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Synthesis, crystal structure and Hirshfeld surface analysis of a coordination compound of cadmium nitrate with 2-aminobenzoxazole

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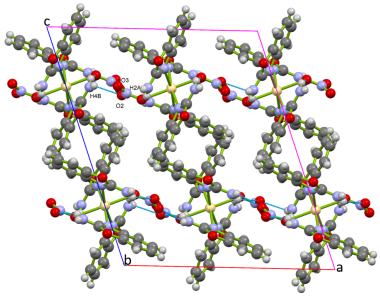
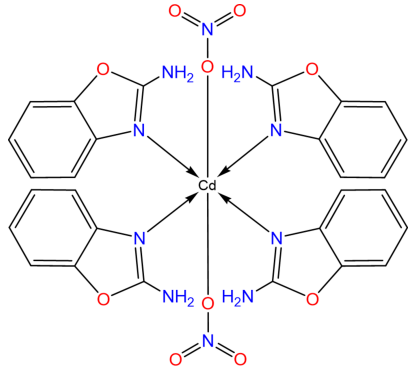
A coordination complex of cadmium nitrate $[Cd(NO_3)_2]$ with 2-aminobenzaxole (2AB; $C_7H_6N_2O$), namely, tetrakis(2-aminobenzoxazole-κN^1)bis(nitrato-κO) cadmium(II), $[Cd(NO_3)_2(2AB)_4]$, has been synthesized from ethanol solutions of $Cd(NO_3)_2{\cdot}H_2O$ and 2AB. The asymmetric unit comprises half a molecule of $[Cd(NO_3)_2(2AB)_4]$, with the Cd^{II} atom positioned on a twofold rotation axis. In the completed molecular complex, four 2AB ligands and two nitrate anions each coordinate monodentately to the Cd^{II} atom, leading to a distorted octahedral coordination environment. The crystal structure of $[Cd(NO_3)_2(2AB)_4]$ exhibits several N—H···O interactions, resulting in the formation of a layered assembly parallel to (001). Hishfeld surface analysis was used to quantify the intermolecular interactions.

1. Chemical context

Benzoxazole is a heterocyclic aromatic compound consisting of a benzene ring fused to an oxazole ring. It has a strong and unpleasant fishy odour, just like pyridine (Katritzky & Pozharskii, 2000; Clayden *et al.*, 2001). Many benzoxazole-based compounds are valued in medicinal and biological research because of their numerous biological activities (Potashman *et al.*, 2007; Šlachtová. & Brulíková, 2018; Razzoqova *et al.*, 2022, 2024), including antimicrobial (Erol *et al.*, 2022), antitumor (Imaizumi *et al.*, 2020), anti-inflammatory (Parlapalli & Manda, 2017), analgesic (Ali *et al.*, 2022; Sattar *et al.*, 2020), antitubercular (Šlachtová & Brulíková, 2018), herbicidal (Sangi *et al.*, 2019), and fungicidal properties (Fan *et al.*, 2022).





At the same time, 2-aminobenzoxazole (2AB) and its derivatives have potent antibacterial and anticancer properties (Paramashivappa *et al.*, 2003; Khajondetchairit *et al.*, 2017; Ouyang *et al.*, 2012). One notable derivative of 2AB is 2-amino-5-chlorobenzoxazole, which has demonstrated muscle relaxant effects and is used as an antispasmodic and uricosuric agent in therapeutic applications (Lynch, 2004).

In the context given above, we present here the synthesis, crystal structure determination and Hirshfeld surface analysis of a coordination complex of 2AB with cadmium nitrate, $[Cd(NO_3)_2(2AB)_4]$.

