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Crystal structure of bis[2-(1*H*-benzimidazol-2-yl-κN^3)aniline-κN]bis(nitrato-κO)cadmium(II)

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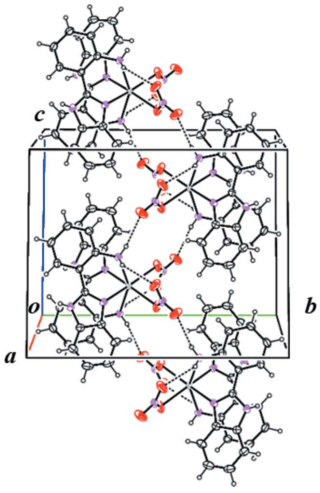
In the title compound, $[Cd(NO_3)_2(C_{13}H_{11}N_3)_2]$, the Cd^{II} atom lies on a twofold rotation axis and is coordinated by four N atoms and two O atoms, provided by two bidentate 2-(1*H*-benzimidazol-2-yl)aniline ligands, and two nitrato O atoms, forming a distorted octahedral geometry [range of bond angles around the Cd atom = 73.82 (2)–106.95 (8)°]. In the ligand, the dihedral angle between the aniline ring and the benzimidazole ring system is 30.43 (7)°. The discrete complex molecule is stabilized by an intramolecular N—H···O hydrogen bond. In the crystal, intermolecular N—H···O hydrogen bonds link the molecules, forming a three-dimensional network.

1. Chemical context

Azole and benzazole derivatives are well-known nitrogen-containing heterocyclic compounds, and are of great interest because of their broad spectrum of biological activity (Esparza-Ruiz *et al.*, 2011; Hock *et al.*, 2013). Imidazole is an azapyrrole in which the nitrogen atoms are separated by one carbon atom. Benzimidazole, a fused heterocycle with benzene and imidazole, is associated with a wide array of pharmacological activities (Akhtar *et al.*, 2017), and benzimidazole derivatives exhibit a wide range of various biological activities. These include bactericidal (Carcanague *et al.*, 2002) and fungicidal (Lezcano *et al.*, 2002; Aghatabay *et al.*, 2007) properties. Their metal complexes have been shown to display antitumor activity and are important biological molecules (Sánchez-Guadarrama *et al.*, 2009; Ramla *et al.*, 2007; Wang *et al.*, 2007). Recently, we reported on the synthesis and structural features of Zn (Kim & Kang, 2015*a*) and Ag (Kim & Kang, 2015*b*) complexes with benzimidazole derivatives. In this work, we have synthesized the title compound and characterized it by single crystal X-ray crystallography.



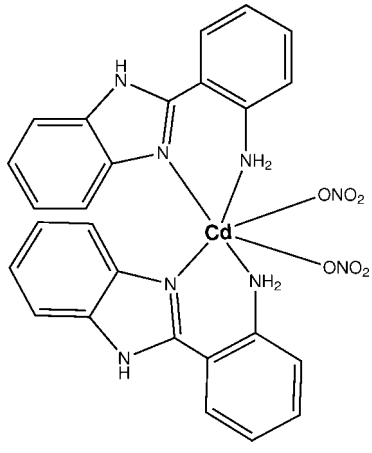


Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N9—H9···O20^{i}	0.75 (3)	2.39 (3)	3.012 (3)	140 (3)
N9—H9···O21^{i}	0.75 (3)	2.51 (3)	3.238 (3)	163 (3)
N17—H17A···O21	0.86 (3)	2.34 (3)	2.973 (3)	131 (2)
N17—H17B···O20^{ii}	0.79 (3)	2.24 (3)	3.024 (3)	170 (3)

