O atoms around the  $\text{Cd}^{\text{II}}$  atom form a slightly distorted square-planar arrangement, with the distorted octahedral coordination sphere being completed by the two pyridine N atoms of the DENA ligands at distances of 2.3336 (13) Å. The dihedral angle between the carboxylate group and the adjacent benzene ring is 8.75 (16)°, while the benzene and pyridine rings are oriented at a dihedral angle of 57.83 (5)°. The water molecules exhibit both intramolecular [to the non-coordinating carboxylate O atom, enclosing an  $S(6)$  hydrogen-bonding motif, where  $\text{O}\cdots\text{O} = 2.670$  (2) Å] and intermolecular [to the amide carbonyl O atom, enclosing an  $R_2^2(16)$  ring motif, where  $\text{O}\cdots\text{O} = 2.781$  (2) Å]  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds. The latter lead to the formation of supramolecular chains propagating along [110].

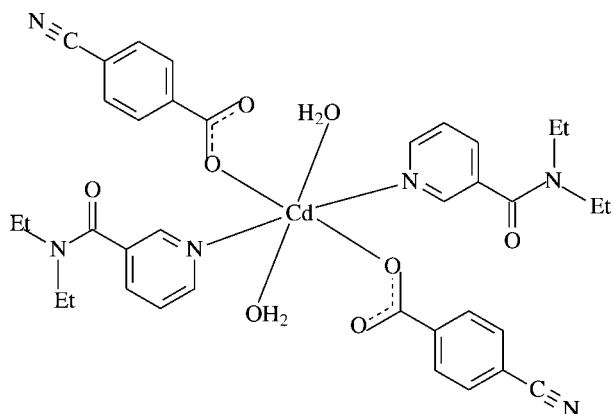
## 1. Chemical context

Nicotinamide (NA) is one form of niacin. A deficiency of this vitamin leads to loss of copper from the body, known as pellagra disease. Pellagra patients show unusually high serum and urinary copper levels (Krishnamachari, 1974). The nicotinic acid derivative *N,N*-diethylnicotinamide (DENA) is an important respiratory stimulant (Bigoli *et al.*, 1972). The crystal structures of some complexes obtained from the reactions of transition metal(II) ions with NA or DENA as ligands, *e.g.*  $[\text{Ni}(\text{NA})_2(\text{C}_7\text{H}_4\text{ClO}_2)_2(\text{H}_2\text{O})_2]$  (Hökelek *et al.*, 2009*a*) and  $[\text{Ni}(\text{DENA})_2(\text{C}_7\text{H}_4\text{ClO}_2)_2(\text{H}_2\text{O})_2]$  (Hökelek *et al.*, 2009*b*), have been determined in our laboratory.

The structure–function–coordination relationships of the arylcarboxylate ion in  $\text{Cd}^{\text{II}}$  complexes of benzoic acid derivatives may change depending on the nature and position of the substituent groups on the benzene ring, the nature of the additional ligand molecule or solvent, and the pH and temperature of synthesis (Shnulin *et al.*, 1981; Nadzhafov *et al.*, 1981; Antsyshkina *et al.*, 1980; Adiwidjaja *et al.*, 1978). When pyridine and its derivatives are used instead of water molecules, the structure is completely different (Catterick *et al.*, 1974). In this context, we synthesized a  $\text{Cd}^{\text{II}}$ -containing compound with 4-cyanobenzoate (CB) and DENA ligands, namely *trans*-diaquabis(4-cyanobenzoato- $\kappa$ O)bis(*N,N*-di-



ethylnicotinamide- $\kappa N$ cadmium,  $[\text{Cd}(\text{CB})_2(\text{DENA})_2(\text{H}_2\text{O})_2]$ , and report herein its crystal structure.



## 2. Structural commentary

The asymmetric unit of the mononuclear title complex contains one  $\text{Cd}^{\text{II}}$  atom located on an inversion centre, one CB ligand, one DENA ligand as well as one water molecule, all ligands coordinating to the  $\text{Cd}^{\text{II}}$  atom in a monodentate mode (Fig. 1).