2. Structural commentary

In the asymmetric unit of $[Cd(NO_3)_2(2AB)_4]$, which consists of half of a complex molecule, the Cd^{II} atom is positioned on a twofold rotation axis (multiplicity 4, Wyckoff letter *e*). In the completed molecule, the Cd^{II} atom coordinates by four 2AB ligands and two nitrate anions, resulting in a distorted octahedral N_4O_2 coordination set (Fig. 1). The four 2AB ligands occupy the equatorial positions and are coordinated monodentately through their aromatic nitrogen donor atoms with Cd—N bond lengths of 2.314 (3) and 2.325 (3) Å. The two axially positioned nitrato ligands are also coordinated in a monodentate fashion with a relatively long Cd—O bond length of 2.418 (3) Å. The dihedral angle formed between the two opposite 2-aminobenzaxazole ligands (labelled in Fig. 1) is 84.85 (17)°. The molecular conformation is stabilized by intramolecular N—H···O hydrogen-bonding interactions involving the coordinated oxygen atom O1 and the non-coordinated oxygen atom O2 (entries #1 and #3 in Table 1).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O1^{i}	0.86	2.26	2.971 (5)	140
N4—H4*B*···O2^{ii}	0.86	2.28	2.822 (6)	121
N2—H2*A*···O2^{i}	0.86	2.11	2.899 (7)	152
N2—H2*B*···O3^{iii}	0.86	2.33	2.953 (6)	129

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

3. Supramolecular features

In the crystal structure of $[Cd(NO_3)_2(2AB)_4]$, intermolecular N—H···O hydrogen bonds involving the non-coordinated O atoms O2 and O3 (entries #2 and #4 in Table 1) lead to the formation of sheets extending parallel to (001), as shown in Fig. 2.

4. Hirshfeld Surface Analysis

Hirshfeld surface (HS) analysis (Spackman & Jayatilaka, 2009) was performed and two-dimensional fingerprint plots (Spackman & McKinnon, 2002) were generated using *CrystalExplorer* (Spackman *et al.*, 2021) to quantify the intermolecular interactions. HS and fingerprint plot analysis conducted for $[Cd(NO_3)_2(2AB)_4]$ are graphically displayed in Fig. 3. The red spots on the HS area of $[Cd(NO_3)_2(2AB)_4]$ confirm the close intermolecular N—H···O contacts (related to entries #2 and #4 in Table 1) between adjacent molecules. The two-dimensional fingerprint plots and their relative

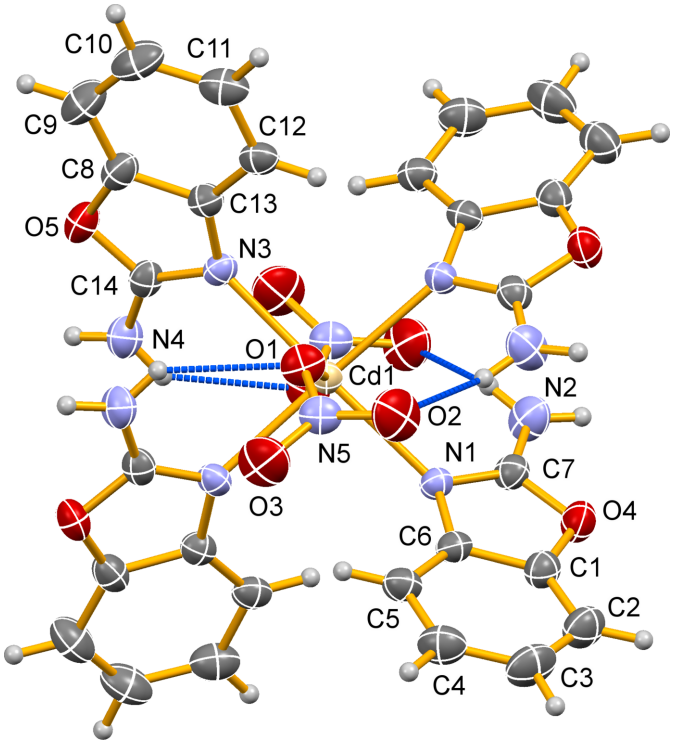


Figure 1
The molecular structure of $[Cd(NO_3)_2(2AB)_4]$ with displacement ellipsoids drawn at the 30% probability level; non-labelled atoms are generated by symmetry code $-x+1, y, -z+\frac{3}{2}$. Intramolecular hydrogen bonds are indicated by dashed blue lines.

