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First seven-coordinate dinuclear Cd^{II} complex featuring bridging 3-aminopyridine and chelating nitrate ligands: crystal structure and Hirshfeld surface analysis

Amani Hind Benahsene,[a]* Belkis Selsebil Yeddiou,[a] Raounek Rouag,[a] Fatiha Guenifa,[a,b] Volker Kahlenberg[c] and Lamia Bendjeddou[a]

[a]Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale, Université Constantine 1 Frères Mentouri, Algeria, [b]École Normale Supérieure Assia Djebar (ENS) de Constantine Ville Universitaire, Ain El Bey Ali Mendjeli, 25000 Constantine, Algeria, and [c]Institute of Mineralogy and Petrography, University of Innsbruck, Innrain 52, A-6020 Innsbruck, Austria. *Correspondence e-mail: amanihind.benahsene@umc.edu.dz

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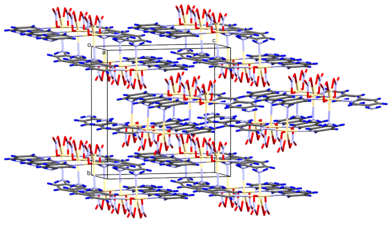
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The title complex, bis(μ-3-aminopyridine)-κ^2N^1:N^3;κ^2N^3:N^1-bis[(3-aminopyridine-κN^1)bis(nitrato-κ^2O,O')cadmium(II)], $[Cd_2(NO_3)_4(3\text{-ampy})_4]$ (3-ampy = 3-aminopyridine, $C_5H_6N_2$), was obtained under hydrothermal conditions and crystallizes in the monoclinic space group $P2_1/n$. The asymmetric unit contains a centrosymmetric dimer formed from two Cd^{II} atoms bridged by a pair of 3-ampy ligands. Each ligand coordinates in a bidentate manner *via* its pyridine N atom and the other through its amino N atom; the second 3-ampy ligand is terminal. Each Cd^{II} atom is seven-coordinate, in a distorted pentagonal-bipyramidal CdN_3O_4 environment completed by two chelating nitrate anions. In the crystal, N—H···O and C—H···O hydrogen bonds link the dimers into layers, which are connected by weaker hydrogen bonds and π–π stacking interactions into a three-dimensional network. Hirshfeld surface analysis shows that H···O/O···H contacts dominate the packing. To our knowledge, this is the first discrete dinuclear Cd^{II}–3-ampy complex and the first with coordinated nitrate anions.

1. Chemical context

Nitrogen-donor ligands are widely used in the design of coordination compounds with diverse structural architectures and properties. Among them, 3-aminopyridine (3-ampy) is particularly versatile because it possesses two potentially coordinating N atoms: the pyridine and amino N atoms. Depending on the metal centre and the reaction conditions, 3-ampy can coordinate in a terminal monodentate fashion through either N atom or act as a bridging ligand through both donor sites (He *et al.*, 2004; Kojima *et al.*, 2009; Goher *et al.*, 2004). Protonated 3-aminopyridinium ions have also been reported in organic–inorganic halocuprate salts containing dinuclear copper(II) anions (Blanchette & Willett, 1988; Willett & Halvorson, 1988). These protonated species are distinct from neutral 3-ampy acting as a coordination ligand.

The coordination chemistry of 3-ampy encompasses compounds with a range of transition-metal centres, including Co^{II}, Ni^{II}, Cu^{II}, Zn^{II}, Cd^{II}, Ag^{I} and Re^{V} (He & Zhu, 2003; Bučar & Meštrović, 2003; He *et al.*, 2004; Kochel, 2006; Qian & Huang, 2006; Pan *et al.*, 2007; Yilmaz *et al.*, 2007). In addition to discrete complexes, 3-ampy has been employed in the construction of extended coordination architectures, ranging from one-dimensional chains to two- and three-dimensional networks, often in combination with bridging anionic ligands (Goher *et al.*, 2004; Mautner *et al.*, 2007; Mautner *et al.*, 2019;



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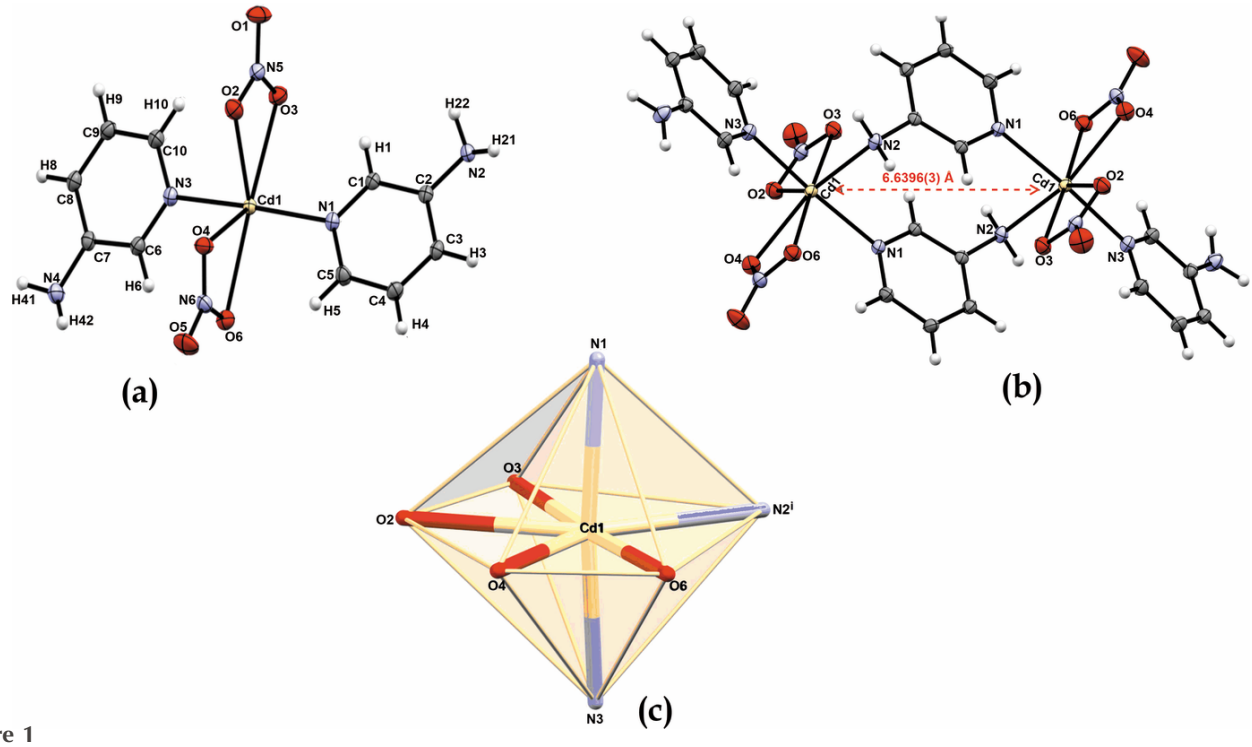
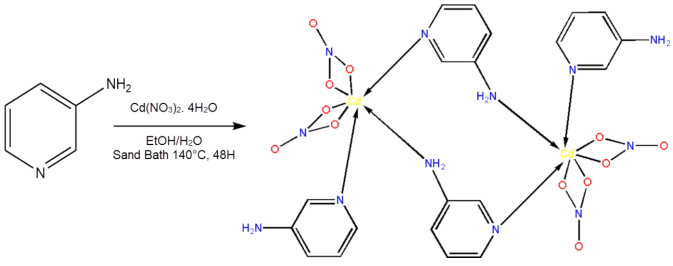