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

2. Structural commentary

The molecular structure of the title complex is shown in Fig. 1. The complex lies about a twofold rotation axis which passes through the Cd^{II} atom, the coordination geometry around which is distorted octahedral with two O atoms of two nitrato ligands and four N atoms of two bidentate 2-(1*H*-benzimidazol-2-yl)aniline ligands. The Cd—N and Cd—O bond lengths [Cd1—N2 = 2.317 (2), Cd1—N17 = 2.437 (2) and Cd1—O19 = 2.3175 (19) Å] are comparable with those of other Cd complexes (Barszcz *et al.*, 2013; Jalilehvand *et al.*, 2009). The bond angles around the Cd1 atom are in the range of 73.82 (8)–106.95 (8)°. The dihedral angle between the benzimidazole (N2/C3–C8/N9/C10) ring system and the aniline (C11–C16/N17) plane in the bidentate ligand is 30.43 (7)°. This twisting is a driving force in the formation of weak Cd1—N17 bonding, this bond being [2.437 (2) Å] a little longer than Cd1—N2 [2.317 (2) Å]. This elongation was also observed in our previous studies of imidazoleaniline–metal complexes (Zn: Kim & Kang, 2015*a*; Ag: Kim & Kang, 2015*b*).

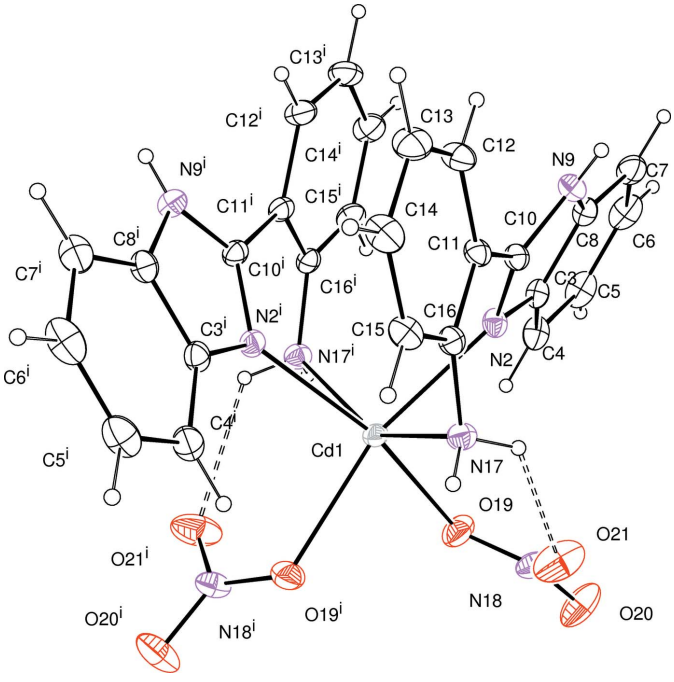


Figure 1
Molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. The intramolecular N—H···O hydrogen bonds are indicated by dashed lines. [Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.]

The N2—C10 bond length of 1.327 (3) Å in the imidazole ring shows double-bond character compared to the other N—C bond lengths [N2—C3 = 1.397 (3), C8—N9 = 1.384 (3) and N9—C10 = 1.355 (3) Å]. The discrete molecule is stabilized by an intramolecular N—H···O hydrogen bond (Table 1).

3. Supramolecular features

In the crystal, molecules are linked by a series of N—H···O interactions. The nitrate group containing oxygen atom O21 forms both intra- and intermolecular hydrogen bonds. Molecules are arranged into a zigzag chain along the *c*-axis direction *via* an N—H···O hydrogen bond (N17—H17B···O20^{ii}; symmetry code as in Table 1; Fig. 2). The other N—H···O hydrogen bonds (N9—H9···O20^{i} and N9—H9···O21^{i}; Table 1) link the molecules into a three-dimensional network (Fig. 3).

