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Synthesis and structure of *catena*-poly[[[bis(pyridin-2-yl)amine]cadmium(II)]-di-μ_2-azido]

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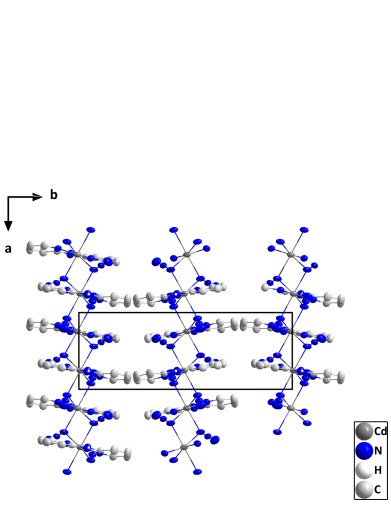
In the title compound, $[Cd(N_3)_2(C_{10}H_9N_3)]_n$, the cadmium(II) ion displays a distorted CdN_6 octahedral geometry arising from one bidentate ligand and four azide ions and forms zigzag polymeric [100] chains *via* the bridging azide ions, both of which show $\mu_{1,1}$ (end-on) coordination. Adjacent chains are linked into layers *via* N—H···N hydrogen bonds. Hirshfeld surface analysis was used to quantify the intermolecular interactions.

1. Chemical context

Cadmium(II) coordination polymers containing polynitrile or pseudohalide ligands have been widely investigated because of their photoluminescence (Addala *et al.*, 2019; Majumder *et al.*, 2017) or photocatalysis (Roy *et al.*, 2017) properties. Generally, the crystal chemistry of the Cd^{II} ion is dominated by coordination numbers of four to six (Setifi *et al.*, 2017; Liu *et al.*, 2016). As for the choice of anionic ligands, pseudohalides are considered as a good linker species. In particular, the azide ligand is an attractive bridging ligand due to the variability of its coordination modes, such as the common $\mu_{1,1}$ (end-on, EO) and $\mu_{1,3}$ (end-to end, EE) modes with single or double azide bridges (Setifi *et al.*, 2025; Merabet *et al.*, 2023). Therefore, such anionic ligands are used for studying magnetochemistry and for the construction of coordination frameworks (Benamara *et al.*, 2021; Merabet *et al.*, 2022).



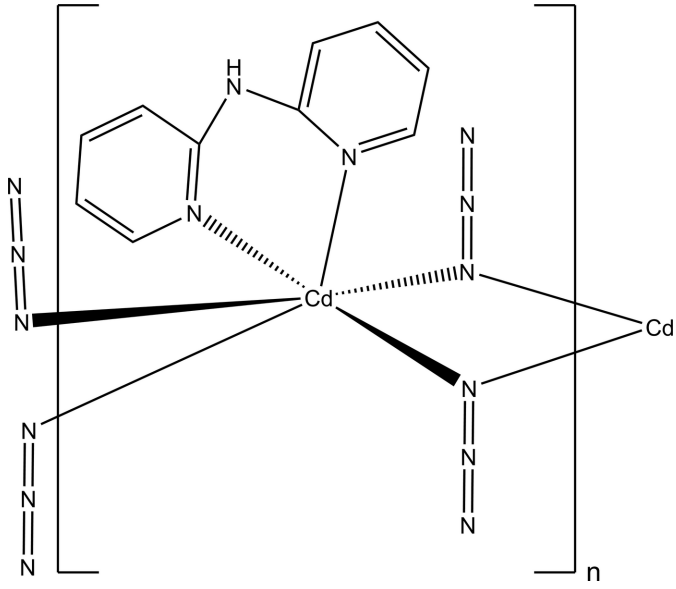


Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.293 (3)	Cd1—N4	2.332 (2)
Cd1—N9	2.330 (2)	Cd1—N1^{i}	2.394 (3)
Cd1—N7	2.330 (2)	Cd1—N4^{ii}	2.436 (3)
N1—Cd1—N9	158.28 (9)	N7—Cd1—N1^{i}	100.49 (10)
N1—Cd1—N7	94.44 (10)	N4—Cd1—N1^{i}	99.89 (10)
N9—Cd1—N7	80.59 (9)	N1—Cd1—N4^{ii}	102.19 (10)
N1—Cd1—N4	95.09 (10)	N9—Cd1—N4^{ii}	98.22 (9)
N9—Cd1—N4	96.82 (9)	N7—Cd1—N4^{ii}	83.17 (9)
N7—Cd1—N4	159.02 (9)	N4—Cd1—N4^{ii}	76.57 (10)
N1—Cd1—N1^{i}	76.52 (11)	N1^{i}—Cd1—N4^{ii}	176.17 (9)
N9—Cd1—N1^{i}	83.57 (9)		

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

As part of our ongoing work in this area, the title one-dimensional Cd^{II} coordination polymer, $[Cd(N_3)_2(C_{10}H_9N_3)]_n$ (**I**), was synthesized and characterized and is reported herein.