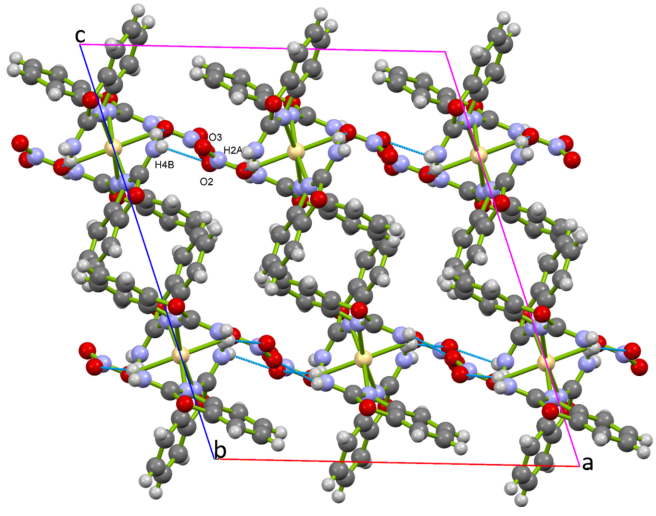


Figure 2
Visualization of the molecular packing in $[Cd(NO_3)_2(2AB)_4]$ in a view along [010]. Intermolecular N—H···O interactions are shows as light-blue dashed lines.

contributions revealed that H···H, O···H, C···H, C···O, O···O and N···H interactions are the main interactions to the HS area. Specifically, the fingerprint plots reveal the presence of close N—H···O contacts in form of two spikes observed near ($d_i + d_e$) ≃ 2.3 Å and C—H contacts as two wings near ($d_i + d_e$) ≃ 2. 8 Å (Fig. 3).

5. Database survey

A survey of the Cambridge Structural Database (CSD, Version 5.46, November 2024; Groom *et al.*, 2016) revealed 17 crystal structures of 2-aminobenzoxazole derivatives. Among these, only two structures involve coordination compounds with zinc (QALXIL; Decken & Gossage, 2005) and cadmium (DIWPIM; Razzoqova *et al.*, 2023). In the zinc complex, the central metal atom coordinates two benzoxazolamine ligands through the aromatic nitrogen atom and two chloro ligands in a distorted tetrahedral coordination environment. In the crystal structure of DIWPIM, which corresponds to $[Cd(2AB)_2(CH_3COO)_2]$, the Cd^{II} atom coordinates by two 2AB ligands and two acetato ligands in a monodentate and bidentate fashion, respectively, forming a distorted octahedral N_2O_4 coordination set.

6. Synthesis and crystallization

$Cd(NO_3)_2{\cdot}H_2O$ (0.308 g, 1 mmol) and 2AB (0.268 g, 2 mmol) were dissolved separately in ethanol (5 ml), mixed together and stirred for 2 h. The obtained colourless solution was filtered and left for crystallization. Single crystals of the complex $[Cd(NO_3)_2(2AB)_4]$ suitable for X-ray analysis were obtained by slow evaporation of the solution over a period of 7 d.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd(NO_3)_2(C_7H_6N_2O)_4]$
M_r	772.97
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	15.9012 (3), 11.0897 (2), 18.9475 (5)
β (°)	109.182 (3)
V (Å^3)	3155.70 (13)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	6.19
Crystal size (mm)	0.10 × 0.08 × 0.06
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix3000
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2020)
T_{min}, T_{max}	0.016, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12616, 3014, 2324
R_{int}	0.084
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.614
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.128, 1.01
No. of reflections	3014
No. of parameters	223
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.56, −0.95

Computer programs: *CrysAlis PRO* (Rigaku OD, 2020), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were treated in a riding model with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