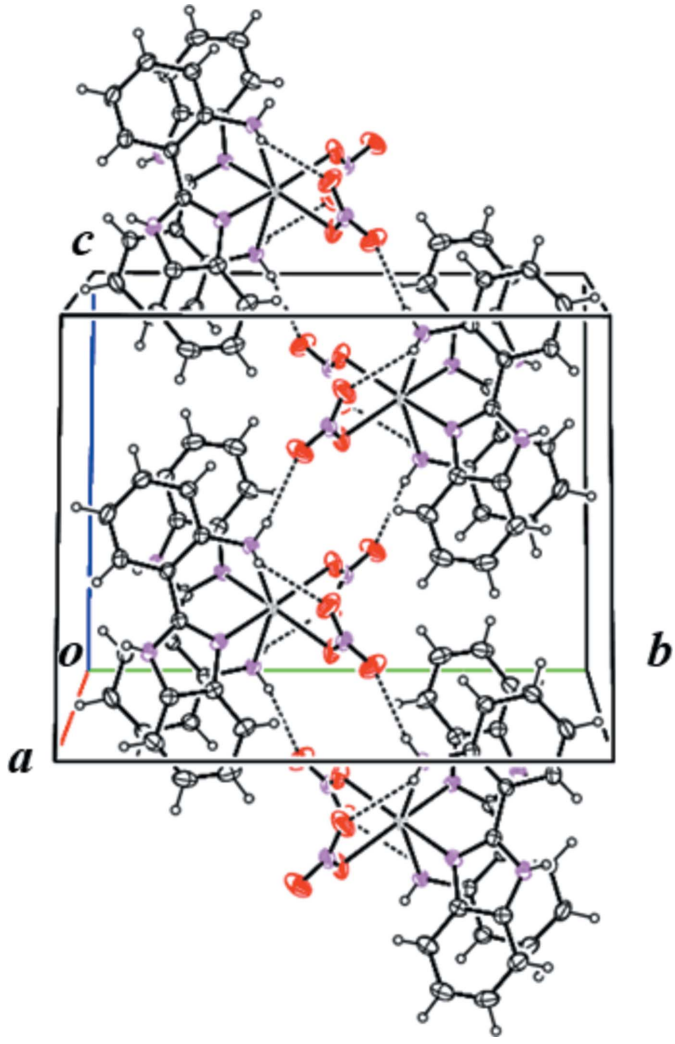


Figure 2
Partial packing diagram of the title compound, showing molecules linked by intermolecular N—H···O hydrogen bonds (dashed lines), viewed along the *a*-axis direction.

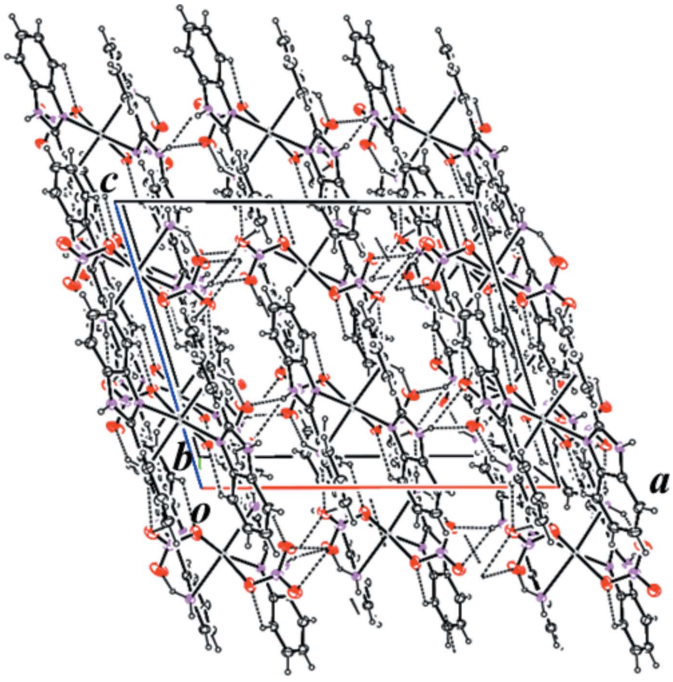


Figure 3
A view along the *b* axis of the crystal packing of the title compound, showing the three-dimensional network linked of molecules linked by N—H···O hydrogen bonds (dashed lines, Table 1).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.40, Feb. 2019; Groom *et al.*, 2016) gave 4678 entries for crystal structures related to benzimidazoles. However, there are only 14 entries involving the ligands 2-(1*H*-benzimidazol-2-yl)aniline or 2-(2-aminophenyl)-1*H*-benzimidazole with a transition metal. These include Ni (refcode EWUZOM; Esparza-Ruiz *et al.*, 2011), Zn [AWOLEE (Eltayeb *et al.*, 2011) and JUFCOE (Kim & Kang, 2015*a*)], Ru (NUNLID; Małecki, 2012) and Re (UYELEQ; Machura *et al.*, 2011).