2. Structural commentary

In compound (**I**), the cadmium ion adopts a distorted CdN_6 octahedral coordination geometry (Table 1) provided by two N atoms from the chelating ligand (N7 and N9) in *cis* positions, two from the $\mu_2;\eta^1$-azide ions in the asymmetric unit and the last two from symmetry generated $\mu_2;\eta^1$-azide ions (N1^{i} at $1-x, 1-y, 1-z$ and N4^{ii} at $2-x, 1-y, 1-z$) (Fig. 1). Part of the distortion results from the small bite angle of the chelating ligand giving an N7—Cd1—N9 angle of 80.59 (9)° while the N1—Cd1—N4 angle, at 95.09 (10)°, is closer to the ideal value. Four Cd—N distances are in the narrow range of 2.293 (3)–2.332 (2) Å but the other two are notably longer at 2.394 (3) Å (Cd1—N1^{i}) and 2.436 (3) Å (Cd1—N4^{ii}) (Fig. 1) making the Cd(μ_2(N$_3$)$_2$)Cd units unsymmetrical. This also leads to two different Cd···Cd distances with Cd1···Cd1^{i} being 3.6812 (4) Å while the Cd1···Cd1^{ii} separation is 3.7432 (4) Å (Fig. 1).

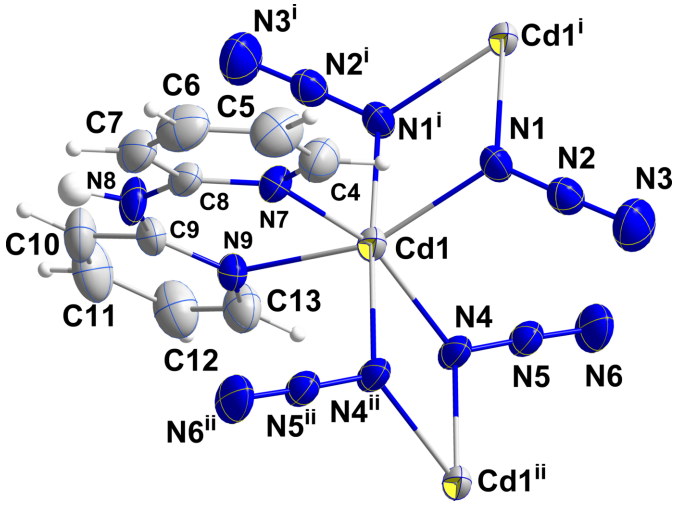


Figure 1
The coordination sphere of the metal ion in (**I**) with 50% probability ellipsoids. Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+2, -y+1, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N8—H8···N6^{iii}	0.89 (1)	2.21 (1)	3.086 (4)	174 (4)

Symmetry code: (iii) $x, y, z+1$.

3. Supramolecular features

In the crystal, the *cis* position of the bridging azide ligands leads to the formation of zigzag chains built up from Cd(μ_2(N$_3$)$_2$)Cd units extending along the *a*-axis direction, which are connected by N8—H8···N6 hydrogen bonds (Table 2) into layers lying parallel to the *ac* plane (Figs. 2 and 3).

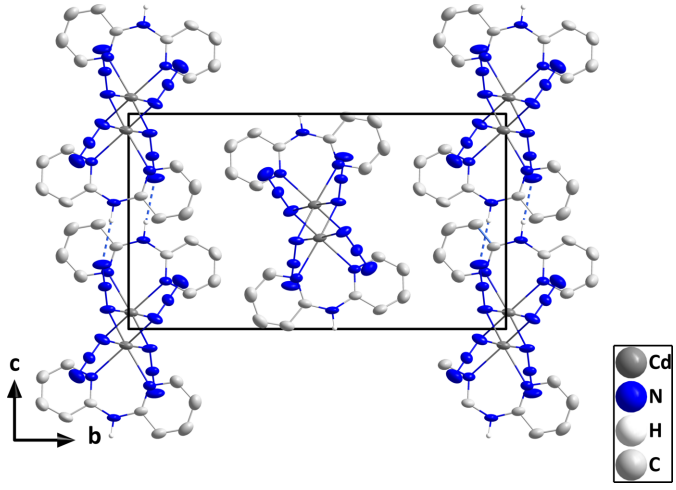


Figure 2
The packing in (**I**) viewed along the *a*-axis direction showing end views of several chains. The N—H···N hydrogen bonds are depicted by dashed lines and non-interacting hydrogen atoms are omitted for clarity.