Figure 1
Views of the title complex, showing (*a*) the molecular structure of the asymmetric unit of the $[Cd(NO_3)_2(3\text{-ampy})_2]_2$ complex, with displacement ellipsoids drawn at the 50% probability level and H atoms shown as spheres of arbitrary radii, (*b*) a dinuclear entity and (*c*) the coordination polyhedra. [Symmetry code: (i) $-x+2, -y+1, -z+1$.]

O'Donovan & LaDuca, 2014; Shen *et al.*, 2015; Wilson *et al.*, 2013; Kartal *et al.*, 2018; Kartal & Şahin, 2021).



In this context, we report the synthesis and crystal structure of a new dinuclear cadmium(II) complex, incorporating 3-ampy and nitrate anions. The structure consists of two inversion-related seven-coordinate Cd^{II} centres linked by *N*,*N*′-bridging 3-ampy ligands. The coordination geometry, supramolecular assembly and intermolecular interactions are discussed, together with a Hirshfeld surface analysis.

2. Structural commentary

The title coordination complex crystallizes in the monoclinic crystal system with the space group $P2_1/n$. The asymmetric unit of the complex contains one Cd^{II} ion coordinated to two 3-aminopyridine (3-ampy) ligand and chelated by two nitrate anions [Fig. 1(*a*)]. A dinuclear complex $[Cd(NO_3)_2(3\text{-ampy})_2]_2$ is generated through the presence of an inversion centre at $(0, \frac{1}{2}, \frac{1}{2})$. The two Cd^{II} atoms are linked by a double 3-ampy bridge forming a centrosymmetric dimer with a Cd1···Cd1^{i} distance of 6.6396 (3) Å [Fig. 1(*b*)].

Table 1
Selected geometric parameters (Å, °).

Cd1—N3	2.2726 (13)	Cd1—O2	2.4495 (13)
Cd1—N1	2.2859 (12)	Cd1—O3	2.5063 (12)
Cd1—O4	2.4067 (12)	Cd1—O6	2.5301 (12)
Cd1—N2^{i}	2.4374 (15)	N2—Cd1^{i}	2.4374 (15)
N3—Cd1—N1	174.79 (5)	N1—Cd1—O3	88.52 (4)
N3—Cd1—O4	91.26 (4)	O4—Cd1—O3	129.47 (4)
N1—Cd1—O4	92.05 (4)	N2^{i}—Cd1—O3	87.22 (4)
N3—Cd1—N2^{i}	88.67 (5)	O2—Cd1—O3	51.82 (4)
N1—Cd1—N2^{i}	86.27 (4)	N3—Cd1—O6	89.42 (4)
O4—Cd1—N2^{i}	143.26 (4)	N1—Cd1—O6	89.44 (4)
N3—Cd1—O2	92.36 (4)	O4—Cd1—O6	52.06 (4)
N1—Cd1—O2	92.28 (4)	O2—Cd1—O6	129.74 (4)
O4—Cd1—O2	77.68 (4)	O3—Cd1—O6	177.49 (4)
N2^{i}—Cd1—O2	139.04 (4)	N5—O4—Cd1	98.29 (10)
N3—Cd1—O3	92.49 (4)		

Symmetry code: (i) $-x+2, -y+1, -z+1$.

The Cd^{II} atom, located in a general position, is hepta-coordinated. The coordination sphere incorporates four O atoms and three N atoms $[CdO_4N_3]$, forming a distorted pentagonal bipyramidal coordination geometry [Fig. 1(*c*)]. The axial positions are occupied by atoms N1 and N3 from the pyridine rings, with axial distances Cd1—N1 = 2.2859 (12) Å and Cd1—N3 = 2.2726 (13) Å, significantly shorter than the equatorial distances [2.4067 (12)–2.5301 (12) Å]. The geometry deviates from a regular pentagon, with bond angles O—Cd—O [51.84 (4)–77.68 (4)°] and N—Cd—O [87.22 (4)–92.49 (4)°] (Table 1) consistent with literature values for

similar cadmium complexes. (Bartholomä *et al.*, 2010; Song *et al.*, 2016; Kovalev *et al.*, 2021; Benahsene *et al.*, 2025).

The 3-ampy ligand exhibits two distinct coordination modes (Fig. 2): mode (I), monodentate coordination through the pyridine N atom, and mode (IV), bridging coordination through both the pyridine and amino N atoms. The latter mode leads to the formation of the dimeric assembly.

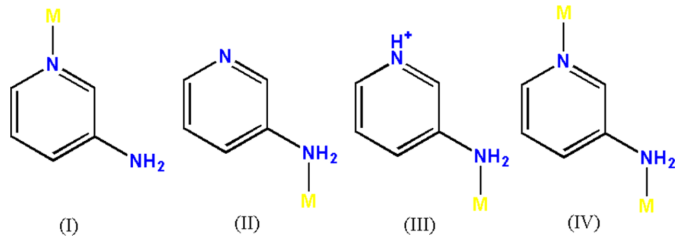


Figure 2
The coordination modes of the 3-aminopyridine ligand.

3. Supramolecular features

The crystal packing consists of shifted dimeric layers parallel to the *ac* plane [Fig. 3(*a*)]. Within each layer, the dimeric entities are arranged along the crystallographic *a* and *c* axes, forming dimeric chains that extend along the *a* axis [Fig. 3(*b*)].