5. Synthesis and crystallization

Chemicals were obtained commercially in reagent grade and used as received. Solvents were dried using standard procedures described in the literature. To a stirred solution of $Cd(NO_3)\cdot 4H_2O$ (0.154 g, 0.5 mmol) in ethanol (20 ml) was added a solution of 2-(1*H*-benzimidazol-2-yl)aniline (0.209 g, 1.0 mmol) in ethanol (10 ml) at 333 K. After 24 h of stirring, the title complex was obtained as a white powder. The powder was filtered off and washed with ethanol. Colourless crystals of the title complex were obtained by slow evaporation of the methanol solvent at room temperature within two weeks.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms of the NH and NH_2 groups were located in a difference-Fourier map and refined freely [refined distances: N—H = 0.75 (3)–0.86 (3) Å]. Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd(NO_3)_2(C_{13}H_{11}N_3)_2]$
M_r	654.91
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	296
a, *b*, *c* (Å)	14.6899 (4), 15.0250 (3), 12.2269 (3)
β (°)	106.8431 (15)
V (Å^3)	2582.90 (11)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.91
Crystal size (mm)	0.15 × 0.13 × 0.12
Data collection	
Diffractometer	Bruker *SMART* CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.546, 0.726
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11727, 3087, 2729
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.035, 0.078, 1.06
No. of reflections	3087
No. of parameters	198
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.82, −0.35

Computer programs: *SMART* and *SAINT* (Bruker, 2012), *SHELXS2013* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015) and *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012).

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Crystal structure of bis[2-(1*H*-benzimidazol-2-yl-κN^3)aniline-κN]bis(nitrato-κO)cadmium(II)

Yongtae Kim and Sung Kwon Kang

Computing details

Data collection: *SMART* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Bis[2-(1*H*-benzimidazol-2-yl-κN^3)aniline-κN]bis(nitrato-κO)cadmium(II)