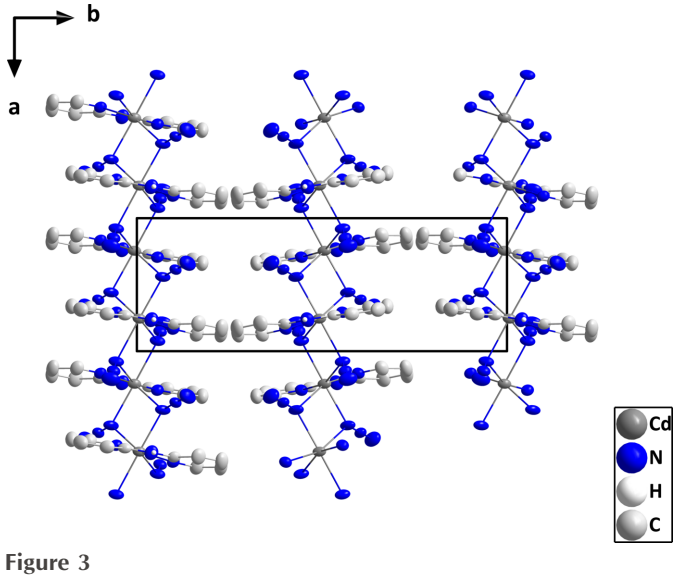


Figure 3
The packing in (**I**) viewed along the *c*-axis direction showing side views of several chains. The N—H···N hydrogen bonds are depicted by dashed lines and non-interacting hydrogen atoms are omitted for clarity.

Table 3
Interatomic distances in Cd(μ-N_3)$_2$ units.

REFCODE	a^1	b^1	c^1	d^1	e^1	f^1	Reference
(I)	2.394 (3)	2.293 (3)	2.332 (2)	2.436 (3)	3.6812 (4)	3.7432 (4)	This work
FEBKED	2.334 (2)	2.399 (2)	2.399 (2)	2.334 (2)	307917 (9)	3.7917 (9)	He & Lu (2004)
FEBKED01	2.312 (3)	2.422 (3)	2.422 (3)	2.312 (3)	3.7728 (2)	3.7728 (2)	Abu-Youssef 2005
OWOGAK	2.445 (2)	2.300 (2)	2.2811 (19)	2.3610 (18)	3.7266 (2)	3.7871 (2)	Marandi *et al.* (2016)
QUXZOZ	2.411 (2)	2.303 (2)	2.303 (2)	2.411 (2)	3.7643 (4)	3.7728 (2)	Chen *et al.* (2010)
UMUSUS	2.367 (4)	2.322 (5)	2.323 (5)	2.367 (4)	3.6327 (9)	3.6327 (9)	Wan *et al.* (2016)
FARZEF	2.283 (6)	2.490 (5)[2]	2.408 (4)[2]	2.326 (6)	3.7351 (6)	3.6992 (7)	Machura *et al.* (2012)
FARZIJ	2.278 (6)	2.376 (4)[2]	2.396 (5)[2]	2.252 (5)	3.6763 (10)	3.6432 (10)	Machura *et al.* (2012)
TEPHUT	2.283 (4)	2.439 (4)[2]	2.471 (3)[2]	2.314 (4)	3.6146 (5)	3.7018 (5)	Bai *et al.* (2013)
GIWYER	2.371 (2)	2.351 (2)	2.351 (2)	2.371 (2)	3.6935 (11)	3.6935 (11)	Goher *et al.* (2008)
GIWYIV	2.369 (5)	2.312 (4)	2.355 (6)	2.326 (5)	3.5665 (19)	3.5516 (19)	Goher *et al.* (2008)
GOYROB	2.3441 (18)	2.3421 (17)	2.3421 (17)	2.3441 (18)	3.5298 (3)	3.5298 (3)	Mautner *et al.* (2015)
KABSUB	2.411 (3)	2.308 (2)	2.411 (3)	2.308 (2)	3.6267 (2)	3.6267 (2)	Yang *et al.* (2010)
WUBSIV	2.359 (6)	2.329 (6)	2.329 (6)	2.585 (6)	3.7050 (16)	3.9291 (16)	Goher *et al.* (2002)

Notes: (1) see Fig. 4*b* for key; (2) distance to μ_3-N_3 ion.

