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Poly[bis(μ-azido-κ^2N^1:N^1)[μ-1,2-bis(imidazol-1-yl)ethane-κ^2N^3:$N^{3'}$]cadmium]

Hai-Yan Li, Peng-Peng Sun and Bao-Long Li*

College of Chemistry, Chemical Engineering and Materials Science, Key Laboratory of Organic Synthesis of Jiangsu Province, Soochow University, Suzhou 215123, People's Republic of China
Correspondence e-mail: libaolong@suda.edu.cn

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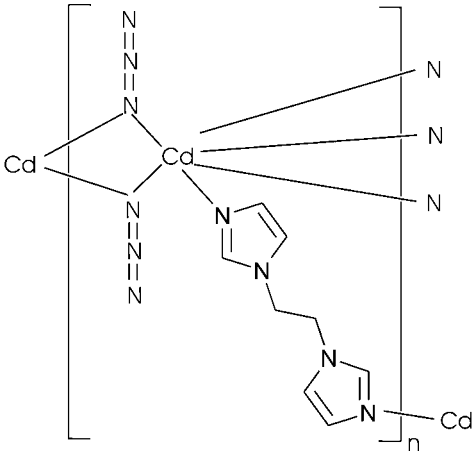
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.004 Å; R factor = 0.023; wR factor = 0.056; data-to-parameter ratio = 13.5.

In the title three-dimensional coordination polymer, $[Cd(N_3)_2(C_8H_{10}N_4)]_n$, the coordination geometry around the Cd^{II} atom is distorted octahedral. The Cd^{II} atom is coordinated by two N atoms from two *cis*-positioned bridging 1,2-bis(imidazol-1-yl)ethane (bime) ligands and four N atoms from four azide anions. Each azide ligand acts in an end-on bridging coordination mode. The azide ligands and Cd^{II} atoms form a one-dimensional zigzag chain constructed from four-membered $[Cd(N_3)_2]_n$ metallacycles extending along the *a* axis. These inorganic chains are connected with four other chains *via* bridging bime ligands to form a three-dimensional coordination network.

Related literature

For coordination polymers with intriguing structures, see: Batten & Robson (1998); Blake *et al.* (1999); Kitagawa *et al.* (2004). For coordination polymers with flexible ligands, see: Hoskins *et al.* (1997*a*,*b*). For azide coordination compounds and polymers, see: Ribas *et al.* (1999); Leibeling *et al.* (2004); Chen & Chen (2002); Mautner *et al.* (1997). For 1,2-bis(imidazol-1-yl)ethane (bime) coordination polymers, see: Zhang *et al.* (2005, 2008); Zhu *et al.* (2010).



Experimental

Crystal data

$[Cd(N_3)_2(C_8H_{10}N_4)]$
M_r = 358.66
Monoclinic, $P2_1/c$
a = 6.4565 (14) Å
b = 18.874 (4) Å
c = 10.449 (2) Å
β = 90.485 (5)°
V = 1273.2 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.72 mm^{-1}
T = 153 K
0.36 × 0.17 × 0.15 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.576, T_{max} = 0.783
12260 measured reflections
2324 independent reflections
2190 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.056
S = 1.09
2324 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N2	2.306 (2)	Cd1—N8	2.345 (2)
Cd1—N4^{i}	2.324 (2)	Cd1—N8^{ii}	2.377 (2)
Cd1—N5	2.340 (2)	Cd1—N5^{iii}	2.397 (2)
N2—Cd1—N5	91.57 (8)		

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2436).

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supporting information

Acta Cryst. (2012). E**68**, m253–m254 [doi:10.1107/S1600536812004370]

Poly[bis(μ-azido-κ^2N^1:N^1)[μ-1,2-bis(imidazol-1-yl)ethane-κ^2N^3:$N^{3\prime}$]cadmium]

Hai-Yan Li, Peng-Peng Sun and Bao-Long Li

S1. Comment

Coordination polymers have been paid great attention for their intriguing structures and potential applications as functional materials (Batten & Robson 1998; Kitagawa *et al.*, 2004). The selection of ligand is very important for the design and construction of the coordination polymers. In contrast to the rigid ligands with little or no conformational freedom when they interact with the metal ions, the flexible ligands can adjust their conformations to the geometric requirements of the metal ions (Hoskins *et al.*, 1997*a,b*).