The two carboxylate O atoms ( $\text{O}2$  and  $\text{O}2^i$ ) [symmetry code: (i)  $-x, -y, -z$ ] of the two symmetry-related monodentate CB anions and water O atoms ( $\text{O}4$  and  $\text{O}4^i$ ) form a slightly distorted square-planar arrangement around the  $\text{Cd}1$  atom, while the slightly distorted octahedral coordination sphere is completed by the two pyridine N atoms ( $\text{N}1$  and  $\text{N}1^i$ ) of two DENA ligands (Fig. 1). The  $\text{Cd}-\text{O}$  bond lengths

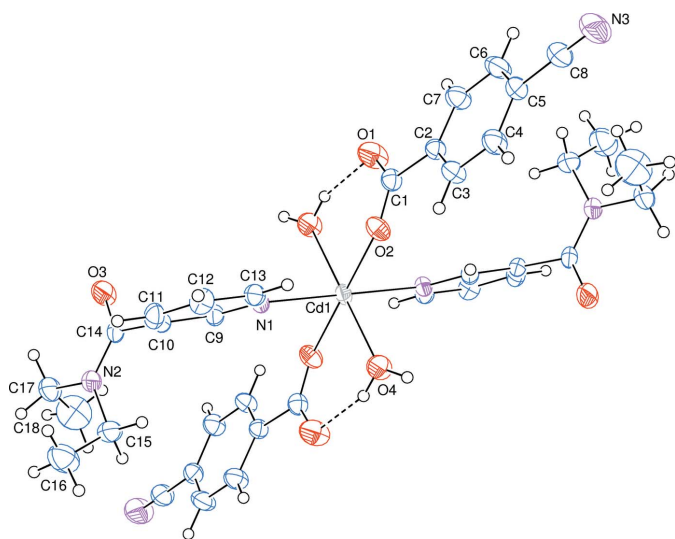


Figure 1

The molecular structure of the title complex with the atom-numbering scheme for the asymmetric unit. Unlabelled atoms are generated by symmetry operation ( $-x, -y, -z$ ). Displacement ellipsoids are drawn at the 50% probability level. Intramolecular  $\text{O}-\text{H}_w \cdots \text{O}_c$  ( $w$  = water,  $c$  = non-coordinating carboxylate O atom) hydrogen bonds, enclosing  $S(6)$  hydrogen-bonding motifs, are shown as dashed lines.

Table 1

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

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O}4-\text{H}41 \cdots \text{O}3^i$	0.78 (3)	2.01 (3)	2.781 (2)	169 (3)
$\text{O}4-\text{H}42 \cdots \text{O}1^{\text{ii}}$	0.87 (3)	1.84 (3)	2.670 (2)	159 (3)

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

involving the water O atoms [ $2.3192(14) \text{\AA}$ ] are *ca*  $0.06 \text{\AA}$  longer than those involving the benzoate oxygen atoms [ $2.2588(12) \text{\AA}$ ]; the  $\text{Cd}-\text{N}$  bond length is the longest with  $2.3336(13) \text{\AA}$  in the  $\text{CdO}_4\text{N}_2$  octahedron. The  $\text{Cd}1$  atom lies  $0.7558(1) \text{\AA}$  below the planar ( $\text{O}1/\text{O}2/\text{C}1$ ) carboxylate group. The  $\text{O}-\text{Cd}-\text{O}$  and  $\text{O}-\text{Cd}-\text{N}$  bond angles range from  $87.54(5)$  to  $92.46(5)^\circ$ . In the carboxylate groups, the  $\text{C}-\text{O}$  bonds of the coordinating O atoms [ $\text{C}1-\text{O}1 = 1.244(2) \text{\AA}$  and  $\text{C}1-\text{O}2 = 1.259(2) \text{\AA}$ ] are  $0.015(2) \text{\AA}$  longer than those of the non-coordinating ones, indicating delocalized bonding arrangements rather than localized single and double bonds. The dihedral angle between the carboxylate group ( $\text{O}1/\text{O}2/\text{C}1$ ) and the adjacent benzene ( $\text{C}2-\text{C}7$ ) ring is  $8.75(16)^\circ$ , while the benzene and pyridine ( $\text{N}1/\text{C}9-\text{C}13$ ) rings are oriented at a dihedral angle of  $57.83(5)^\circ$ .