4. Database survey

A search of the Cambridge Structural Database [CSD, updated to September 2025 (Groom *et al.*, 2016)] with the search fragment shown in Fig. 4*a* gave 65 hits, 21 of which contained coordinated azide ions. Of these, 16 were considered most similar to the title compound while one was monomeric and the remaining four contained exclusively Cd—N═N═N—Cd bridging units. Table 3 lists the title compound and the most similar ones with pertinent geometric details. The compounds with refcodes FEBKED to UMUSUS contain a chelating ligand similar to that in the title compound so that the two Cd(μ_2(N_3)$_2$)Cd units are *cis* to one another and unsymmetrically bridged as well. The Cd—N distances are comparable although the short–long pattern is not always in the same order. Except for OWOGAK, which has two different Cd···Cd separations as is the case with the title molecule, the Cd···Cd separations are equivalent by symmetry. For FARZEF, FARZIJ and TERHUT, pairs of Cd ions are bridged either by one μ_2;η^1-N_3 ion and one μ_3;η^1-N_3 ion or by two μ_3;η^1-N_3 ions. Here, the Cd—N distances to the μ_2;η^1-N_3 ion are comparable to the shorter ones seen in (**I**) but those to the μ_3;η^1-N_3 grouping are noticeably longer as expected. The last group contains Cd(μ_2(N_3)$_2$)Cd units which are *trans* to one another but the bridging units are still unsymmetrical except for GOYROD where site symmetry requires them to be symmetrical.

5. Hirshfeld surface analysis

A Hirshfeld surface (HS) analysis was performed using CrystalExplorer (Spackman *et al.*, 2021) to explore the intermolecular interactions in the crystal of (**I**). Descriptions and interpretations of the plots obtained have been published (Tan *et al.*, 2019). The d_{norm} HS for a portion of one chain is shown in Fig. 5 with the bright red spots on the right side showing the sites of N—Cd bonds that continue the chain. The red spots on the top of the surface indicate the locations of the N—H···N hydrogen bonds, which connect the chains. Fig. 6 shows the two-dimensional fingerprint plots with Fig. 6*a* showing all intermolecular interactions. This is characterized by two pairs of sharp peaks and a broader central one. Delineation of these

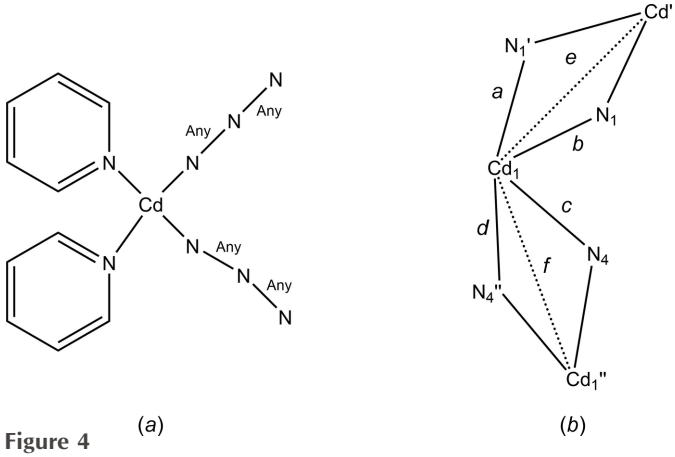


Figure 4
(*a*) The search fragment used where 'Any' refers to any bond type (single, double or delocalized) in the CSD search, and (*B*) the key for column headings in Table 3.

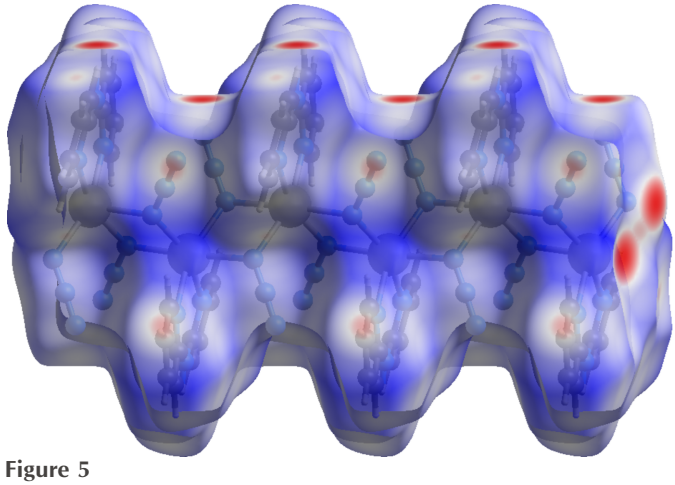


Figure 5
The d_{norm} Hirshfeld surface for (**I**).