The short anion ligand azide (N_3^-) is widely used to construct novel coordination polymers because its versatile coordination modes and the ability to mediate strong magnetic coupling (Ribas *et al.*, 1999; Leibeling *et al.*, 2004).

In our previous studies, we synthesized two Cd^{II} coordination polymers with the flexible ligand 1,2-bis(imidazol-1-yl)ethane (bime; Zhang *et al.*, 2005; Zhang *et al.*, 2008) and one Cu^{II} coordination polymer (Zhu *et al.*, 2010). In order to extend our work, in the present paper we report the preparation and crystal structure of a novel three-dimensional cadmium(II) coordination polymer $[Cd(bime)(N_3)_2]_n$ (I) with the flexible ligand bime and short anion ligand azide.

The structure of (I) is a novel three-dimensional network. Each Cd^{II} atom is coordinated by six nitrogen atoms: two from two bime ligands in the *cis*-positions and the remaining four from four azide anions, in a distorted octahedral geometry (Fig. 1, Table 1).

The Cd—N bond lengths are in the range of 2.306 (2) - 2.397 (2) Å and do not vary much. The Cd—N (bime) lengths of 2.306 (2) and 2.324 (2)Å are corresponding to the values 2.2769 (17)Å in $[Cd(bime)dca)_2]_n$ (dca = dicyanamide; Zhang, *et al.*, 2005) and 2.2748 (18) Å in $[Cd(phba)_2(bime)(H_2O)_2]_n$ (phba = 4-hydroxybenzoate; Zhang *et al.*, 2008). There are two symmetry independent azide ligands and they both act in end-on (EO) bridging coordination mode. The EO-azide ligands are linear and asymmetric [bond angles N5—N6—N7 = 177.5 (3)° and N8—N9—N10 = 178.4 (3)°, bond lengths N5—N6 = 1.195 (3) Å, N6—N7 = 1.158 (3) Å, N8—N9 = 1.166 (3) Å and N9—N10 = 1.177 (4) Å].

The Cd—N (azide) bond lengths of 2.340 (2) to 2.397 (2)Å are similar to the corresponding values of 2.258 (7) and 2.335 (6) Å in $[Cd(picolinato)(N_3]_n$ with only EO-azide (Mautner *et al.*, 1997) and 2.404 (3) to 2.474 (3) Å in $[Cd(N_3)(4\text{-}aba)(H_2O)]_n$ with μ-1,1,3-azide (4-abaH = 4-aminobenzoic acid; Chen & Chen, 2002). The cis N—Cd—N bond angles are in the range of 74.11 (9) to 98.95 (8)°, deviating much from 90°.

A pair of azide ligands bridge the Cd^{II} atoms to form a $[Cd_2(N_3)_2]$ four-membered metallacycle. The neighboring metallacycles have a common Cd^{II} atom and form a one-dimensional inorganic zigzag chain $[Cd(N_3)_2]_n$ (Fig. 2). The Cd1···Cd1# and Cd1···Cd1& separations *via* the EO-azide ligands are 3.6804 (7) and 3.7688 (7) Å, respectively. There is one symmetry independent bime ligand in (I). The bime ligands exhibits the anti-conformation with the torsion angle N1—C1—C2—N3 of 179.4 (2)°. The Cd···Cd distances between Cd^{II} atoms bridged *via* bime ligands are 11.5566 (15) Å.

The bime ligands attached to the $[Cd(N_3)_2]_n$ chain point in four different directions (Fig. 3) binding to adjacent $[Cd(N_3)_2$ chain and generating a three-dimensional network (Fig. 4).

S2. Experimental

An aqueous (20 mL) solution of $Cd(NO_3)_2 \cdot 4H_2O$ (0.50 mmol) and NaN_3 (1.0 mmol) was added to one side of a "H-shape" tube, and a methanolic solution (20 mL) of bime (0.50 mmol) was added to the another side of the "H-shape" tube. Colourless crystal were obtained after about one month. Anal. Calcd. for $C_8H_{10}CdN_{10}$: C, 26.79; H, 2.81; N, 39.06%. Found: C, 26.68; H, 2.72; N, 38.98%.