## 3. Supramolecular features

Intramolecular  $\text{O}-\text{H}_w \cdots \text{O}_c$  ( $w$  = water,  $c$  = non-coordinating carboxylate O atom) hydrogen bonds (Table 1) link the water molecules by one of their H atoms to the CB anions, enclosing  $S(6)$  hydrogen-bonding motifs (Fig. 1). The other water H atom is involved in intermolecular  $\text{O}-\text{H}_w \cdots \text{O}_{\text{DENA}}$  ( $\text{O}_{\text{DENA}}$  = carbonyl O atom of  $N,N'$ -diethylnicotinamide) hydrogen bonds (Table 1), enclosing  $R_2^2(16)$  ring motifs, leading to the formation of infinite chains (Fig. 2) propagating along the  $[110]$  direction (Fig. 3).

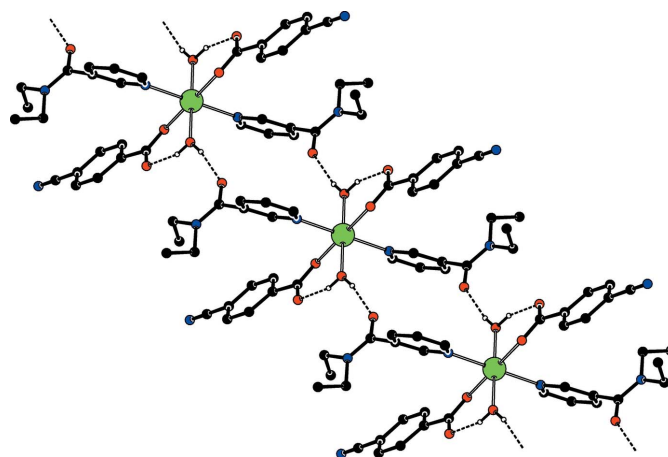
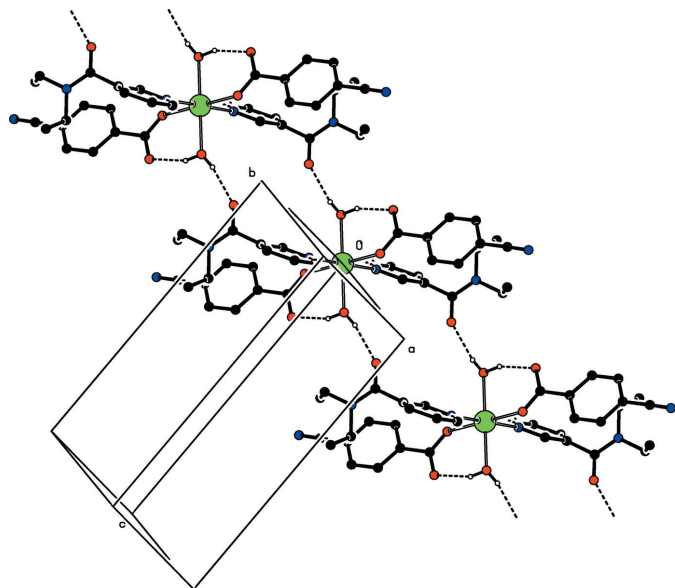


Figure 2

Part of the supramolecular chain of the title compound. Intermolecular  $\text{O}-\text{H}_w \cdots \text{O}_{\text{DENA}}$  ( $\text{O}_{\text{DENA}}$  = carbonyl O atom of  $N,N'$ -diethylnicotinamide) hydrogen bonds, enclosing  $R_2^2(16)$  ring motifs, are shown as dashed lines. Non-bonding H atoms have been omitted for clarity.



**Figure 3**  
Part of the crystal structure. Intra- and intermolecular [O—H<sub>w</sub> ··· O<sub>c</sub> and O—H<sub>w</sub> ··· O<sub>DENA</sub>, respectively] hydrogen bonds are shown as dashed lines (see Table 1). Non-bonding H atoms have been omitted for clarity.