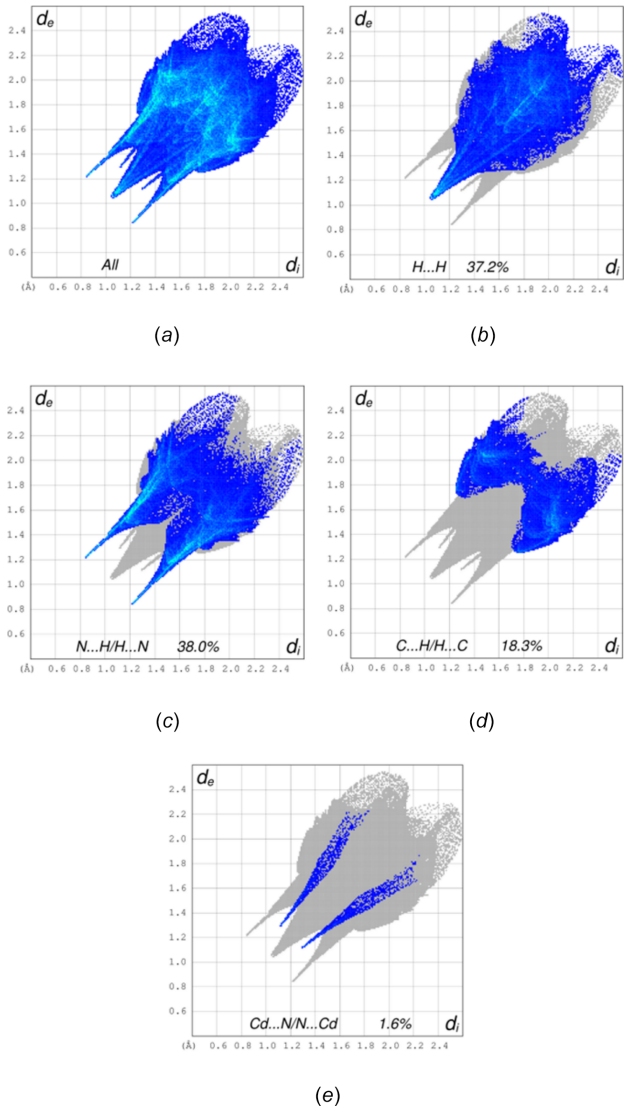


Figure 6
Two-dimensional fingerprint plots for (**I**) showing all interactions (*a*) and those delineated into H···H (*b*), N···H/H···N (*c*), C···H/H···C (*d*) and Cd—N (*e*) interactions.

into specific atom···atom interactions shows the central peak to represent H···H interactions at 37.2% of the total and the pair with tips at $d_e + d_i \simeq 2.2$ Å (Fig. 6*c*) consistent with the N—H···N hydrogen bonds at 38.0% of the total. The C···H/H···C interactions constitute 18.3% of the total and appear as a pair of broad peaks at $d_e + d_i \simeq 3$ Å (Fig. 6*d*). These do not appear to represent any *specific* interactions as calculations of intermolecular distances do not show any C—H···π(ring) interactions to be present. Finally, the pair of sharp peaks with $d_e + d_i \simeq 2.4$ Å (Fig. 6*e*) can be attributed to the Cd—N bonds mentioned above that continue the chain beyond that fragment used in the calculation of the HS.

6. Synthesis and crystallization

The title compound was prepared under solvothermal conditions from a mixture of cadmium(II) nitrate tetrahydrate (62 mg, 0.20 mmol), 2,2′-dipyridylamine (17 mg, 0.10 mmol), sodium azide (26 mg, 0.40 mmol), N,N-dimethylformamide (10 ml) and water (7 ml), which was sonicated for 30min. Then the reaction mixture was transferred to a Teflon-lined stainless steel reactor and heated to 403 K for 2 days. After cooling to room temperature at a rate of 10 K h^{-1}, colourless block-shaped crystals of (**I**) were collected.