The complex exhibits a total of eight hydrogen bonds, comprising N—H···O and C—H···O interactions (Table 2). Within the same chain, adjacent dimeric entities are connected

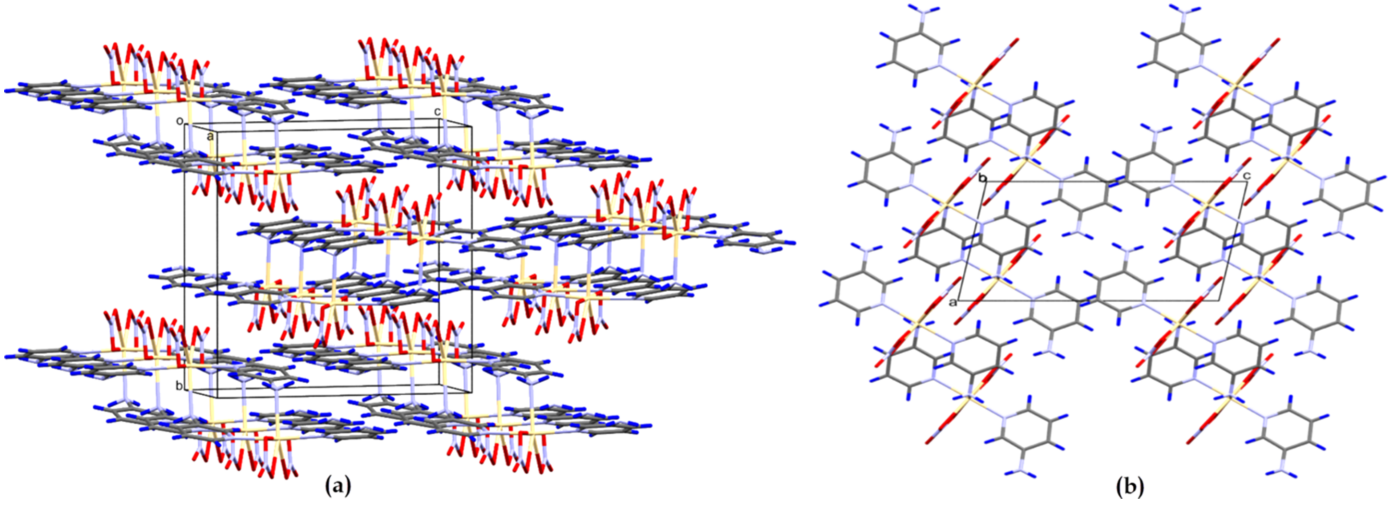


Figure 3
Packing view of the title coordination complex, showing (*a*) the crystal packing and (*b*) the dimeric layers.

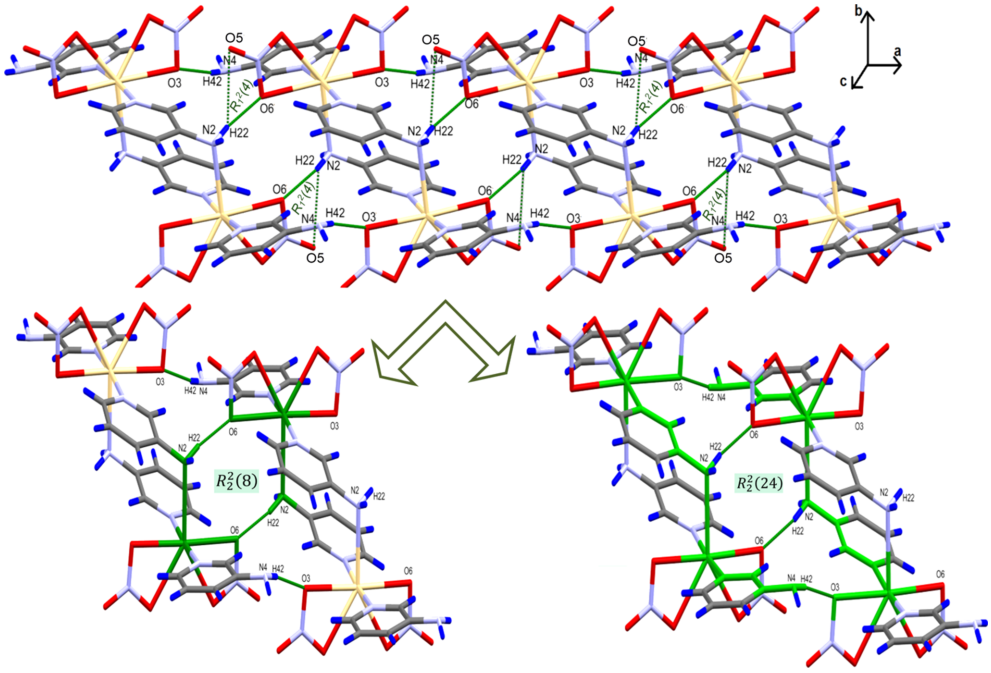


Figure 4
Part of the crystal structure showing the junction between dimeric entities through N4—H42···O3^{v} and N2—H22···O6^{iii} hydrogen bonds with $R_1^2(4)$, $R_2^2(8)$ and $R_2^2(24)$ motifs. The ring used for the graph set is shown in green. [Symmetry codes: (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (v) $x-1, y, z$.]

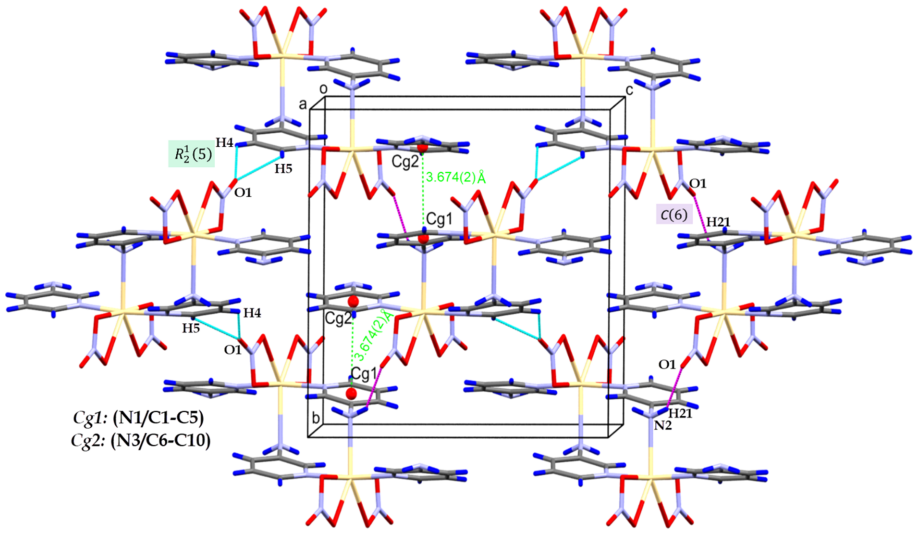


Figure 5
Part of the crystal structure showing the interactions between dimeric layers through N2—H21···O1^{ii}, C4—H4···O1^{vi} and C5—H5···O1^{vi} hydrogen bonds, and π–π intermolecular interactions. *Cg*1 is the centroid of the N1/C1–C5 ring and *Cg*2 of the N3/C6–C10 ring, and the *Cg*1···*Cg*2 distance is 3.674 (2) Å. [Symmetry codes: (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (vi) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.]