#### 4. Synthesis and crystallization

The title compound was prepared by the reaction of CdSO<sub>4</sub>·8/3H<sub>2</sub>O (0.64 g, 2.5 mmol) in H<sub>2</sub>O (50 ml) and diethylnicotinamide (0.89 g, 5 mmol) in H<sub>2</sub>O (10 ml) with sodium 4-cyanobenzoate (0.85 g, 5 mmol) in H<sub>2</sub>O (100 ml). The mixture was filtered and set aside to crystallize at ambient temperature for several days, giving colourless single crystals.

#### 5. Refinement

Experimental details including the crystal data, data collection and refinement are summarized in Table 2. Atoms H41 and H42 (for H<sub>2</sub>O) were located in a difference Fourier map and were refined freely. The C-bound H atoms were positioned geometrically with C—H = 0.93, 0.97 and 0.96 Å, for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = k \times U_{\text{eq}}(\text{C})$ , where  $k = 1.5$  for methyl H atoms and  $k = 1.2$  for aromatic and methylene H-atoms.

#### Acknowledgements

The authors acknowledge the Scientific and Technological Research Application and Research Center, Sinop University, Turkey, for the use of the Bruker D8 QUEST diffractometer. This work was supported financially by Kafkas University, Scientific Research Projects Coordinator (project No. 2016-FM-49).

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	[Cd(C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O) <sub>2</sub> (C <sub>8</sub> H <sub>4</sub> NO <sub>2</sub> ) <sub>2</sub> ·(H <sub>2</sub> O) <sub>2</sub> ]
$M_r$	797.16
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	296
$a, b, c$ (Å)	7.5125 (2), 8.6671 (3), 15.3079 (5)
$\alpha, \beta, \gamma$ (°)	86.198 (3), 76.249 (4), 74.730 (3)
$V$ (Å <sup>3</sup> )	933.97 (5)
$Z$	1
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	0.64
Crystal size (mm)	0.15 × 0.11 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2012)
$T_{\text{min}}, T_{\text{max}}$	0.595, 0.746
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	46611, 4638, 4538
$R_{\text{int}}$	0.044
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.027, 0.068, 1.09
No. of reflections	4638
No. of parameters	243
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.42, -1.02

Computer programs: APEX2 and SAINT (Bruker, 2012), SHELXS97 and SHELXL97 (Sheldrick, 2008), ORTEP-3 for Windows and WinGX (Farrugia, 2012) and PLATON (Spek, 2009).

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## supporting information

*Acta Cryst.* (2016). E72, 1827-1829 [https://doi.org/10.1107/S2056989016018247]

## Crystal structure of *trans*-diaquabis(4-cyanobenzoato- $\kappa$ O)bis(*N,N*-diethylnicotinamide- $\kappa$ N)cadmium

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### Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINTE* (Bruker, 2012); data reduction: *SAINTE* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

### *trans*-Diaquabis(4-cyanobenzoato- $\kappa$ O)bis(*N,N*-diethylnicotinamide- $\kappa$ N)cadmium

#### Crystal data

[Cd(C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>O)<sub>2</sub>(C<sub>8</sub>H<sub>4</sub>NO<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]

$M_r = 797.16$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 7.5125$  (2) Å

$b = 8.6671$  (3) Å

$c = 15.3079$  (5) Å

$\alpha = 86.198$  (3)°

$\beta = 76.249$  (4)°

$\gamma = 74.730$  (3)°

$V = 933.97$  (5) Å<sup>3</sup>

$Z = 1$

$F(000) = 410$

$D_x = 1.417$  Mg m<sup>-3</sup>

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

Cell parameters from 9549 reflections

$\theta = 3.3$ – $28.4$ °

$\mu = 0.64$  mm<sup>-1</sup>

$T = 296$  K

Block, colourless

$0.15 \times 0.11 \times 0.10$  mm

#### Data collection

Bruker APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2012)

$T_{\min} = 0.595$ ,  $T_{\max} = 0.746$

46611 measured reflections

4638 independent reflections

4538 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 28.4$ °,  $\theta_{\min} = 3.3$ °

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -20 \rightarrow 20$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.068$

$S = 1.09$

4638 reflections

243 parameters

0 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

$$w = 1/[\sigma^2(F_o^2) + (0.0332P)^2 + 0.4012P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.42 \text{ e } \text{Å}^{-3}$

$$\Delta\rho_{\min} = -1.02 \text{ e } \text{Å}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick, 2008),  $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.063 (3)

*Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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  $F^2 > 2\sigma(F^2)$  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<sup>2</sup>)*

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.0000	0.0000	0.0000	0.03023 (7)
O1	0.1214 (2)	0.0630 (2)	-0.22948 (11)	0.0618 (4)
O2	0.25363 (17)	0.01600 (17)	-0.11090 (8)	0.0414 (3)
O3	-0.5079 (2)	0.6289 (2)	0.12687 (10)	0.0600 (4)
O4	0.1904 (2)	-0.1246 (2)	0.09660 (10)	0.0536 (4)
H41	0.281 (4)	-0.194 (3)	0.0977 (17)	0.054 (7)*
H42	0.106 (4)	-0.123 (3)	0.147 (2)	0.064 (8)*
N1	-0.01528 (19)	0.24366 (16)	0.06156 (9)	0.0312 (3)
N2	-0.4728 (2)	0.58766 (18)	0.27019 (10)	0.0400 (3)
N3	1.1521 (3)	-0.2028 (3)	-0.46792 (15)	0.0799 (7)
C1	0.2592 (2)	0.0188 (2)	-0.19381 (12)	0.0349 (3)
C2	0.4546 (2)	-0.03711 (19)	-0.25493 (11)	0.0324 (3)
C3	0.6144 (2)	-0.0663 (2)	-0.21992 (12)	0.0388 (4)
H3	0.6008	-0.0560	-0.1584	0.047*
C4	0.7941 (3)	-0.1105 (2)	-0.27535 (13)	0.0431 (4)
H4	0.9008	-0.1289	-0.2515	0.052*
C5	0.8134 (3)	-0.1272 (2)	-0.36706 (12)	0.0412 (4)
C6	0.6546 (3)	-0.1021 (3)	-0.40264 (13)	0.0498 (5)
H6	0.6684	-0.1152	-0.4639	0.060*
C7	0.4760 (3)	-0.0575 (3)	-0.34684 (13)	0.0449 (4)
H7	0.3694	-0.0409	-0.3706	0.054*
C8	1.0022 (3)	-0.1694 (3)	-0.42433 (14)	0.0546 (5)
C9	-0.1852 (2)	0.33349 (19)	0.10302 (11)	0.0317 (3)
H9	-0.2919	0.2972	0.1045	0.038*
C10	-0.2092 (2)	0.47761 (19)	0.14372 (11)	0.0322 (3)
C11	-0.0502 (3)	0.5326 (2)	0.13986 (13)	0.0410 (4)
H11	-0.0611	0.6289	0.1666	0.049*
C12	0.1253 (3)	0.4418 (2)	0.09551 (13)	0.0413 (4)
H12	0.2339	0.4768	0.0916	0.050*
C13	0.1368 (2)	0.2986 (2)	0.05715 (11)	0.0347 (3)
H13	0.2549	0.2382	0.0272	0.042*