Crystal data

$[Cd(NO_3)_2(C_{13}H_{11}N_3)_2]$
$M_r = 654.91$
Monoclinic, $C2/c$
$a = 14.6899$ (4) Å
$b = 15.0250$ (3) Å
$c = 12.2269$ (3) Å
$\beta = 106.8431$ (15)°
$V = 2582.90$ (11) Å^3
$Z = 4$
$F(000) = 1320$
$D_x = 1.684$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5554 reflections
$\theta = 2.4$–$28.0°$
$\mu = 0.91$ mm^{-1}
$T = 296$ K
Block, colourless
0.15 × 0.13 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
$T_{min} = 0.546$, $T_{max} = 0.726$
11727 measured reflections
3087 independent reflections
2729 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.0°$
$h = -19 \rightarrow 17$
$k = -19 \rightarrow 20$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.078$
$S = 1.06$
3087 reflections
198 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 0.8298P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.82$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.62214 (2)	0.7500	0.03198 (10)
N2	0.59443 (14)	0.72062 (13)	0.68561 (17)	0.0345 (4)
C3	0.60535 (16)	0.72958 (16)	0.5763 (2)	0.0357 (5)
C4	0.57954 (19)	0.6718 (2)	0.4835 (2)	0.0470 (7)
H4	0.5507	0.6173	0.4877	0.056*
C5	0.5990 (2)	0.6994 (2)	0.3847 (3)	0.0562 (8)
H5	0.5826	0.6628	0.3206	0.067*
C6	0.6425 (2)	0.7807 (2)	0.3793 (3)	0.0594 (8)
H6	0.6538	0.7970	0.3110	0.071*
C7	0.6695 (2)	0.8379 (2)	0.4705 (3)	0.0495 (7)
H7	0.6997	0.8917	0.4663	0.059*
C8	0.64909 (17)	0.81075 (17)	0.5695 (2)	0.0373 (5)
N9	0.66350 (16)	0.85021 (15)	0.67542 (19)	0.0380 (5)
H9	0.696 (2)	0.889 (2)	0.697 (3)	0.054 (10)*
C10	0.62989 (16)	0.79434 (15)	0.7417 (2)	0.0323 (5)
C11	0.62624 (16)	0.81778 (15)	0.8566 (2)	0.0334 (5)
C12	0.6159 (2)	0.90724 (18)	0.8829 (2)	0.0443 (6)
H12	0.6155	0.9506	0.8285	0.053*
C13	0.6065 (2)	0.93253 (19)	0.9865 (3)	0.0540 (7)
H13	0.5984	0.9922	1.0017	0.065*
C14	0.6090 (2)	0.86845 (19)	1.0683 (3)	0.0520 (7)
H14	0.6028	0.8852	1.1390	0.062*
C15	0.62043 (18)	0.78054 (18)	1.0463 (2)	0.0428 (6)
H15	0.6230	0.7383	1.1027	0.051*
C16	0.62832 (16)	0.75354 (16)	0.9400 (2)	0.0331 (5)
N17	0.63122 (16)	0.66172 (14)	0.9164 (2)	0.0367 (5)
H17A	0.674 (2)	0.6453 (18)	0.885 (3)	0.040 (8)*
H17B	0.640 (2)	0.6314 (18)	0.972 (3)	0.037 (8)*
N18	0.63805 (17)	0.48486 (14)	0.6968 (2)	0.0457 (5)
O19	0.55302 (15)	0.50697 (13)	0.6581 (2)	0.0584 (6)
O20	0.67211 (17)	0.43131 (17)	0.6449 (2)	0.0793 (8)
O21	0.6875 (2)	0.51407 (17)	0.7877 (2)	0.0861 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02785 (14)	0.02431 (13)	0.04112 (16)	0.000	0.00582 (10)	0.000
N2	0.0292 (11)	0.0388 (11)	0.0348 (11)	−0.0043 (8)	0.0083 (8)	−0.0076 (9)
C3	0.0269 (12)	0.0433 (14)	0.0362 (14)	0.0012 (9)	0.0078 (10)	−0.0038 (11)

C4	0.0370 (15)	0.0591 (18)	0.0432 (16)	−0.0004 (12)	0.0090 (11)	−0.0138 (13)
C5	0.0521 (18)	0.076 (2)	0.0366 (16)	0.0124 (15)	0.0060 (13)	−0.0119 (15)
C6	0.066 (2)	0.079 (2)	0.0350 (16)	0.0263 (17)	0.0172 (14)	0.0110 (16)
C7	0.0522 (18)	0.0522 (17)	0.0479 (17)	0.0117 (13)	0.0205 (13)	0.0133 (14)
C8	0.0321 (13)	0.0434 (14)	0.0361 (14)	0.0049 (10)	0.0092 (10)	0.0016 (11)
N9	0.0379 (12)	0.0354 (11)	0.0402 (12)	−0.0066 (9)	0.0107 (9)	−0.0014 (10)
C10	0.0267 (12)	0.0323 (12)	0.0351 (13)	−0.0033 (9)	0.0046 (9)	−0.0005 (10)
C11	0.0320 (13)	0.0318 (12)	0.0355 (13)	−0.0066 (9)	0.0084 (10)	−0.0045 (10)
C12	0.0547 (17)	0.0322 (12)	0.0476 (16)	−0.0077 (11)	0.0175 (13)	−0.0027 (12)
C13	0.070 (2)	0.0368 (15)	0.0595 (19)	−0.0068 (13)	0.0257 (16)	−0.0164 (14)
C14	0.066 (2)	0.0513 (17)	0.0434 (16)	−0.0139 (14)	0.0238 (14)	−0.0129 (13)
C15	0.0465 (16)	0.0441 (15)	0.0365 (15)	−0.0082 (11)	0.0097 (11)	−0.0019 (11)
C16	0.0265 (12)	0.0341 (12)	0.0357 (13)	−0.0047 (9)	0.0042 (9)	−0.0031 (10)
N17	0.0372 (13)	0.0329 (11)	0.0374 (13)	0.0007 (9)	0.0068 (10)	0.0019 (10)
N18	0.0556 (15)	0.0329 (11)	0.0444 (14)	0.0093 (10)	0.0079 (11)	−0.0038 (10)
O19	0.0457 (12)	0.0411 (11)	0.0832 (16)	0.0077 (8)	0.0105 (11)	−0.0139 (10)
O20	0.0740 (16)	0.0897 (19)	0.0650 (15)	0.0407 (14)	0.0059 (12)	−0.0261 (14)
O21	0.099 (2)	0.0681 (16)	0.0665 (17)	0.0171 (14)	−0.0153 (14)	−0.0294 (13)