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H21···O1^{ii}	0.88	2.52	3.273 (2)	143
N2—H21···O2^{ii}	0.88	2.57	3.2645 (18)	136
N2—H22···O5^{iii}	0.91	2.61	3.280 (2)	131
N2—H22···O6^{iii}	0.91	2.16	3.0601 (17)	175
N4—H41···O4^{iv}	0.88	2.58	3.3268 (19)	144
N4—H42···O3^{v}	0.83	2.27	3.0922 (18)	177
C4—H4···O1^{vi}	0.93	2.59	3.166 (2)	121
C5—H5···O1^{vi}	0.93	2.58	3.166 (2)	122

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

through three strong and moderate N—H···O hydrogen bonds, giving rise to $R_1^2(4)$, $R_2^2(8)$ and $R_2^2(24)$ ring motifs that propagate parallel to the *a*-axis direction (Fig. 4).

Interlayer connectivity between dimeric layers parallel to the *ac* plane is established by one moderate N—H···O hydrogen bond and two weak C—H···O interactions, generating infinite *C*(6) chains and $R_2^1(5)$ ring motifs, respectively (Fig. 5). These interactions, together with two intermolecular π–π stacking interactions between the pyridine ring centroids, with a centroid-to-centroid distance of 3.674 (2) Å, contribute to the formation of >a three-dimensional supramolecular network (Fig. 5).

4. Hirshfeld surface analysis

Hirshfeld surface analysis using *CrystalExplorer21* (Spackman *et al.*, 2021) was used to illustrate and quantify the interactions in the crystal structure of the complex. The analysis generated Hirshfeld surfaces mapped over d_{norm}, shape index and curvedness, alongside two-dimensional fingerprint plots (2D-FPs).

The d_{norm} surfaces (Fig. 6) were plotted over the range −0.54 to 1.49 a.u. with transparency to allow visualization of

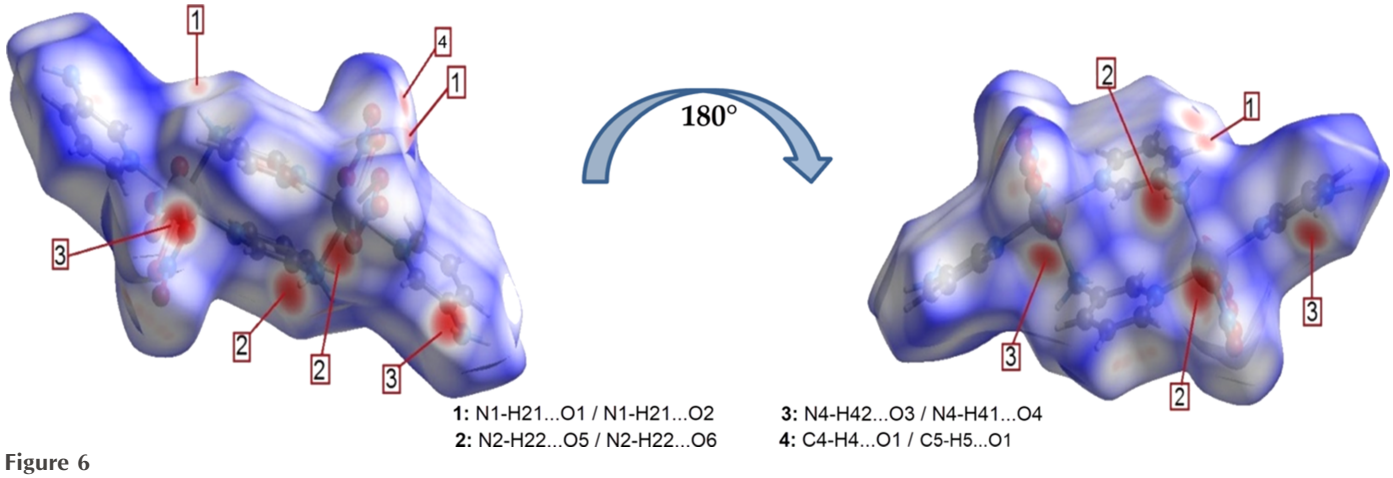


Figure 6
Hirshfeld surface of the studied complex mapped over d_{norm}, showing the intermolecular interactions.

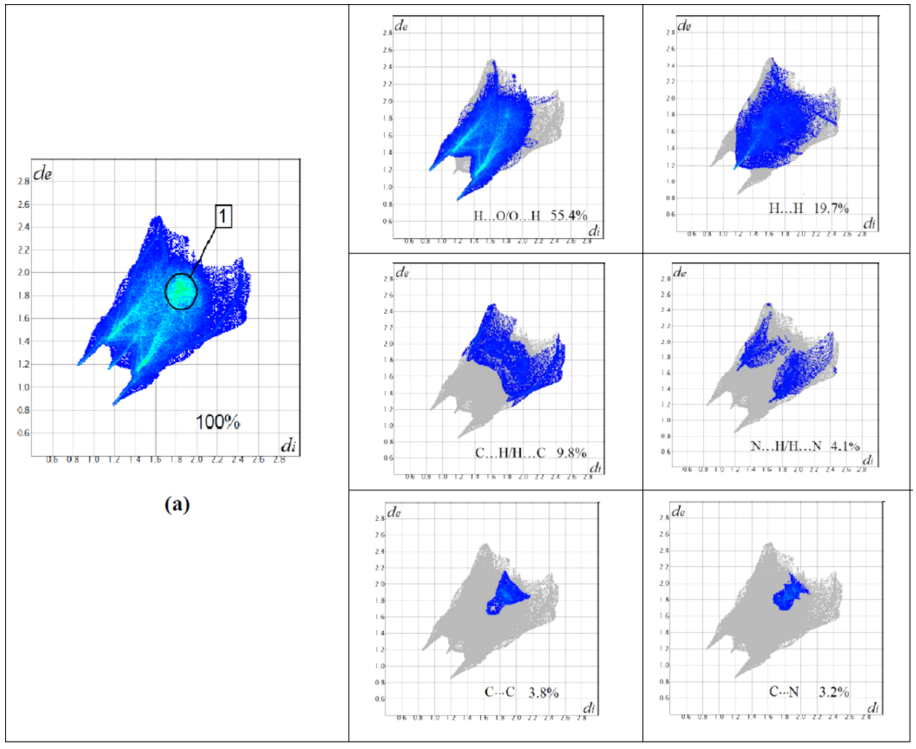


Figure 7
Two-dimensional fingerprint plots of the different contacts in the studied complex and their contributions to the total surface.

the molecular structures. Red spots on the d_{norm} surface correspond to intermolecular H···O contacts, while blue regions indicate regions too distant for interaction.