C14	-0.4097 (2)	0.57261 (19)	0.18114 (11)	0.0357 (3)
C15	-0.3659 (3)	0.5045 (3)	0.33602 (13)	0.0504 (5)
H15A	-0.2440	0.4405	0.3041	0.060*
H15B	-0.4343	0.4325	0.3716	0.060*
C16	-0.3345 (4)	0.6172 (4)	0.39795 (18)	0.0699 (7)
H16A	-0.2536	0.5578	0.4353	0.105*
H16B	-0.4540	0.6715	0.4351	0.105*
H16C	-0.2757	0.6942	0.3630	0.105*
C17	-0.6711 (3)	0.6737 (3)	0.30629 (14)	0.0497 (5)
H17A	-0.7148	0.7492	0.2615	0.060*
H17B	-0.6784	0.7340	0.3588	0.060*
C18	-0.7992 (4)	0.5630 (5)	0.3320 (3)	0.0889 (9)
H18A	-0.9278	0.6245	0.3520	0.133*
H18B	-0.7624	0.4932	0.3796	0.133*
H18C	-0.7892	0.5003	0.2808	0.133*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cd1	0.02713 (10)	0.02936 (10)	0.03006 (10)	-0.00088 (6)	-0.00360 (6)	-0.00758 (6)
O1	0.0332 (7)	0.0956 (13)	0.0485 (8)	-0.0023 (7)	-0.0093 (6)	-0.0017 (8)
O2	0.0319 (6)	0.0535 (7)	0.0368 (6)	-0.0134 (5)	0.0008 (5)	-0.0081 (5)
O3	0.0519 (8)	0.0668 (10)	0.0434 (7)	0.0231 (7)	-0.0171 (6)	-0.0088 (7)
O4	0.0356 (7)	0.0698 (10)	0.0435 (8)	0.0135 (7)	-0.0154 (6)	-0.0032 (7)
N1	0.0306 (6)	0.0294 (6)	0.0299 (6)	-0.0027 (5)	-0.0043 (5)	-0.0043 (5)
N2	0.0396 (8)	0.0360 (7)	0.0348 (7)	0.0049 (6)	-0.0053 (6)	-0.0024 (6)
N3	0.0532 (12)	0.0997 (18)	0.0569 (12)	0.0069 (12)	0.0145 (10)	0.0032 (12)
C1	0.0303 (8)	0.0347 (8)	0.0379 (8)	-0.0093 (6)	-0.0026 (6)	-0.0019 (6)
C2	0.0316 (8)	0.0321 (7)	0.0316 (7)	-0.0088 (6)	-0.0025 (6)	-0.0002 (6)
C3	0.0349 (8)	0.0493 (10)	0.0304 (8)	-0.0102 (7)	-0.0034 (6)	-0.0040 (7)
C4	0.0319 (8)	0.0531 (11)	0.0403 (9)	-0.0068 (7)	-0.0045 (7)	-0.0029 (8)
C5	0.0382 (9)	0.0396 (9)	0.0366 (9)	-0.0040 (7)	0.0030 (7)	-0.0005 (7)
C6	0.0509 (11)	0.0634 (13)	0.0281 (8)	-0.0073 (9)	-0.0025 (7)	-0.0041 (8)
C7	0.0399 (9)	0.0581 (11)	0.0353 (9)	-0.0084 (8)	-0.0102 (7)	-0.0019 (8)
C8	0.0476 (11)	0.0586 (12)	0.0410 (10)	0.0007 (9)	0.0049 (9)	0.0023 (9)
C9	0.0305 (7)	0.0277 (7)	0.0343 (8)	-0.0040 (6)	-0.0053 (6)	-0.0027 (6)
C10	0.0369 (8)	0.0266 (7)	0.0286 (7)	0.0011 (6)	-0.0087 (6)	-0.0012 (6)
C11	0.0485 (10)	0.0296 (8)	0.0475 (10)	-0.0071 (7)	-0.0173 (8)	-0.0066 (7)
C12	0.0383 (9)	0.0404 (9)	0.0499 (10)	-0.0132 (7)	-0.0154 (8)	0.0004 (8)
C13	0.0309 (8)	0.0366 (8)	0.0330 (8)	-0.0033 (6)	-0.0065 (6)	-0.0001 (6)
C14	0.0382 (8)	0.0266 (7)	0.0358 (8)	0.0039 (6)	-0.0086 (7)	-0.0048 (6)
C15	0.0534 (11)	0.0517 (11)	0.0361 (9)	0.0024 (9)	-0.0098 (8)	0.0041 (8)
C16	0.0641 (15)	0.0883 (19)	0.0550 (13)	-0.0054 (13)	-0.0218 (12)	-0.0106 (13)
C17	0.0414 (10)	0.0518 (11)	0.0422 (10)	0.0050 (8)	-0.0007 (8)	-0.0062 (8)
C18	0.0602 (16)	0.111 (3)	0.097 (2)	-0.0325 (17)	-0.0083 (16)	-0.003 (2)