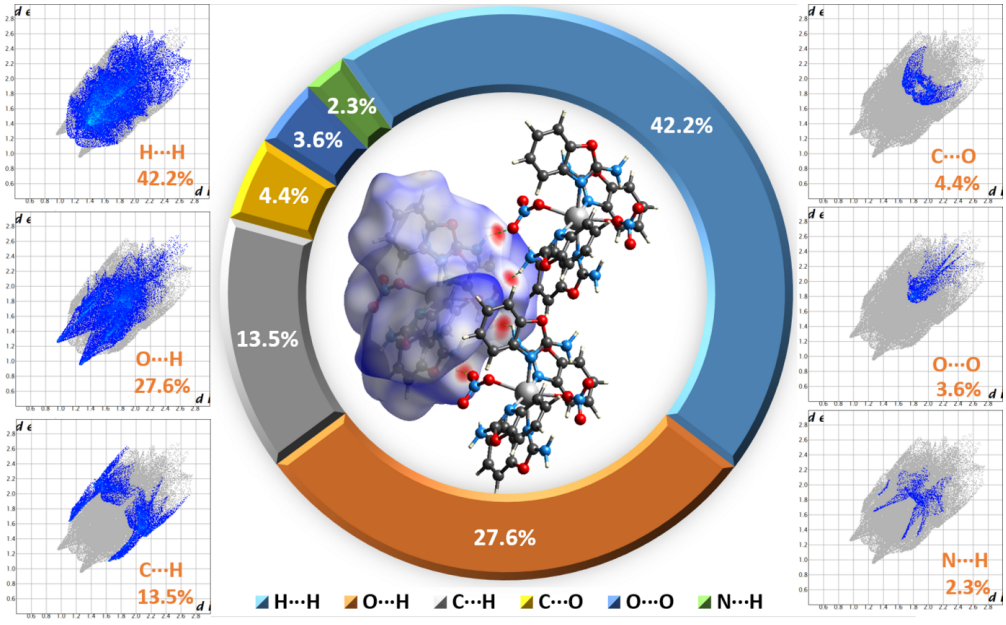


Figure 3
View of HS and two-dimensional fingerprint plots of $[Cd(NO_3)_2(2AB)_4]$.

Acknowledgements

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supporting information

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Synthesis, crystal structure and Hirshfeld surface analysis of a coordination compound of cadmium nitrate with 2-aminobenzoxazole

Surayyo Razzoqova, Yodgor Ruzimov, Akobir Toshov, Batirbay Torambetov, Aziz Ibragimov, Jamshid Ashurov and Shakhnoza Kadirova

Computing details

Tetrakis(2-aminobenzoxazole-κN^1)bis(nitrato-κO)cadmium(II)

Crystal data

$[Cd(NO_3)_2(C_7H_6N_2O)_4]$
$M_r = 772.97$
Monoclinic, $C2/c$
$a = 15.9012$ (3) Å
$b = 11.0897$ (2) Å
$c = 18.9475$ (5) Å
$\beta = 109.182$ (3)°
$V = 3155.70$ (13) Å^3
$Z = 4$
$F(000) = 1560$
$D_x = 1.627$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 4500 reflections
$\theta = 4.9$–$70.8°$
$\mu = 6.19$ mm^{-1}
$T = 293$ K
Block, colourless
0.10 × 0.08 × 0.06 mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix3000 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2020)
$T_{min} = 0.016$, $T_{max} = 1.000$
12616 measured reflections
3014 independent reflections
2324 reflections with $I > 2\sigma(I)$
$R_{int} = 0.084$
$\theta_{max} = 71.1°$, $\theta_{min} = 4.9°$
$h = -19 \rightarrow 19$
$k = -13 \rightarrow 13$
$l = -22 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.128$
$S = 1.01$
3014 reflections
223 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0631P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.95$ e Å^{-3}
Extinction correction: SHELXL (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00041 (6)