The two-dimensional FPs (Fig. 7) reveals the dominant role of H···O/O···H contacts (55.4%), followed by H···H interactions (19.7%) and C···H/H···C contacts (9.8%). Analysis in curvedness [Fig. 8(*a*)] and shape index modes [Fig. 8(*b*)] identifies π–π interactions (3.8% of surface contacts) between adjacent pyridine rings, confirming aromatic stacking as a secondary contributor to the crystal packing.

This quantitative assessment demonstrates that hydrogen bonding is the primary determinant of the supramolecular architecture, with π–π stacking providing structural reinforcement.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.01, November 2025, including the September 2026 updates; Groom *et al.*, 2016) was performed using *ConQuest*, targeting transition-metal-containing structures featuring 3-aminopyridine (3-ampy). The search returned 142 hits, of which 15 corresponded to cadmium-containing coordination complexes.

The reported Cd^{II}–3-ampy structures exhibit a variety of coordination environments and structural arrangements. The mononuclear complex $[CdCl_2(3\text{-ampy})_4]$ contains six-coordinate Cd^{II}, with the 3-ampy ligands coordinated through their pyridine N atoms (He *et al.*, 2004). In the sulfate and azide compounds, $\{[Cd(3\text{-ampy})(H_2O)_4](SO_4)\cdot H_2O\}_n$ and [Cd(3-

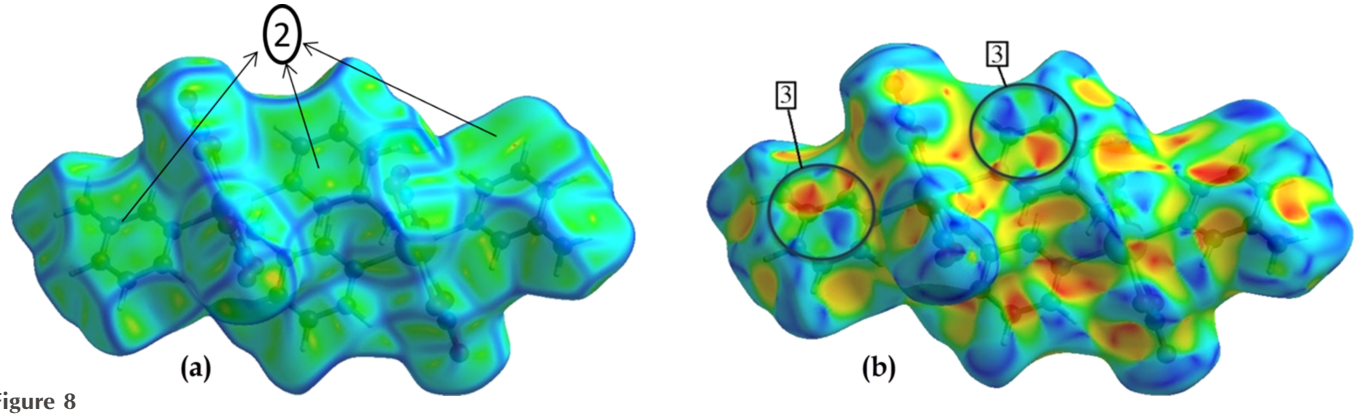


Figure 8
Hirshfeld surface of the studied complex mapped over (*a*) curvedness and (*b*) shape index.

ampy)$(N_3)_2]_n$, respectively, 3-ampy acts as a bridging ligand through both N atoms, resulting in one- and three-dimensional coordination architectures (Goher *et al.*, 2004). In the Hofmann-type compounds $[Cd(3\text{-ampy})_2Ni(CN)_4]$ and $[Cd(3\text{-ampy})_2Cd(\mu_4\text{-}CN)_4]_n$, 3-ampy coordinates in a terminal monodentate fashion through the pyridine N atom (Kartal *et al.*, 2018; Kartal & Şahin, 2021). Other reported Cd^{II}–3-ampy coordination polymers incorporate carboxylate ligands (O'Donovan & LaDuca, 2014; Shen *et al.*, 2015; Wilson *et al.*, 2013), as well as thiocyanate, dicyanamide and sulfate anions (Saber *et al.*, 2012; Mautner *et al.*, 2019; Mautner *et al.*, 2021; Goher *et al.*, 2004).

Seven-coordinate Cd^{II} centres coordinated by 3-ampy have previously been reported in two polymeric carboxylate structures (Shen *et al.*, 2015; Wilson *et al.*, 2013), in which the high coordination number is achieved through chelating carboxylate groups. Furthermore, although Cd_2N_2 units occur in the azide-based coordination polymer reported by Goher *et al.* (2004), these units are linked into an extended three-dimensional network rather than forming discrete dinuclear complexes.

The title compound therefore exhibits a distinct combination of structural features. It consists of a discrete centrosymmetric dinuclear complex in which two symmetry-related 3-ampy ligands bridge the Cd^{II} centres through their pyridine and amino N atoms, while additional 3-ampy ligands coordinate terminally through their pyridine N atoms. Each Cd^{II} centre is seven-coordinate, with its coordination sphere completed by two chelating nitrate anions. No previously reported Cd^{II}–3-ampy structure featuring coordinated nitrate anions was identified in the CSD survey. To the best of our knowledge, the title compound is thus the first reported discrete dinuclear Cd^{II}–3-ampy complex combining *N*:*N*′-bridging 3-ampy ligands, seven-coordinate Cd^{II} centres and coordinated nitrate anions.