*Geometric parameters (Å, °)*

Cd1—O2	2.2588 (12)	C6—H6	0.9300
Cd1—O2 <sup>i</sup>	2.2588 (12)	C7—H7	0.9300
Cd1—O4	2.3192 (14)	C8—N3	1.138 (3)
Cd1—O4 <sup>i</sup>	2.3192 (14)	C9—C10	1.383 (2)
Cd1—N1	2.3336 (13)	C9—H9	0.9300
Cd1—N1 <sup>i</sup>	2.3336 (13)	C10—C11	1.386 (3)
O2—C1	1.259 (2)	C10—C14	1.508 (2)
O3—C14	1.233 (2)	C11—C12	1.384 (3)
O4—H41	0.78 (3)	C11—H11	0.9300
O4—H42	0.87 (3)	C12—H12	0.9300
N1—C9	1.340 (2)	C13—C12	1.382 (3)
N1—C13	1.335 (2)	C13—H13	0.9300
N2—C15	1.471 (2)	C14—N2	1.336 (2)
N2—C17	1.469 (2)	C15—C16	1.503 (3)
C1—O1	1.244 (2)	C15—H15A	0.9700
C2—C1	1.516 (2)	C15—H15B	0.9700
C2—C3	1.386 (2)	C16—H16A	0.9600
C2—C7	1.395 (2)	C16—H16B	0.9600
C3—C4	1.384 (2)	C16—H16C	0.9600
C3—H3	0.9300	C17—C18	1.503 (4)
C4—H4	0.9300	C17—H17A	0.9700
C5—C4	1.390 (3)	C17—H17B	0.9700
C5—C6	1.387 (3)	C18—H18A	0.9600
C5—C8	1.446 (3)	C18—H18B	0.9600
C6—C7	1.380 (3)	C18—H18C	0.9600
O2 <sup>i</sup> —Cd1—O2	180.00 (6)	C6—C7—H7	119.9
O2—Cd1—O4	92.15 (5)	N3—C8—C5	178.6 (3)
O2 <sup>i</sup> —Cd1—O4	87.85 (5)	N1—C9—C10	123.03 (15)
O2—Cd1—O4 <sup>i</sup>	87.85 (5)	N1—C9—H9	118.5
O2 <sup>i</sup> —Cd1—O4 <sup>i</sup>	92.15 (5)	C10—C9—H9	118.5
O2—Cd1—N1	92.46 (5)	C9—C10—C11	118.26 (15)
O2 <sup>i</sup> —Cd1—N1	87.54 (5)	C9—C10—C14	117.30 (15)
O2—Cd1—N1 <sup>i</sup>	87.54 (5)	C11—C10—C14	124.12 (15)
O2 <sup>i</sup> —Cd1—N1 <sup>i</sup>	92.46 (5)	C10—C11—H11	120.5
O4—Cd1—O4 <sup>i</sup>	180.00 (5)	C12—C11—C10	118.93 (16)
O4—Cd1—N1	87.91 (6)	C12—C11—H11	120.5
O4 <sup>i</sup> —Cd1—N1	92.09 (6)	C11—C12—H12	120.5
O4—Cd1—N1 <sup>i</sup>	92.09 (6)	C13—C12—C11	119.07 (16)
O4 <sup>i</sup> —Cd1—N1 <sup>i</sup>	87.91 (6)	C13—C12—H12	120.5
N1 <sup>i</sup> —Cd1—N1	180.00 (11)	N1—C13—C12	122.42 (16)
C1—O2—Cd1	125.35 (11)	N1—C13—H13	118.8
Cd1—O4—H41	141.0 (19)	C12—C13—H13	118.8
Cd1—O4—H42	101.5 (18)	O3—C14—N2	123.71 (16)
H41—O4—H42	110 (3)	O3—C14—C10	117.33 (15)
C9—N1—Cd1	118.45 (11)	N2—C14—C10	118.94 (14)