S3. Refinement

H atoms were placed in idealized positions and refined as riding, with C—H distances of 0.99Å (ethyl) and 0.95Å (imidazole) with $U_{iso}(H) = 1.2U_{eq}(C)$.

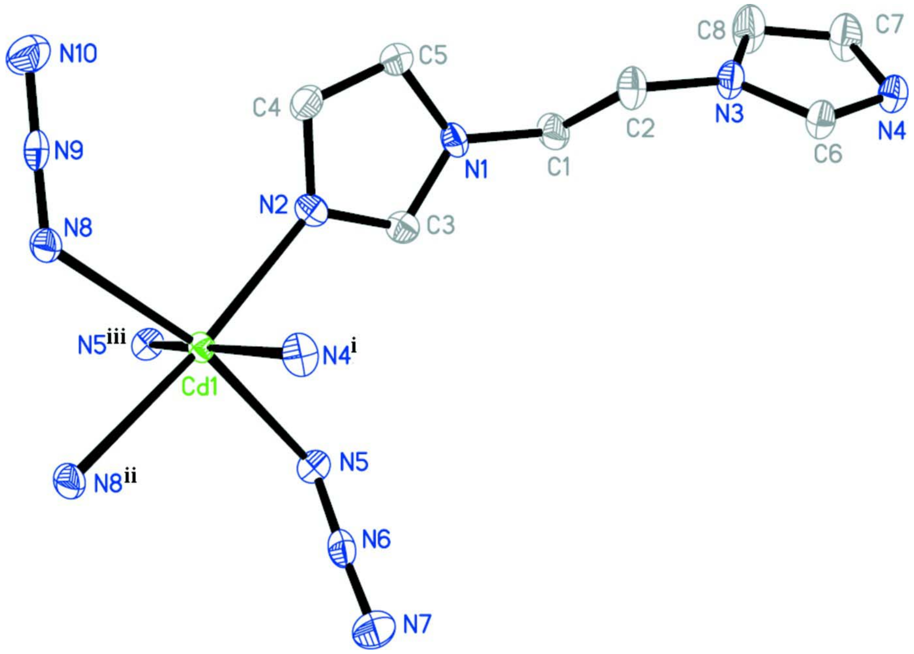

Figure 1

The coordination environment of Cd1 in (I) with displacement ellipsoids drawn at the 50% probability level [symmetry codes: (i) $x - 1, -y + 3/2, z + 1/2$; (ii) $-x, -y + 1, -z + 1$; (iii) $-x + 1, -y + 1, -z + 1$].

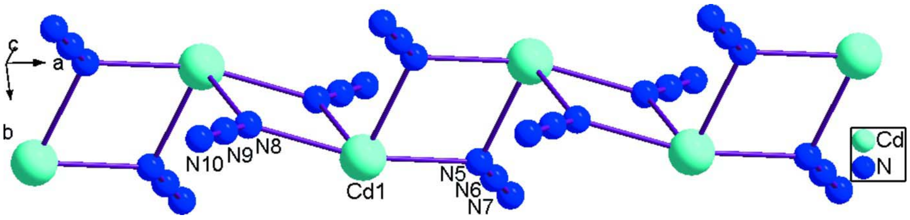

Figure 2

The one-dimensional inorganic chain with bridging EO-azide ligands running along the a axis.