Table 4
Experimental details.

Crystal data	
Chemical formula	$[Cd(N_3)_3(C_{10}H_9N_3)]$
M_r	367.66
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, b, c (Å)	6.6655 (5), 18.5106 (17), 10.5746 (9)
β (°)	93.612 (3)
V (Å^3)	1302.13 (19)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.68
Crystal size (mm)	0.34 × 0.21 × 0.17
Data collection	
Diffractometer	Bruker D8 Quest PHOTON 100 CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.796, 0.877
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	64159, 6322, 5357
R_{int}	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.835
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.096, 1.37
No. of reflections	6322
No. of parameters	185
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.19, −1.10

Computer programs: *APEX4* and *SAINT* (Bruker, 2018), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012), *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. The N-bound H atom was located in a difference map and its position was freely refined. The C-bound H atoms were located geometrically (C—H = 0.93 Å) and refined as riding atoms.

Acknowledgements

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supporting information

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Synthesis and structure of *catena*-poly[[[bis(pyridin-2-yl)amine]cadmium(II)]-di-μ_2-azido]

Zouaoui Setifi, Fatima Setifi, Joel T. Mague and Mohammed Hadi Al-Douh

Computing details

***catena*-Poly[[[bis(pyridin-2-yl)amine]cadmium(II)]-di-μ_2-azido]**

Crystal data

$[Cd(N_3)_3(C_{10}H_9N_3)]$
M_r = 367.66
Monoclinic, $P2_1/c$
a = 6.6655 (5) Å
b = 18.5106 (17) Å
c = 10.5746 (9) Å
β = 93.612 (3)°
V = 1302.13 (19) Å^3
Z = 4
$F(000)$ = 720
D_x = 1.875 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9995 reflections
θ = 3.0–32.3°
μ = 1.68 mm^{-1}
T = 298 K
Block, colourless
0.34 × 0.21 × 0.17 mm

Data collection

Bruker D8 Quest PHOTON 100 CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.796, T_{max} = 0.877
64159 measured reflections
6322 independent reflections
5357 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 36.4°, θ_{min} = 2.9°
h = −11→8
k = −30→30
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.096
S = 1.37
6322 reflections
185 parameters
1 restraint
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 2.1586P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.19 e Å^{-3}
$\Delta\rho_{min}$ = −1.10 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.

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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 Å) and were included as riding contributions with isotropic displacement parameters 1.2 times those of the attached atoms. That attached to nitrogen was placed in a location derived from a difference map and refined with a DFIX 0.89 0.01 instruction