6. Synthesis and crystallization

3-Aminopyridine ($C_5H_6N_2$, 0.5 mmol, 0.04705 g) and cadmium nitrate tetrahydrate [$Cd(NO_3)_2{\cdot}4H_2O$, 0.5 mmol, 0.1542 g] were dissolved in a 1:1 (*v*/*v*) mixture of ethanol and distilled water (20 ml). The solution was stirred at room temperature for 15 min, then transferred to a sealed tube and heated in a sand bath at 140 °C for 48 h. The tube was subsequently allowed to cool to room temperature over 48 h. Transparent prismatic crystals suitable for single-crystal X-ray diffraction analysis were obtained in approximately 45% yield, based on cadmium nitrate.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Aromatic H atoms were placed at calculated positions and refined using a riding model, with C—H bond lengths fixed at 0.93 Å. The two amino H atoms were initially located in the difference Fourier map and subsequently refined using a geometrically constrained model.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Cd_2(NO_3)_4(C_5H_6N_2)_4]$
M_r	849.32
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	273
a, b, c (Å)	8.1799 (2), 13.0955 (3), 13.5180 (3)
β (°)	100.441 (1)
V (Å^3)	1424.07 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.58
Crystal size (mm)	0.20 × 0.20 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.697, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11199, 2882, 2587
R_{int}	0.016
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.015, 0.038, 1.09
No. of reflections	2882
No. of parameters	210
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.44, −0.24

Computer programs: *APEX2* (Bruker, 2011), *SAINT* (Bruker, 2011), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *WinGX* (Farrugia, 2012) and *Mercury* (Macrae *et al.*,2020).

The isotropic displacement parameters of all H atoms were set to $U_{iso}(H) = 1.2U_{eq}(C)$ and $U_{iso} = 1.5U_{eq}(N)$, depending on the atom to which each H atom is bonded.

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References

Bartholomä, M., Cheung, H. & Zubieta, J. (2010). *Acta Cryst.* E**66**, m1197.
Benahsene, A. H., Bendjeddou, L., Kahlenberg, V., Zouchoune, B., Carcelli, M., Viappiani, C., Rouag, R., Guenifa, F. & Henchiri, R. (2025). *Polyhedron* **279**, 117606.
Blanchette, J. T. & Willett, R. D. (1988). *Inorg. Chem.* **27**, 843–849.
Bruker (2011). *APEX2* and *SAINT*. Bruker AXS Inc, Madison, Wisconsin, USA.
Bučar, D.-K. & Meštrović, E. (2003). *Acta Cryst.* E**59**, m985–m987.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Goher, M. A. S., Hafez, A. K., Abu-Youssef, M. A. M., Badr, A. M. A., Gspan, C. & Mautner, F. A. (2004). *Polyhedron* **23**, 2349–2356.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

He, H.-Y. & Zhu, L.-G. (2003). *Acta Cryst.* E**59**, m1192–m1193.
He, X., Lu, C.-Z., Yu, Y.-Q., Chen, S.-M., Wu, X.-Y. & Liu, J.-H. (2004). *Acta Cryst.* E**60**, m1639–m1640.
Kartal, Z. & Şahin, O. (2021). *Turk. J. Chem.* **45**, 942–955.
Kartal, Z., Şahin, O. & Yavuz, A. (2018). *J. Mol. Struct.* **1171**, 578–586.
Kochel, A. (2006). *Acta Cryst.* E**62**, m1740–m1742.
Kojima, T., Nakanishi, T., Honda, T., Harada, R., Shiro, M. & Fukuzumi, S. (2009). *Eur. J. Inorg. Chem.* pp. 727–734.
Kovalev, V. V., Kokunov, Y. V., Shmelev, M. A., Voronina, Y. K., Kiskin, M. A., Popov, L. D. & Eremenko, I. L. (2021). *Russ. J. Coord. Chem.* **47**, 272–279.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. 10.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
Mautner, F. A., Goher, M. A. S., Moustafa, H. E., Abu-Youssef, M. A. M. & Öhrström, L. (2007). *Polyhedron* **26**, 2703–2712.
Mautner, F. A., Jantscher, P., Fischer, R. C., Torvisco, A., Vicente, R., Karsili, T. N. V. & Massoud, S. S. (2019). *Polyhedron* **166**, 36–43.
Mautner, F. A., Jantscher, P. V., Fischer, R. C., Torvisco, A., Reichmann, K., Salem, N. M. H., Gordon, K. J., Louka, F. R. & Massoud, S. S. (2021). *Crystals* **11**, 181.
O'Donovan, M. E. & LaDuca, R. L. (2014). *J. Mol. Struct.* **1070**, 1–8.
Pan, W.-L., Niu, X.-L., Tang, W. & Hu, C.-W. (2007). *Acta Cryst.* E**63**, m304–m305.
Qian, H.-F. & Huang, W. (2006). *Acta Cryst.* C**62**, m349–m351.
Saber, M. R., Abu-Youssef, M. A. M., Goher, M. A. S., Sabra, B. A., Hafez, A. K., Badr, A. M. A. & Mautner, F. A. (2012). *J. Mol. Struct.* **1014**, 1–7.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Shen, Y., Ma, N., Wu, L. & Song, H.-H. (2015). *Inorg. Chim. Acta* **429**, 51–60.
Song, X.-Q., Cheng, G.-Q. & Liu, Y.-A. (2016). *Inorg. Chim. Acta* **450**, 386–394.
Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.
Willett, R. D. & Halvorson, K. (1988). *Acta Cryst.* C**44**, 2068–2071.
Wilson, J. A., Uebler, J. W. & LaDuca, R. L. (2013). *CrystEngComm* **15**, 5218–5225.
Yilmaz, V. T., Hamamci, S. & Kazak, C. (2007). *Acta Cryst.* E**63**, m3000.

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First seven-coordinate dinuclear Cd^{II} complex featuring bridging 3-aminopyridine and chelating nitrate ligands: crystal structure and Hirshfeld surface analysis

Amani Hind Benahsene, Belkis Selsebil Yeddiou, Raounek Rouag, Fatiha Guenifa, Volker Kahlenberg and Lamia Bendjeddou

Computing details

Bis(*μ*-3-aminopyridine)-*κ*^{2}*N*^{1}:*N*^{3};*κ*^{2}*N*^{3}:*N*^{1})bis[(3-aminopyridine-*κN*^{1})bis(nitrato-*κ*^{2}*O*,*O*′)cadmium(II)]