Geometric parameters (Å, º)

Cd1—N2	2.317 (2)	N9—C10	1.355 (3)
Cd1—N2^{i}	2.317 (2)	N9—H9	0.75 (3)
Cd1—O19	2.3175 (19)	C10—C11	1.464 (3)
Cd1—O19^{i}	2.3175 (19)	C11—C16	1.398 (3)
Cd1—N17	2.437 (2)	C11—C12	1.401 (3)
Cd1—N17^{i}	2.437 (2)	C12—C13	1.368 (4)
N2—C10	1.327 (3)	C12—H12	0.9300
N2—C3	1.397 (3)	C13—C14	1.381 (4)
C3—C4	1.392 (4)	C13—H13	0.9300
C3—C8	1.392 (3)	C14—C15	1.368 (4)
C4—C5	1.384 (4)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.398 (4)
C5—C6	1.389 (5)	C15—H15	0.9300
C5—H5	0.9300	C16—N17	1.413 (3)
C6—C7	1.373 (4)	N17—H17A	0.86 (3)
C6—H6	0.9300	N17—H17B	0.79 (3)
C7—C8	1.390 (4)	N18—O20	1.218 (3)
C7—H7	0.9300	N18—O21	1.219 (3)
C8—N9	1.384 (3)	N18—O19	1.246 (3)
N2—Cd1—N2^{i}	100.60 (10)	C7—C8—C3	122.0 (3)
N2—Cd1—O19	89.64 (8)	C10—N9—C8	108.1 (2)
N2^{i}—Cd1—O19	163.78 (7)	C10—N9—H9	125 (3)
N2—Cd1—O19^{i}	163.78 (7)	C8—N9—H9	125 (3)
N2^{i}—Cd1—O19^{i}	89.64 (8)	N2—C10—N9	111.4 (2)
O19—Cd1—O19^{i}	83.39 (11)	N2—C10—C11	125.3 (2)
N2—Cd1—N17	73.82 (8)	N9—C10—C11	123.1 (2)