C13—N1—Cd1	123.28 (11)	N2—C15—C16	112.93 (19)
C13—N1—C9	118.27 (14)	N2—C15—H15A	109.0
C14—N2—C15	124.30 (15)	N2—C15—H15B	109.0
C14—N2—C17	118.61 (15)	C16—C15—H15A	109.0
C17—N2—C15	116.50 (16)	C16—C15—H15B	109.0
O1—C1—O2	126.45 (16)	H15A—C15—H15B	107.8
O1—C1—C2	117.84 (16)	C15—C16—H16A	109.5
O2—C1—C2	115.71 (15)	C15—C16—H16B	109.5
C3—C2—C1	120.04 (15)	C15—C16—H16C	109.5
C3—C2—C7	119.33 (16)	H16A—C16—H16B	109.5
C7—C2—C1	120.63 (16)	H16A—C16—H16C	109.5
C2—C3—H3	119.6	H16B—C16—H16C	109.5
C4—C3—C2	120.80 (16)	N2—C17—C18	112.4 (2)
C4—C3—H3	119.6	N2—C17—H17A	109.1
C3—C4—C5	119.28 (17)	N2—C17—H17B	109.1
C3—C4—H4	120.4	C18—C17—H17A	109.1
C5—C4—H4	120.4	C18—C17—H17B	109.1
C4—C5—C8	118.55 (19)	H17A—C17—H17B	107.9
C6—C5—C4	120.48 (17)	C17—C18—H18A	109.5
C6—C5—C8	120.97 (18)	C17—C18—H18B	109.5
C5—C6—H6	120.1	C17—C18—H18C	109.5
C7—C6—C5	119.80 (17)	H18A—C18—H18B	109.5
C7—C6—H6	120.1	H18A—C18—H18C	109.5
C2—C7—H7	119.9	H18B—C18—H18C	109.5
C6—C7—C2	120.28 (17)		
O2—Cd1—N1—C9	148.84 (12)	C7—C2—C1—O2	172.21 (17)
O2 <sup>i</sup> —Cd1—N1—C9	-31.16 (12)	C1—C2—C3—C4	-177.11 (17)
O2—Cd1—N1—C13	-30.80 (13)	C7—C2—C3—C4	2.0 (3)
O2 <sup>i</sup> —Cd1—N1—C13	149.20 (13)	C1—C2—C7—C6	177.33 (19)
O4—Cd1—N1—C9	-119.09 (12)	C3—C2—C7—C6	-1.7 (3)
O4 <sup>i</sup> —Cd1—N1—C9	60.91 (12)	C2—C3—C4—C5	-0.6 (3)
O4—Cd1—N1—C13	61.26 (13)	C6—C5—C4—C3	-0.9 (3)
O4 <sup>i</sup> —Cd1—N1—C13	-118.74 (13)	C8—C5—C4—C3	178.4 (2)
O4—Cd1—O2—C1	152.29 (15)	C4—C5—C6—C7	1.2 (3)
O4 <sup>i</sup> —Cd1—O2—C1	-27.71 (15)	C8—C5—C6—C7	-178.2 (2)
N1—Cd1—O2—C1	-119.71 (14)	C5—C6—C7—C2	0.2 (3)
N1 <sup>i</sup> —Cd1—O2—C1	60.29 (14)	N1—C9—C10—C11	1.2 (2)
Cd1—O2—C1—O1	24.2 (3)	N1—C9—C10—C14	175.06 (15)
Cd1—O2—C1—C2	-156.03 (11)	C9—C10—C11—C12	0.1 (3)
Cd1—N1—C9—C10	178.26 (12)	C14—C10—C11—C12	-173.25 (17)
C13—N1—C9—C10	-2.1 (2)	C9—C10—C14—O3	-67.2 (2)
Cd1—N1—C13—C12	-178.75 (13)	C9—C10—C14—N2	111.03 (19)
C9—N1—C13—C12	1.6 (2)	C11—C10—C14—O3	106.3 (2)
C14—N2—C15—C16	122.5 (2)	C11—C10—C14—N2	-75.5 (2)
C17—N2—C15—C16	-66.5 (3)	C10—C11—C12—C13	-0.6 (3)
C14—N2—C17—C18	95.2 (3)	N1—C13—C12—C11	-0.3 (3)
C15—N2—C17—C18	-76.3 (3)	O3—C14—N2—C17	1.0 (3)



C3—C2—C1—O1	171.04 (18)	O3—C14—N2—C15	171.9 (2)
C3—C2—C1—O2	-8.7 (2)	C10—C14—N2—C17	-177.05 (17)
C7—C2—C1—O1	-8.0 (3)	C10—C14—N2—C15	-6.2 (3)

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

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O4—H41 $\cdots$ O3 <sup>ii</sup>	0.78 (3)	2.01 (3)	2.781 (2)	169 (3)
O4—H42 $\cdots$ O1 <sup>i</sup>	0.87 (3)	1.84 (3)	2.670 (2)	159 (3)

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