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.75506 (3)	0.49321 (2)	0.57654 (2)	0.03175 (6)
N1	0.5582 (4)	0.56986 (17)	0.4517 (3)	0.0413 (6)
N2	0.6135 (4)	0.60430 (14)	0.3655 (3)	0.0355 (5)
N3	0.6614 (6)	0.6371 (2)	0.2803 (3)	0.0616 (9)
N4	0.9227 (4)	0.44425 (16)	0.4095 (2)	0.0366 (5)
N5	0.8521 (4)	0.43719 (15)	0.3032 (2)	0.0342 (5)
N6	0.7900 (5)	0.4295 (2)	0.2006 (3)	0.0570 (9)
N7	0.7069 (4)	0.55560 (14)	0.7636 (2)	0.0339 (5)
N8	0.7629 (5)	0.46074 (16)	0.9133 (2)	0.0414 (6)
H8	0.762 (6)	0.454 (2)	0.9962 (11)	0.045 (11)*
N9	0.8345 (4)	0.40164 (14)	0.7223 (2)	0.0323 (5)
C4	0.6731 (6)	0.6269 (2)	0.7451 (4)	0.0472 (8)
H4	0.656367	0.643523	0.662142	0.057*
C5	0.6618 (7)	0.6763 (2)	0.8408 (4)	0.0566 (10)
H5	0.638413	0.724920	0.823253	0.068*
C6	0.6862 (6)	0.6517 (2)	0.9641 (4)	0.0553 (10)
H6	0.679635	0.683707	1.031517	0.066*
C7	0.7197 (5)	0.5804 (2)	0.9861 (3)	0.0447 (7)
H7	0.735825	0.563157	1.068661	0.054*
C8	0.7299 (4)	0.53278 (17)	0.8829 (3)	0.0329 (5)
C9	0.7960 (4)	0.39917 (17)	0.8450 (3)	0.0332 (6)
C10	0.7921 (7)	0.3336 (2)	0.9106 (3)	0.0513 (9)
H10	0.764813	0.333059	0.995747	0.062*
C11	0.8280 (8)	0.2708 (2)	0.8499 (4)	0.0619 (11)
H11	0.823748	0.226957	0.892713	0.074*
C12	0.8711 (7)	0.2726 (2)	0.7232 (4)	0.0566 (10)
H12	0.898021	0.230431	0.679391	0.068*
C13	0.8726 (6)	0.3382 (2)	0.6654 (3)	0.0467 (8)
H13	0.902013	0.339522	0.580567	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02633 (9)	0.04938 (12)	0.01945 (8)	−0.00229 (9)	0.00072 (6)	0.00442 (8)
N1	0.0259 (11)	0.0631 (18)	0.0341 (13)	−0.0045 (11)	−0.0051 (9)	0.0172 (12)
N2	0.0291 (11)	0.0394 (13)	0.0372 (13)	−0.0044 (9)	−0.0038 (9)	0.0049 (10)
N3	0.062 (2)	0.070 (2)	0.053 (2)	−0.0140 (18)	0.0035 (16)	0.0210 (17)
N4	0.0270 (11)	0.0641 (17)	0.0191 (9)	−0.0058 (11)	0.0044 (8)	−0.0026 (10)
N5	0.0303 (11)	0.0491 (14)	0.0236 (10)	−0.0058 (10)	0.0051 (8)	−0.0022 (9)
N6	0.0508 (18)	0.095 (3)	0.0247 (13)	−0.0106 (17)	−0.0029 (12)	−0.0051 (14)
N7	0.0343 (12)	0.0438 (13)	0.0242 (10)	0.0019 (10)	0.0063 (9)	0.0015 (9)
N8	0.0583 (18)	0.0509 (15)	0.0151 (10)	0.0058 (13)	0.0025 (10)	0.0018 (9)
N9	0.0336 (12)	0.0432 (13)	0.0199 (9)	0.0037 (10)	0.0003 (8)	0.0015 (8)
C4	0.051 (2)	0.0485 (19)	0.0424 (18)	0.0033 (15)	0.0094 (15)	0.0066 (14)
C5	0.064 (3)	0.0426 (19)	0.064 (3)	0.0026 (17)	0.013 (2)	−0.0035 (17)
C6	0.057 (2)	0.059 (2)	0.050 (2)	−0.0026 (18)	0.0113 (18)	−0.0211 (18)
C7	0.0459 (18)	0.060 (2)	0.0286 (14)	−0.0002 (15)	0.0059 (13)	−0.0081 (13)
C8	0.0283 (12)	0.0488 (16)	0.0219 (11)	−0.0007 (11)	0.0043 (9)	−0.0042 (10)
C9	0.0322 (13)	0.0451 (16)	0.0216 (11)	0.0021 (11)	−0.0029 (9)	0.0033 (10)
C10	0.070 (3)	0.055 (2)	0.0283 (15)	0.0042 (18)	−0.0020 (15)	0.0111 (14)
C11	0.088 (3)	0.045 (2)	0.051 (2)	0.005 (2)	−0.011 (2)	0.0118 (17)
C12	0.076 (3)	0.0447 (19)	0.047 (2)	0.0089 (18)	−0.0083 (19)	−0.0075 (16)
C13	0.058 (2)	0.0513 (19)	0.0302 (15)	0.0069 (16)	−0.0013 (14)	−0.0050 (13)

Geometric parameters (Å, º)

Cd1—N1	2.293 (3)	C4—C5	1.369 (5)
Cd1—N9	2.330 (2)	C4—H4	0.9300
Cd1—N7	2.330 (2)	C5—C6	1.382 (6)
Cd1—N4	2.332 (2)	C5—H5	0.9300
Cd1—N1^{i}	2.394 (3)	C6—C7	1.355 (6)
Cd1—N4^{ii}	2.436 (3)	C6—H6	0.9300
N1—N2	1.190 (4)	C7—C8	1.408 (4)
N2—N3	1.148 (4)	C7—H7	0.9300
N4—N5	1.199 (3)	C9—C10	1.399 (5)
N5—N6	1.145 (4)	C10—C11	1.357 (6)
N7—C8	1.330 (4)	C10—H10	0.9300
N7—C4	1.352 (4)	C11—C12	1.389 (6)
N8—C9	1.375 (4)	C11—H11	0.9300
N8—C8	1.386 (4)	C12—C13	1.361 (5)
N8—H8	0.885 (10)	C12—H12	0.9300
N9—C9	1.339 (3)	C13—H13	0.9300
N9—C13	1.351 (4)		
N1—Cd1—N9	158.28 (9)	C13—N9—Cd1	112.2 (2)
N1—Cd1—N7	94.44 (10)	N7—C4—C5	124.2 (4)
N9—Cd1—N7	80.59 (9)	N7—C4—H4	117.9
N1—Cd1—N4	95.09 (10)	C5—C4—H4	117.9