N2^{i}—Cd1—N17	88.10 (7)	C16—C11—C12	118.4 (2)
O19—Cd1—N17	106.95 (8)	C16—C11—C10	122.3 (2)
O19^{i}—Cd1—N17	94.19 (8)	C12—C11—C10	119.2 (2)
N2—Cd1—N17^{i}	88.10 (7)	C13—C12—C11	121.8 (3)
N2^{i}—Cd1—N17^{i}	73.82 (8)	C13—C12—H12	119.1
O19—Cd1—N17^{i}	94.18 (8)	C11—C12—H12	119.1
O19^{i}—Cd1—N17^{i}	106.95 (8)	C12—C13—C14	119.2 (3)
N17—Cd1—N17^{i}	151.75 (10)	C12—C13—H13	120.4
C10—N2—C3	106.1 (2)	C14—C13—H13	120.4
C10—N2—Cd1	122.79 (16)	C15—C14—C13	120.6 (3)
C3—N2—Cd1	129.23 (15)	C15—C14—H14	119.7
C4—C3—C8	121.3 (2)	C13—C14—H14	119.7
C4—C3—N2	129.8 (2)	C14—C15—C16	120.7 (3)
C8—C3—N2	109.0 (2)	C14—C15—H15	119.6
C5—C4—C3	116.7 (3)	C16—C15—H15	119.6
C5—C4—H4	121.7	C15—C16—C11	119.2 (2)
C3—C4—H4	121.7	C15—C16—N17	119.2 (2)
C4—C5—C6	121.3 (3)	C11—C16—N17	121.4 (2)
C4—C5—H5	119.3	C16—N17—Cd1	110.21 (15)
C6—C5—H5	119.3	C16—N17—H17A	116.2 (19)
C7—C6—C5	122.7 (3)	Cd1—N17—H17A	93 (2)
C7—C6—H6	118.6	C16—N17—H17B	113 (2)
C5—C6—H6	118.6	Cd1—N17—H17B	118 (2)
C6—C7—C8	116.1 (3)	H17A—N17—H17B	105 (3)
C6—C7—H7	122.0	O20—N18—O21	119.1 (3)
C8—C7—H7	122.0	O20—N18—O19	119.7 (2)
N9—C8—C7	132.5 (3)	O21—N18—O19	121.1 (2)
N9—C8—C3	105.5 (2)	N18—O19—Cd1	117.12 (17)

C10—N2—C3—C4	−179.5 (3)	C8—N9—C10—N2	0.1 (3)
Cd1—N2—C3—C4	−15.2 (4)	C8—N9—C10—C11	−174.8 (2)
C10—N2—C3—C8	0.4 (3)	N2—C10—C11—C16	31.7 (4)
Cd1—N2—C3—C8	164.74 (16)	N9—C10—C11—C16	−154.1 (2)
C8—C3—C4—C5	−0.4 (4)	N2—C10—C11—C12	−145.3 (2)
N2—C3—C4—C5	179.5 (3)	N9—C10—C11—C12	28.9 (4)
C3—C4—C5—C6	0.3 (4)	C16—C11—C12—C13	−1.0 (4)
C4—C5—C6—C7	0.6 (5)	C10—C11—C12—C13	176.1 (3)
C5—C6—C7—C8	−1.2 (4)	C11—C12—C13—C14	1.3 (5)
C6—C7—C8—N9	−178.7 (3)	C12—C13—C14—C15	−0.2 (5)
C6—C7—C8—C3	1.1 (4)	C13—C14—C15—C16	−1.0 (5)
C4—C3—C8—N9	179.5 (2)	C14—C15—C16—C11	1.3 (4)
N2—C3—C8—N9	−0.4 (3)	C14—C15—C16—N17	−174.2 (3)
C4—C3—C8—C7	−0.3 (4)	C12—C11—C16—C15	−0.2 (3)
N2—C3—C8—C7	179.8 (2)	C10—C11—C16—C15	−177.2 (2)
C7—C8—N9—C10	180.0 (3)	C12—C11—C16—N17	175.1 (2)
C3—C8—N9—C10	0.2 (3)	C10—C11—C16—N17	−1.9 (3)
C3—N2—C10—N9	−0.3 (3)	C15—C16—N17—Cd1	120.8 (2)
Cd1—N2—C10—N9	−165.88 (16)	C11—C16—N17—Cd1	−54.5 (3)

C3—N2—C10—C11	174.4 (2)	O20—N18—O19—Cd1	−172.3 (2)
Cd1—N2—C10—C11	8.8 (3)	O21—N18—O19—Cd1	9.7 (3)

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*
N9—H9···O20^{ii}	0.75 (3)	2.39 (3)	3.012 (3)	140 (3)
N9—H9···O21^{ii}	0.75 (3)	2.51 (3)	3.238 (3)	163 (3)
N17—H17*A*···O21	0.86 (3)	2.34 (3)	2.973 (3)	131 (2)
N17—H17*B*···O20^{iii}	0.79 (3)	2.24 (3)	3.024 (3)	170 (3)

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