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	0.500000	0.24505 (3)	0.750000	0.04211 (19)
O5	0.5198 (2)	−0.0974 (3)	0.6354 (2)	0.0633 (9)
O4	0.5320 (2)	0.5949 (3)	0.8680 (2)	0.0650 (9)
O1	0.3406 (2)	0.2156 (3)	0.7009 (2)	0.0639 (9)
N1	0.5181 (2)	0.3989 (3)	0.8371 (2)	0.0461 (8)
N3	0.5049 (2)	0.0945 (3)	0.6668 (2)	0.0470 (8)
N5	0.2779 (2)	0.2434 (4)	0.7254 (3)	0.0572 (11)
N4	0.6112 (2)	−0.0366 (4)	0.7492 (2)	0.0625 (11)
H4A	0.629684	0.016170	0.784177	0.075*
H4B	0.634011	−0.107721	0.755194	0.075*
O2	0.2525 (3)	0.3475 (4)	0.7173 (3)	0.1036 (16)
N2	0.6252 (3)	0.5215 (4)	0.8094 (3)	0.0752 (13)
H2A	0.645052	0.464034	0.788780	0.090*
H2B	0.647782	0.592541	0.812309	0.090*
O3	0.2472 (3)	0.1686 (5)	0.7563 (3)	0.1067 (16)
C5	0.3927 (3)	0.3589 (5)	0.8882 (3)	0.0590 (12)
H5	0.386358	0.277102	0.876857	0.071*
C6	0.4556 (3)	0.4272 (4)	0.8722 (2)	0.0483 (10)
C13	0.4434 (3)	0.0736 (4)	0.5961 (3)	0.0487 (10)
C7	0.5601 (3)	0.5007 (4)	0.8366 (3)	0.0527 (11)
C12	0.3822 (3)	0.1470 (5)	0.5465 (3)	0.0560 (11)
H12	0.374376	0.226672	0.558271	0.067*
C1	0.4640 (3)	0.5490 (4)	0.8903 (3)	0.0591 (12)
C2	0.4121 (4)	0.6093 (5)	0.9230 (3)	0.0768 (16)
H2	0.418750	0.691342	0.933603	0.092*
C11	0.3324 (3)	0.0975 (6)	0.4779 (3)	0.0754 (16)
H11	0.291093	0.145209	0.442908	0.091*
C14	0.5477 (3)	−0.0084 (4)	0.6863 (3)	0.0501 (11)
C8	0.4530 (3)	−0.0457 (4)	0.5772 (3)	0.0595 (12)
C4	0.3384 (4)	0.4174 (6)	0.9221 (3)	0.0793 (17)
H4	0.294517	0.373897	0.933595	0.095*
C3	0.3487 (4)	0.5396 (7)	0.9391 (4)	0.087 (2)
H3	0.311723	0.575692	0.962182	0.105*
C10	0.3436 (4)	−0.0227 (7)	0.4611 (4)	0.086 (2)
H10	0.308806	−0.053870	0.415260	0.103*
C9	0.4051 (4)	−0.0967 (6)	0.5107 (3)	0.0831 (18)
H9	0.413245	−0.176568	0.499456	0.100*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0425 (2)	0.0410 (3)	0.0463 (3)	0.000	0.01946 (17)	0.000
O5	0.068 (2)	0.0510 (17)	0.074 (2)	0.0032 (16)	0.0276 (18)	−0.0150 (17)
O4	0.073 (2)	0.0507 (18)	0.074 (2)	−0.0063 (16)	0.0271 (18)	−0.0097 (17)
O1	0.0380 (16)	0.081 (2)	0.075 (2)	0.0023 (15)	0.0215 (16)	−0.0023 (18)
N1	0.0500 (19)	0.0458 (18)	0.046 (2)	−0.0011 (16)	0.0208 (16)	−0.0034 (16)
N3	0.0495 (18)	0.0491 (19)	0.047 (2)	0.0014 (16)	0.0214 (16)	−0.0052 (16)
N5	0.0346 (17)	0.077 (3)	0.060 (2)	0.0003 (18)	0.0162 (17)	0.000 (2)
N4	0.059 (2)	0.053 (2)	0.075 (3)	0.0158 (18)	0.022 (2)	0.002 (2)
O2	0.100 (3)	0.096 (3)	0.126 (4)	0.050 (3)	0.053 (3)	0.018 (3)
N2	0.068 (3)	0.073 (3)	0.094 (4)	−0.025 (2)	0.039 (3)	−0.017 (3)
O3	0.107 (3)	0.113 (4)	0.126 (4)	−0.044 (3)	0.074 (3)	−0.008 (3)
C5	0.063 (3)	0.066 (3)	0.053 (3)	0.001 (2)	0.026 (2)	0.002 (2)
C6	0.049 (2)	0.056 (2)	0.041 (2)	0.006 (2)	0.0149 (18)	−0.0022 (19)
C13	0.046 (2)	0.054 (2)	0.049 (3)	−0.0074 (19)	0.0186 (19)	−0.003 (2)
C7	0.053 (2)	0.052 (2)	0.051 (3)	−0.007 (2)	0.014 (2)	−0.007 (2)
C12	0.058 (3)	0.067 (3)	0.049 (3)	−0.005 (2)	0.025 (2)	−0.001 (2)
C1	0.062 (3)	0.055 (3)	0.058 (3)	0.008 (2)	0.018 (2)	−0.001 (2)
C2	0.084 (4)	0.073 (4)	0.077 (4)	0.017 (3)	0.032 (3)	−0.009 (3)
C11	0.061 (3)	0.106 (5)	0.060 (3)	−0.008 (3)	0.019 (3)	0.003 (3)
C14	0.046 (2)	0.048 (2)	0.062 (3)	0.0033 (18)	0.025 (2)	−0.004 (2)
C8	0.062 (3)	0.058 (3)	0.067 (3)	−0.007 (2)	0.031 (2)	−0.015 (2)
C4	0.075 (3)	0.100 (5)	0.071 (4)	−0.005 (3)	0.035 (3)	0.000 (3)
C3	0.083 (4)	0.103 (5)	0.084 (4)	0.027 (4)	0.038 (3)	−0.017 (4)
C10	0.073 (4)	0.114 (5)	0.067 (4)	−0.019 (4)	0.019 (3)	−0.033 (4)
C9	0.079 (4)	0.084 (4)	0.086 (5)	−0.016 (3)	0.027 (3)	−0.035 (3)