Crystal data

$[Cd_2(NO_3)_4(C_5H_6N_2)_4]$
M_r = 849.32
Monoclinic, $P2_1/n$
a = 8.1799 (2) Å
b = 13.0955 (3) Å
c = 13.5180 (3) Å
β = 100.441 (1)°
V = 1424.07 (6) Å^3
Z = 2
$F(000)$ = 840
D_x = 1.981 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2882 reflections
θ = 5.1–26.4°
μ = 1.58 mm^{-1}
T = 273 K
Prism, colorless
0.2 × 0.2 × 0.1 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2015)
T_{min} = 0.697, T_{max} = 0.746
11199 measured reflections
2882 independent reflections
2587 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 26.4°, θ_{min} = 5.1°
h = −9→10
k = −16→14
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.038
S = 1.09
2882 reflections
210 parameters
0 restraints
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0164P)^2 + 0.6403P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 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	0.68740 (2)	0.63024 (2)	0.36679 (2)	0.01378 (5)
O4	0.52043 (14)	0.76753 (10)	0.41279 (8)	0.0212 (3)
N2	1.28163 (15)	0.55491 (11)	0.63043 (9)	0.0154 (3)
H21	1.3466	0.5789	0.6848	0.023*
H22	1.3205	0.5761	0.5752	0.023*
O2	0.82763 (14)	0.78131 (10)	0.31546 (8)	0.0221 (3)
O3	0.94568 (15)	0.63757 (9)	0.29167 (9)	0.0209 (3)
O6	0.43340 (14)	0.61791 (9)	0.44867 (9)	0.0204 (3)
N3	0.52084 (17)	0.61615 (11)	0.21342 (10)	0.0165 (3)
N1	0.85218 (16)	0.62875 (10)	0.52262 (9)	0.0145 (3)
O5	0.30785 (15)	0.75465 (11)	0.48771 (10)	0.0311 (3)
O1	1.04893 (16)	0.78031 (12)	0.24830 (10)	0.0327 (3)
N4	0.08435 (17)	0.56886 (12)	0.10418 (10)	0.0217 (3)
H42	0.0513	0.5870	0.1556	0.033*
H41	0.0295	0.5908	0.0459	0.033*
C6	0.3577 (2)	0.59751 (13)	0.20409 (11)	0.0170 (3)
H6	0.3129	0.5893	0.2621	0.020*
C10	0.5866 (2)	0.62834 (13)	0.12995 (12)	0.0186 (3)
H10	0.6996	0.6421	0.1363	0.022*
C1	1.01493 (19)	0.60731 (12)	0.53263 (11)	0.0136 (3)
H1	1.0630	0.6061	0.4753	0.016*
C8	0.3230 (2)	0.60128 (13)	0.02486 (11)	0.0178 (3)
H8	0.2577	0.5956	−0.0388	0.021*
N6	0.94378 (16)	0.73424 (12)	0.28473 (9)	0.0177 (3)
C9	0.4907 (2)	0.62101 (13)	0.03509 (12)	0.0186 (3)
H9	0.5390	0.6293	−0.0216	0.022*
N5	0.41755 (16)	0.71478 (12)	0.44979 (10)	0.0178 (3)
C4	0.8768 (2)	0.61716 (13)	0.70101 (11)	0.0180 (3)
H4	0.8275	0.6230	0.7576	0.022*
C2	1.11416 (19)	0.58686 (12)	0.62500 (11)	0.0140 (3)
C5	0.7845 (2)	0.63390 (13)	0.60592 (12)	0.0178 (3)
H5	0.6721	0.6492	0.5995	0.021*
C7	0.2519 (2)	0.58983 (13)	0.11054 (11)	0.0160 (3)
C3	1.0427 (2)	0.59172 (13)	0.71081 (11)	0.0158 (3)
H3	1.1058	0.5780	0.7738	0.019*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01206 (7)	0.01692 (7)	0.01223 (6)	0.00097 (4)	0.00185 (4)	0.00119 (4)
O4	0.0185 (5)	0.0225 (7)	0.0242 (6)	−0.0016 (5)	0.0083 (5)	0.0036 (5)
N2	0.0138 (6)	0.0168 (7)	0.0151 (6)	−0.0005 (5)	0.0008 (5)	0.0012 (5)
O2	0.0203 (6)	0.0227 (7)	0.0244 (6)	0.0045 (5)	0.0070 (5)	−0.0003 (5)
O3	0.0239 (6)	0.0173 (7)	0.0229 (6)	0.0020 (5)	0.0082 (5)	0.0032 (5)
O6	0.0216 (6)	0.0192 (7)	0.0212 (5)	−0.0002 (5)	0.0064 (5)	0.0006 (5)
N3	0.0169 (6)	0.0171 (8)	0.0149 (6)	0.0005 (5)	0.0015 (5)	0.0010 (5)
N1	0.0152 (6)	0.0135 (7)	0.0143 (6)	0.0002 (5)	0.0013 (5)	0.0005 (5)
O5	0.0231 (6)	0.0322 (8)	0.0427 (8)	0.0060 (6)	0.0185 (6)	−0.0032 (6)
O1	0.0264 (7)	0.0357 (9)	0.0398 (7)	−0.0095 (6)	0.0161 (6)	0.0078 (6)
N4	0.0182 (7)	0.0300 (9)	0.0162 (6)	−0.0022 (6)	0.0016 (5)	0.0002 (6)
C6	0.0192 (8)	0.0177 (9)	0.0144 (7)	0.0006 (7)	0.0041 (6)	0.0011 (6)
C10	0.0162 (7)	0.0206 (9)	0.0191 (7)	0.0012 (7)	0.0035 (6)	0.0019 (7)
C1	0.0157 (7)	0.0108 (8)	0.0144 (7)	−0.0011 (6)	0.0031 (6)	−0.0006 (6)
C8	0.0215 (8)	0.0170 (9)	0.0138 (7)	0.0012 (7)	0.0002 (6)	−0.0005 (6)
N6	0.0165 (6)	0.0210 (8)	0.0149 (6)	−0.0024 (6)	0.0010 (5)	0.0025 (5)
C9	0.0228 (8)	0.0177 (9)	0.0163 (7)	0.0020 (7)	0.0064 (6)	0.0013 (6)
N5	0.0136 (6)	0.0225 (8)	0.0171 (6)	0.0014 (6)	0.0020 (5)	−0.0005 (6)
C4	0.0212 (8)	0.0201 (9)	0.0133 (7)	−0.0004 (7)	0.0047 (6)	−0.0028 (6)
C2	0.0157 (7)	0.0090 (8)	0.0171 (7)	−0.0012 (6)	0.0020 (6)	−0.0006 (6)
C5	0.0155 (7)	0.0193 (9)	0.0188 (7)	0.0024 (6)	0.0034 (6)	−0.0024 (6)
C7	0.0175 (7)	0.0121 (8)	0.0176 (7)	0.0002 (6)	0.0010 (6)	0.0002 (6)
C3	0.0193 (7)	0.0144 (8)	0.0125 (7)	−0.0010 (6)	−0.0003 (6)	−0.0002 (6)

Geometric parameters (Å, º)