N9—Cd1—N4	96.82 (9)	C4—C5—C6	117.9 (4)
N7—Cd1—N4	159.02 (9)	C4—C5—H5	121.0
N1—Cd1—N1^{i}	76.52 (11)	C6—C5—H5	121.0
N9—Cd1—N1^{i}	83.57 (9)	C7—C6—C5	119.4 (3)
N7—Cd1—N1^{i}	100.49 (10)	C7—C6—H6	120.3
N4—Cd1—N1^{i}	99.89 (10)	C5—C6—H6	120.3
N1—Cd1—N4^{ii}	102.19 (10)	C6—C7—C8	119.5 (3)
N9—Cd1—N4^{ii}	98.22 (9)	C6—C7—H7	120.2
N7—Cd1—N4^{ii}	83.17 (9)	C8—C7—H7	120.2
N4—Cd1—N4^{ii}	76.57 (10)	N7—C8—N8	122.2 (3)
N1^{i}—Cd1—N4^{ii}	176.17 (9)	N7—C8—C7	121.8 (3)
N2—N1—Cd1	125.4 (2)	N8—C8—C7	115.9 (3)
N2—N1—Cd1^{i}	118.4 (2)	N9—C9—N8	121.8 (3)
Cd1—N1—Cd1^{i}	103.48 (11)	N9—C9—C10	121.4 (3)
N3—N2—N1	178.0 (3)	N8—C9—C10	116.8 (3)
N5—N4—Cd1	125.1 (2)	C11—C10—C9	120.0 (3)
N5—N4—Cd1^{ii}	113.66 (19)	C11—C10—H10	120.0
Cd1—N4—Cd1^{ii}	103.43 (10)	C9—C10—H10	120.0
N6—N5—N4	177.9 (4)	C10—C11—C12	119.3 (4)
C8—N7—C4	117.1 (3)	C10—C11—H11	120.4
C8—N7—Cd1	129.3 (2)	C12—C11—H11	120.4
C4—N7—Cd1	113.1 (2)	C13—C12—C11	117.6 (4)
C9—N8—C8	134.7 (2)	C13—C12—H12	121.2
C9—N8—H8	115 (3)	C11—C12—H12	121.2
C8—N8—H8	111 (2)	N9—C13—C12	124.7 (3)
C9—N9—C13	117.1 (3)	N9—C13—H13	117.7
C9—N9—Cd1	128.1 (2)	C12—C13—H13	117.7

C8—N7—C4—C5	0.2 (5)	C13—N9—C9—N8	177.4 (3)
Cd1—N7—C4—C5	−172.7 (3)	Cd1—N9—C9—N8	−22.4 (4)
N7—C4—C5—C6	−0.1 (6)	C13—N9—C9—C10	−1.1 (5)
C4—C5—C6—C7	−0.1 (6)	Cd1—N9—C9—C10	159.0 (3)
C5—C6—C7—C8	0.2 (6)	C8—N8—C9—N9	11.1 (6)
C4—N7—C8—N8	179.2 (3)	C8—N8—C9—C10	−170.3 (4)
Cd1—N7—C8—N8	−9.2 (4)	N9—C9—C10—C11	0.1 (6)
C4—N7—C8—C7	0.0 (4)	N8—C9—C10—C11	−178.5 (4)
Cd1—N7—C8—C7	171.5 (2)	C9—C10—C11—C12	0.9 (7)
C9—N8—C8—N7	6.0 (6)	C10—C11—C12—C13	−0.8 (7)
C9—N8—C8—C7	−174.7 (4)	C9—N9—C13—C12	1.2 (6)
C6—C7—C8—N7	−0.2 (5)	Cd1—N9—C13—C12	−162.0 (3)
C6—C7—C8—N8	−179.5 (3)	C11—C12—C13—N9	−0.2 (7)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N8—H8···N6^{iii}	0.89 (1)	2.21 (1)	3.086 (4)	174 (4)

Symmetry code: (iii) x, y, z+1.