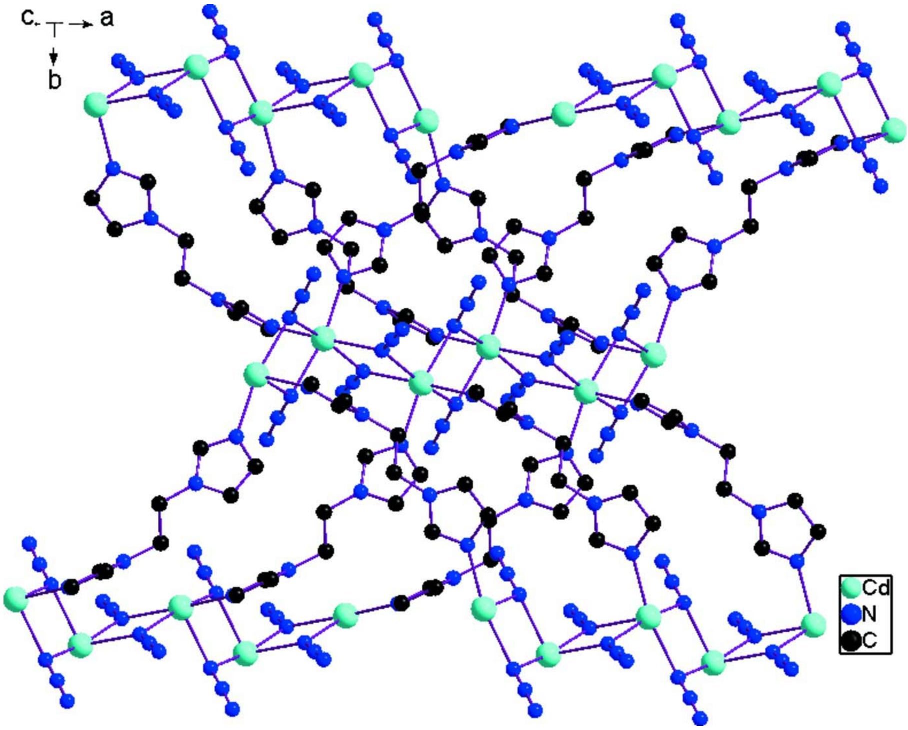

Figure 3

Inorganic $[Cd(N_3)_2]_n$ chains bridged by bime ligands.

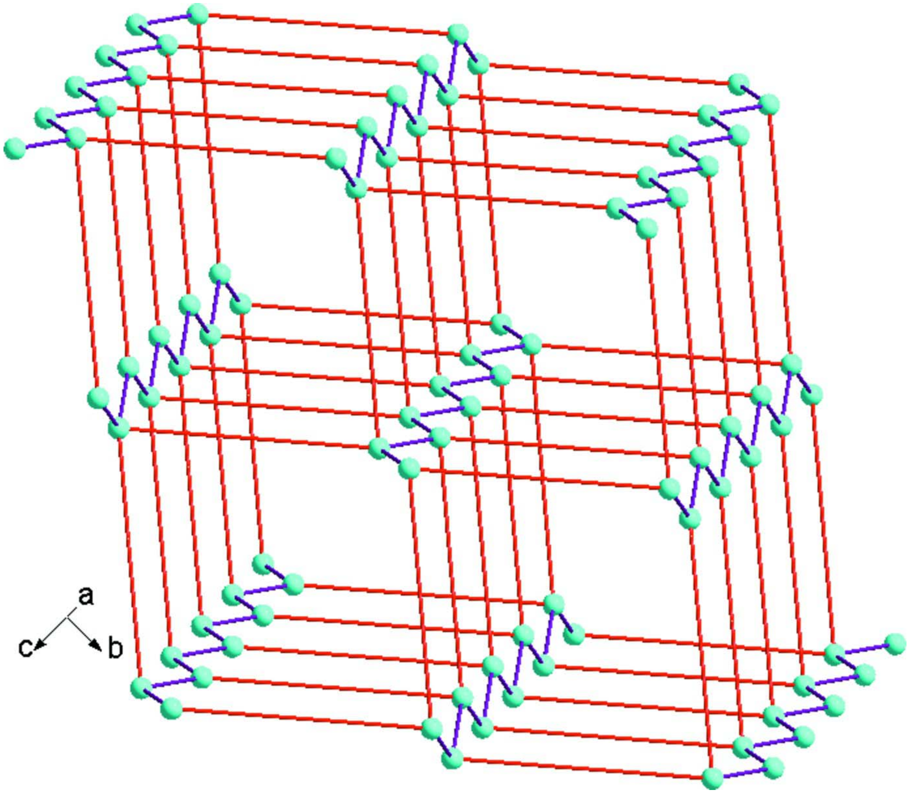

Figure 4

A three-dimensional topology of (I). The long sticks represent the bime ligands and the short ones the pair of EO-azide ligands.