Cd1—N3	2.2726 (13)	O1—N6	1.2247 (18)
Cd1—N1	2.2859 (12)	N4—C7	1.385 (2)
Cd1—O4	2.4067 (12)	N4—H42	0.8251
Cd1—N2^{i}	2.4374 (15)	N4—H41	0.8808
Cd1—O2	2.4495 (13)	C6—C7	1.401 (2)
Cd1—O3	2.5063 (12)	C6—H6	0.9300
Cd1—O6	2.5301 (12)	C10—C9	1.380 (2)
O4—N5	1.2601 (18)	C10—H10	0.9300
N2—C2	1.4215 (19)	C1—C2	1.386 (2)
N2—Cd1^{i}	2.4374 (15)	C1—H1	0.9300
N2—H21	0.8834	C8—C9	1.378 (2)
N2—H22	0.9062	C8—C7	1.395 (2)
O2—N6	1.2641 (18)	C8—H8	0.9300
O3—N6	1.2694 (19)	C9—H9	0.9300
O6—N5	1.2756 (19)	C4—C3	1.380 (2)
N3—C6	1.340 (2)	C4—C5	1.385 (2)
N3—C10	1.345 (2)	C4—H4	0.9300
N1—C1	1.343 (2)	C2—C3	1.392 (2)
N1—C5	1.343 (2)	C5—H5	0.9300

O5—N5	1.2278 (18)	C3—H3	0.9300
N3—Cd1—N1	174.79 (5)	C7—N4—H41	109.2
N3—Cd1—O4	91.26 (4)	H42—N4—H41	117.9
N1—Cd1—O4	92.05 (4)	N3—C6—C7	122.67 (14)
N3—Cd1—N2^{i}	88.67 (5)	N3—C6—H6	118.7
N1—Cd1—N2^{i}	86.27 (4)	C7—C6—H6	118.7
O4—Cd1—N2^{i}	143.26 (4)	N3—C10—C9	121.65 (15)
N3—Cd1—O2	92.36 (4)	N3—C10—H10	119.2
N1—Cd1—O2	92.28 (4)	C9—C10—H10	119.2
O4—Cd1—O2	77.68 (4)	N1—C1—C2	122.61 (14)
N2^{i}—Cd1—O2	139.04 (4)	N1—C1—H1	118.7
N3—Cd1—O3	92.49 (4)	C2—C1—H1	118.7
N1—Cd1—O3	88.52 (4)	C9—C8—C7	119.61 (14)
O4—Cd1—O3	129.47 (4)	C9—C8—H8	120.2
N2^{i}—Cd1—O3	87.22 (4)	C7—C8—H8	120.2
O2—Cd1—O3	51.82 (4)	O1—N6—O2	121.09 (15)
N3—Cd1—O6	89.42 (4)	O1—N6—O3	121.39 (15)
N1—Cd1—O6	89.44 (4)	O2—N6—O3	117.51 (13)
O4—Cd1—O6	52.06 (4)	C8—C9—C10	119.63 (15)
N2^{i}—Cd1—O6	91.20 (4)	C8—C9—H9	120.2
O2—Cd1—O6	129.74 (4)	C10—C9—H9	120.2
O3—Cd1—O6	177.49 (4)	O5—N5—O4	121.59 (15)
N5—O4—Cd1	98.29 (10)	O5—N5—O6	120.76 (14)
C2—N2—Cd1^{i}	112.96 (10)	O4—N5—O6	117.63 (13)
C2—N2—H21	111.5	C3—C4—C5	119.21 (15)
Cd1^{i}—N2—H21	107.2	C3—C4—H4	120.4
C2—N2—H22	110.2	C5—C4—H4	120.4
Cd1^{i}—N2—H22	105.5	C1—C2—C3	118.43 (14)
H21—N2—H22	109.2	C1—C2—N2	120.32 (14)
N6—O2—Cd1	96.76 (10)	C3—C2—N2	121.12 (13)
N6—O3—Cd1	93.91 (9)	N1—C5—C4	122.16 (15)
N5—O6—Cd1	92.01 (9)	N1—C5—H5	118.9
C6—N3—C10	119.07 (13)	C4—C5—H5	118.9
C6—N3—Cd1	121.53 (10)	N4—C7—C8	121.77 (14)
C10—N3—Cd1	119.40 (10)	N4—C7—C6	120.84 (14)
C1—N1—C5	118.51 (13)	C8—C7—C6	117.36 (14)
C1—N1—Cd1	120.19 (10)	C4—C3—C2	119.02 (14)
C5—N1—Cd1	120.56 (10)	C4—C3—H3	120.5
C7—N4—H42	111.2	C2—C3—H3	120.5
C10—N3—C6—C7	0.2 (3)	Cd1—O6—N5—O4	1.06 (12)
Cd1—N3—C6—C7	179.13 (13)	N1—C1—C2—C3	−1.9 (2)
C6—N3—C10—C9	−0.7 (3)	N1—C1—C2—N2	173.86 (15)
Cd1—N3—C10—C9	−179.69 (13)	Cd1^{i}—N2—C2—C1	−93.71 (15)
C5—N1—C1—C2	2.3 (2)	Cd1^{i}—N2—C2—C3	81.92 (16)
Cd1—N1—C1—C2	−167.83 (12)	C1—N1—C5—C4	−0.5 (2)
Cd1—O2—N6—O1	178.44 (12)	Cd1—N1—C5—C4	169.63 (13)

Cd1—O2—N6—O3	−0.50 (13)	C3—C4—C5—N1	−1.7 (3)
Cd1—O3—N6—O1	−178.45 (12)	C9—C8—C7—N4	−179.30 (16)
Cd1—O3—N6—O2	0.48 (13)	C9—C8—C7—C6	−1.1 (3)
C7—C8—C9—C10	0.6 (3)	N3—C6—C7—N4	178.97 (16)
N3—C10—C9—C8	0.4 (3)	N3—C6—C7—C8	0.7 (3)
Cd1—O4—N5—O5	177.30 (12)	C5—C4—C3—C2	2.1 (3)
Cd1—O4—N5—O6	−1.12 (13)	C1—C2—C3—C4	−0.4 (2)
Cd1—O6—N5—O5	−177.38 (12)	N2—C2—C3—C4	−176.08 (15)

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H21···O1^{ii}	0.88	2.52	3.273 (2)	143
N2—H21···O2^{ii}	0.88	2.57	3.2645 (18)	136
N2—H22···O5^{iii}	0.91	2.61	3.280 (2)	131
N2—H22···O6^{iii}	0.91	2.16	3.0601 (17)	175
N4—H41···O4^{iv}	0.88	2.58	3.3268 (19)	144
N4—H42···O3^{v}	0.83	2.27	3.0922 (18)	177
C4—H4···O1^{vi}	0.93	2.59	3.166 (2)	121
C5—H5···O1^{vi}	0.93	2.58	3.166 (2)	122

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