Geometric parameters (Å, º)

Cd1—O1^{i}	2.418 (3)	N2—C7	1.319 (6)
Cd1—O1	2.418 (3)	C5—H5	0.9300
Cd1—N1^{i}	2.325 (3)	C5—C6	1.365 (6)
Cd1—N1	2.325 (3)	C5—C4	1.396 (7)
Cd1—N3	2.314 (3)	C6—C1	1.390 (6)
Cd1—N3^{i}	2.314 (3)	C13—C12	1.375 (6)
O5—C14	1.350 (5)	C13—C8	1.392 (6)
O5—C8	1.380 (6)	C12—H12	0.9300
O4—C7	1.349 (5)	C12—C11	1.392 (7)
O4—C1	1.381 (6)	C1—C2	1.358 (7)
O1—N5	1.269 (5)	C2—H2	0.9300
N1—C6	1.401 (6)	C2—C3	1.383 (8)
N1—C7	1.314 (5)	C11—H11	0.9300
N3—C13	1.395 (6)	C11—C10	1.396 (9)
N3—C14	1.318 (5)	C8—C9	1.363 (7)
N5—O2	1.217 (5)	C4—H4	0.9300
N5—O3	1.206 (6)	C4—C3	1.391 (8)

N4—H4A	0.8600	C3—H3	0.9300
N4—H4B	0.8600	C10—H10	0.9300
N4—C14	1.322 (6)	C10—C9	1.381 (9)
N2—H2A	0.8600	C9—H9	0.9300
N2—H2B	0.8600		

O1—Cd1—O1^{i}	164.46 (17)	C1—C6—N1	108.1 (4)
N1—Cd1—O1^{i}	87.51 (12)	C12—C13—N3	132.4 (4)
N1—Cd1—O1	104.00 (12)	C12—C13—C8	119.9 (4)
N1^{i}—Cd1—O1^{i}	104.00 (12)	C8—C13—N3	107.7 (4)
N1^{i}—Cd1—O1	87.51 (12)	N1—C7—O4	114.8 (4)
N1^{i}—Cd1—N1	85.58 (18)	N1—C7—N2	128.3 (4)
N3—Cd1—O1	84.62 (12)	N2—C7—O4	116.9 (4)
N3—Cd1—O1^{i}	84.18 (13)	C13—C12—H12	121.2
N3^{i}—Cd1—O1	84.18 (13)	C13—C12—C11	117.6 (5)
N3^{i}—Cd1—O1^{i}	84.63 (12)	C11—C12—H12	121.2
N3—Cd1—N1	171.33 (11)	O4—C1—C6	107.7 (4)
N3^{i}—Cd1—N1	94.01 (14)	C2—C1—O4	127.7 (5)
N3^{i}—Cd1—N1^{i}	171.33 (11)	C2—C1—C6	124.6 (5)
N3—Cd1—N1^{i}	94.01 (14)	C1—C2—H2	122.5
N3^{i}—Cd1—N3	87.70 (18)	C1—C2—C3	115.0 (6)
C14—O5—C8	104.7 (4)	C3—C2—H2	122.5
C7—O4—C1	104.9 (4)	C12—C11—H11	119.6
N5—O1—Cd1	132.6 (3)	C12—C11—C10	120.8 (6)
C6—N1—Cd1	124.1 (3)	C10—C11—H11	119.6
C7—N1—Cd1	124.8 (3)	N3—C14—O5	114.5 (4)
C7—N1—C6	104.6 (4)	N3—C14—N4	129.0 (4)
C13—N3—Cd1	127.1 (3)	N4—C14—O5	116.5 (4)
C14—N3—Cd1	124.3 (3)	O5—C8—C13	108.1 (4)
C14—N3—C13	105.1 (4)	C9—C8—O5	128.0 (5)
O2—N5—O1	116.9 (5)	C9—C8—C13	123.9 (5)
O3—N5—O1	120.2 (5)	C5—C4—H4	119.5
O3—N5—O2	122.9 (5)	C3—C4—C5	121.0 (6)
H4A—N4—H4B	120.0	C3—C4—H4	119.5
C14—N4—H4A	120.0	C2—C3—C4	122.2 (6)
C14—N4—H4B	120.0	C2—C3—H3	118.9
H2A—N2—H2B	120.0	C4—C3—H3	118.9
C7—N2—H2A	120.0	C11—C10—H10	119.1
C7—N2—H2B	120.0	C9—C10—C11	121.8 (5)
C6—C5—H5	121.5	C9—C10—H10	119.1
C6—C5—C4	117.0 (5)	C8—C9—C10	116.0 (6)
C4—C5—H5	121.5	C8—C9—H9	122.0
C5—C6—N1	131.8 (4)	C10—C9—H9	122.0
C5—C6—C1	120.2 (5)		