Poly[bis(μ-azido-κ^2N^1:N^1)[μ-1,2-bis(imidazol-1- yl)ethane-κ^2N^3:$N^{3'}$]cadmium]

Crystal data

$[Cd(N_3)_2(C_8H_{10}N_4)]$
M_r = 358.66
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 6.4565 (14) Å
b = 18.874 (4) Å
c = 10.449 (2) Å
β = 90.485 (5)°
V = 1273.2 (5) Å^3
Z = 4
$F(000)$ = 704
D_x = 1.871 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71070 Å
Cell parameters from 4950 reflections
θ = 3.2–25.4°
μ = 1.72 mm^{-1}
T = 153 K
Block, colourless
0.36 × 0.17 × 0.15 mm

Data collection

Rigaku Mercury CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan
(REQAB; Jacobson, 1998)
T_{min} = 0.576, T_{max} = 0.783
12260 measured reflections
2324 independent reflections
2190 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.3°, θ_{min} = 3.2°
$h = -7 \rightarrow 7$
$k = -22 \rightarrow 21$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.056$
$S = 1.09$
2324 reflections
172 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0271P)^2 + 1.003P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.68$ e Å^{-3}
$\Delta\rho_{\min} = -0.39$ e Å^{-3}

Special details

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

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Cd1	0.25318 (3)	0.538064 (9)	0.443664 (17)	0.01313 (8)
N1	0.6247 (3)	0.60924 (12)	0.1163 (2)	0.0180 (5)
N2	0.4047 (3)	0.56039 (12)	0.2487 (2)	0.0173 (5)
N3	0.9231 (4)	0.75635 (12)	−0.0341 (2)	0.0214 (5)
N4	1.1350 (4)	0.84573 (12)	−0.0646 (2)	0.0203 (5)
N5	0.5555 (3)	0.57080 (12)	0.5537 (2)	0.0174 (5)
N6	0.5556 (4)	0.61004 (12)	0.6435 (2)	0.0210 (5)
N7	0.5618 (5)	0.64938 (15)	0.7285 (3)	0.0419 (8)
N8	−0.0515 (3)	0.48306 (13)	0.3709 (2)	0.0194 (5)
N9	−0.0800 (3)	0.46469 (11)	0.2657 (2)	0.0163 (5)
N10	−0.1107 (4)	0.44775 (15)	0.1588 (3)	0.0344 (7)
C1	0.8087 (4)	0.64601 (16)	0.0693 (3)	0.0228 (6)
H1A	0.8769	0.6170	0.0030	0.027*
H1B	0.9085	0.6534	0.1405	0.027*
C2	0.7448 (4)	0.71673 (15)	0.0134 (3)	0.0244 (6)
H2A	0.6452	0.7088	−0.0578	0.029*
H2B	0.6742	0.7450	0.0798	0.029*
C3	0.5867 (4)	0.59166 (14)	0.2384 (3)	0.0182 (6)
H3A	0.6786	0.6005	0.3081	0.022*
C4	0.3236 (4)	0.55828 (15)	0.1267 (3)	0.0212 (6)
H4A	0.1927	0.5388	0.1039	0.025*
C5	0.4581 (4)	0.58817 (15)	0.0439 (3)	0.0223 (6)
H5A	0.4405	0.5934	−0.0460	0.027*
C6	0.9741 (4)	0.82267 (14)	−0.0004 (3)	0.0202 (6)
H6A	0.9028	0.8497	0.0621	0.024*

C7	1.1899 (5)	0.79080 (16)	−0.1438 (3)	0.0322 (8)
H7A	1.3012	0.7917	−0.2027	0.039*
C8	1.0618 (5)	0.73543 (17)	−0.1252 (3)	0.0350 (8)
H8A	1.0667	0.6908	−0.1669	0.042*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01024 (12)	0.01476 (13)	0.01442 (12)	0.00040 (7)	0.00091 (8)	0.00122 (7)
N1	0.0179 (12)	0.0179 (12)	0.0184 (12)	−0.0024 (9)	0.0052 (10)	0.0028 (9)
N2	0.0180 (12)	0.0174 (11)	0.0164 (12)	0.0028 (10)	0.0023 (10)	0.0012 (10)
N3	0.0223 (13)	0.0169 (12)	0.0251 (13)	−0.0057 (10)	0.0059 (11)	−0.0022 (10)
N4	0.0184 (12)	0.0173 (12)	0.0252 (13)	−0.0019 (10)	0.0036 (10)	−0.0013 (10)
N5	0.0156 (12)	0.0167 (12)	0.0199 (12)	0.0020 (9)	−0.0006 (10)	−0.0020 (10)
N6	0.0192 (13)	0.0205 (13)	0.0233 (14)	−0.0054 (10)	0.0037 (10)	0.0033 (11)
N7	0.063 (2)	0.0351 (17)	0.0281 (16)	−0.0174 (15)	0.0124 (14)	−0.0144 (13)
N8	0.0136 (12)	0.0269 (13)	0.0178 (13)	−0.0039 (10)	0.0006 (10)	0.0029 (11)
N9	0.0108 (11)	0.0136 (12)	0.0246 (15)	−0.0019 (8)	0.0031 (10)	0.0020 (10)
N10	0.0336 (16)	0.0459 (17)	0.0238 (16)	−0.0125 (13)	0.0015 (12)	−0.0103 (13)
C1	0.0167 (14)	0.0288 (16)	0.0231 (15)	−0.0040 (12)	0.0042 (12)	0.0038 (12)
C2	0.0205 (15)	0.0215 (15)	0.0312 (16)	−0.0055 (12)	0.0040 (13)	0.0020 (13)
C3	0.0161 (14)	0.0204 (14)	0.0182 (14)	0.0016 (11)	−0.0005 (11)	0.0010 (11)
C4	0.0203 (15)	0.0209 (14)	0.0222 (15)	−0.0042 (12)	−0.0011 (12)	−0.0031 (12)
C5	0.0252 (16)	0.0241 (15)	0.0177 (14)	−0.0061 (12)	0.0001 (12)	−0.0012 (12)
C6	0.0199 (15)	0.0161 (14)	0.0247 (15)	−0.0019 (11)	0.0056 (12)	−0.0025 (11)
C7	0.0392 (19)	0.0233 (16)	0.0345 (18)	−0.0055 (14)	0.0204 (15)	−0.0058 (13)
C8	0.049 (2)	0.0218 (16)	0.0344 (18)	−0.0084 (15)	0.0219 (16)	−0.0103 (14)

Geometric parameters (Å, º)

Cd1—N2	2.306 (2)	N5—Cd1^{iii}	2.397 (2)
Cd1—N4^{i}	2.324 (2)	N6—N7	1.158 (3)
Cd1—N5	2.340 (2)	N8—N9	1.166 (3)
Cd1—N8	2.345 (2)	N8—Cd1^{ii}	2.377 (2)
Cd1—N8^{ii}	2.377 (2)	N9—N10	1.177 (4)
Cd1—N5^{iii}	2.397 (2)	C1—C2	1.513 (4)
N1—C3	1.343 (3)	C1—H1A	0.9900
N1—C5	1.369 (4)	C1—H1B	0.9900
N1—C1	1.464 (4)	C2—H2A	0.9900
N2—C3	1.320 (4)	C2—H2B	0.9900
N2—C4	1.375 (4)	C3—H3A	0.9500
N3—C6	1.341 (3)	C4—C5	1.355 (4)
N3—C8	1.370 (4)	C4—H4A	0.9500
N3—C2	1.463 (4)	C5—H5A	0.9500
N4—C6	1.316 (4)	C6—H6A	0.9500
N4—C7	1.375 (4)	C7—C8	1.348 (4)
N4—Cd1^{iv}	2.324 (2)	C7—H7A	0.9500
N5—N6	1.195 (3)	C8—H8A	0.9500