Cd1—O1—N5—O2	79.2 (6)	C13—N3—C14—O5	−0.8 (5)
Cd1—O1—N5—O3	−99.7 (5)	C13—N3—C14—N4	−178.2 (5)
Cd1—N1—C6—C5	26.7 (6)	C13—C12—C11—C10	0.9 (8)

Cd1—N1—C6—C1	−151.9 (3)	C13—C8—C9—C10	−0.6 (9)
Cd1—N1—C7—O4	152.3 (3)	C7—O4—C1—C6	1.0 (5)
Cd1—N1—C7—N2	−27.5 (7)	C7—O4—C1—C2	−177.8 (5)
Cd1—N3—C13—C12	22.8 (7)	C7—N1—C6—C5	179.3 (5)
Cd1—N3—C13—C8	−158.9 (3)	C7—N1—C6—C1	0.7 (5)
Cd1—N3—C14—O5	159.4 (3)	C12—C13—C8—O5	178.4 (4)
Cd1—N3—C14—N4	−18.0 (7)	C12—C13—C8—C9	0.5 (8)
O5—C8—C9—C10	−178.0 (5)	C12—C11—C10—C9	−1.1 (9)
O4—C1—C2—C3	179.8 (5)	C1—O4—C7—N1	−0.6 (5)
N1—C6—C1—O4	−1.1 (5)	C1—O4—C7—N2	179.2 (4)
N1—C6—C1—C2	177.8 (5)	C1—C2—C3—C4	−0.9 (9)
N3—C13—C12—C11	177.5 (5)	C11—C10—C9—C8	0.8 (9)
N3—C13—C8—O5	−0.2 (5)	C14—O5—C8—C13	−0.2 (5)
N3—C13—C8—C9	−178.1 (5)	C14—O5—C8—C9	177.5 (5)
C5—C6—C1—O4	−179.9 (4)	C14—N3—C13—C12	−177.7 (5)
C5—C6—C1—C2	−1.0 (8)	C14—N3—C13—C8	0.6 (5)
C5—C4—C3—C2	0.5 (10)	C8—O5—C14—N3	0.6 (5)
C6—N1—C7—O4	−0.1 (5)	C8—O5—C14—N4	178.4 (4)
C6—N1—C7—N2	−179.8 (5)	C8—C13—C12—C11	−0.7 (7)
C6—C5—C4—C3	−0.3 (8)	C4—C5—C6—N1	−177.9 (5)
C6—C1—C2—C3	1.1 (8)	C4—C5—C6—C1	0.5 (7)

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*
N4—H4*A*···O1^{i}	0.86	2.26	2.971 (5)	140
N4—H4*B*···O2^{ii}	0.86	2.28	2.822 (6)	121
N2—H2*A*···O2^{i}	0.86	2.11	2.899 (7)	152
N2—H2*B*···O3^{iii}	0.86	2.33	2.953 (6)	129

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