N2—Cd1—N4^{i}	86.36 (8)	Cd1—N8—Cd1^{ii}	105.89 (9)
N2—Cd1—N5	91.57 (8)	N8—N9—N10	178.4 (3)
N4^{i}—Cd1—N5	92.36 (8)	N1—C1—C2	109.1 (2)
N2—Cd1—N8	98.95 (8)	N1—C1—H1A	109.9
N4^{i}—Cd1—N8	97.56 (8)	C2—C1—H1A	109.9
N5—Cd1—N8	165.94 (8)	N1—C1—H1B	109.9
N2—Cd1—N8^{ii}	171.89 (8)	C2—C1—H1B	109.9
N4^{i}—Cd1—N8^{ii}	90.38 (8)	H1A—C1—H1B	108.3
N5—Cd1—N8^{ii}	95.98 (8)	N3—C2—C1	111.7 (2)
N8—Cd1—N8^{ii}	74.11 (9)	N3—C2—H2A	109.3
N2—Cd1—N5^{iii}	86.80 (8)	C1—C2—H2A	109.3
N4^{i}—Cd1—N5^{iii}	168.07 (8)	N3—C2—H2B	109.3
N5—Cd1—N5^{iii}	78.07 (8)	C1—C2—H2B	109.3
N8—Cd1—N5^{iii}	93.15 (8)	H2A—C2—H2B	107.9
N8^{ii}—Cd1—N5^{iii}	97.62 (8)	N2—C3—N1	111.0 (2)
C3—N1—C5	107.7 (2)	N2—C3—H3A	124.5
C3—N1—C1	126.2 (2)	N1—C3—H3A	124.5
C5—N1—C1	126.1 (2)	C5—C4—N2	109.8 (2)
C3—N2—C4	105.6 (2)	C5—C4—H4A	125.1
C3—N2—Cd1	122.58 (18)	N2—C4—H4A	125.1
C4—N2—Cd1	130.74 (18)	C4—C5—N1	105.8 (2)
C6—N3—C8	106.9 (2)	C4—C5—H5A	127.1
C6—N3—C2	125.5 (2)	N1—C5—H5A	127.1
C8—N3—C2	127.5 (2)	N4—C6—N3	111.6 (2)
C6—N4—C7	105.4 (2)	N4—C6—H6A	124.2
C6—N4—Cd1^{iv}	123.63 (18)	N3—C6—H6A	124.2
C7—N4—Cd1^{iv}	130.37 (19)	C8—C7—N4	109.6 (3)
N6—N5—Cd1	122.96 (18)	C8—C7—H7A	125.2
N6—N5—Cd1^{iii}	121.70 (18)	N4—C7—H7A	125.2
Cd1—N5—Cd1^{iii}	101.93 (8)	C7—C8—N3	106.4 (3)
N7—N6—N5	177.5 (3)	C7—C8—H8A	126.8
N9—N8—Cd1	124.23 (19)	N3—C8—H8A	126.8
N9—N8—Cd1^{ii}	129.46 (19)		

C3—N1—C1—C2	−116.5 (3)	C3—N1—C5—C4	0.1 (3)
C5—N1—C1—C2	61.8 (4)	C1—N1—C5—C4	−178.4 (3)
C6—N3—C2—C1	−125.8 (3)	C7—N4—C6—N3	−0.1 (3)
C8—N3—C2—C1	58.2 (4)	Cd1^{iv}—N4—C6—N3	172.20 (18)
N1—C1—C2—N3	179.4 (2)	C8—N3—C6—N4	0.5 (3)
C4—N2—C3—N1	−0.1 (3)	C2—N3—C6—N4	−176.2 (3)
Cd1—N2—C3—N1	−169.59 (17)	C6—N4—C7—C8	−0.5 (4)
C5—N1—C3—N2	0.0 (3)	Cd1^{iv}—N4—C7—C8	−172.0 (2)
C1—N1—C3—N2	178.6 (2)	N4—C7—C8—N3	0.8 (4)
C3—N2—C4—C5	0.2 (3)	C6—N3—C8—C7	−0.8 (4)

Cd1—N2—C4—C5	168.5 (2)	C2—N3—C8—C7	175.9 (3)
N2—C4—C5—N1	−0.2 (3)		

Symmetry codes: (i) $x-1, -y+3/2, z+1/2$; (ii) $-x, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $x+1, -y+3/2, z-1/2$.