

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

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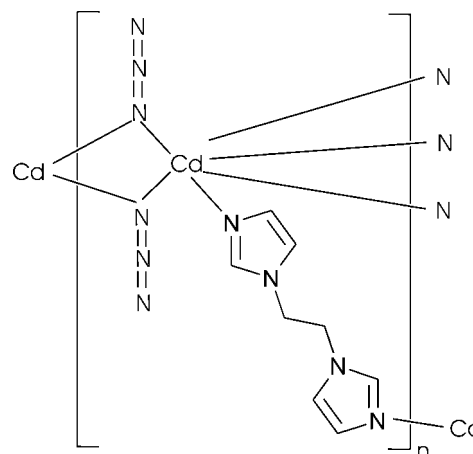
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Key indicators: single-crystal X-ray study; $T = 153$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.023; wR factor = 0.056; data-to-parameter ratio = 13.5.

In the title three-dimensional coordination polymer, $[\text{Cd}(\text{N}_3)_2(\text{C}_8\text{H}_{10}\text{N}_4)]_n$, 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 $[\text{Cd}(\text{N}_3)_2]_n$ 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); Leibelng *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

$[\text{Cd}(\text{N}_3)_2(\text{C}_8\text{H}_{10}\text{N}_4)]$
 $M_r = 358.66$

Monoclinic, $P2_1/c$
 $a = 6.4565$ (14) Å
 $b = 18.874$ (4) Å
 $c = 10.449$ (2) Å
 $\beta = 90.485$ (5)°

$V = 1273.2$ (5) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 1.72$ mm⁻¹
 $T = 153$ K
 $0.36 \times 0.17 \times 0.15$ mm

Data collection

Rigaku Mercury CCD
diffractometer
Absorption correction: multi-scan
(*REQAB*; Jacobson, 1998)
 $T_{\text{min}} = 0.576$, $T_{\text{max}} = 0.783$

12260 measured reflections
2324 independent reflections
2190 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

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
 $\Delta\rho_{\text{max}} = 0.68$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.39$ 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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supplementary materials

Acta Cryst. (2012). E68, m253–m254 [doi:10.1107/S1600536812004370]

Poly[bis(μ -azido- κ^2 N¹:N¹)[μ -1,2-bis(imidazol-1-yl)ethane- κ^2 N³:N^{3'}]cadmium]**Hai-Yan Li, Peng-Peng Sun and Bao-Long Li****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 (N₃⁻) 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; Leibelng *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)(N₃)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)(H₂O)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)(N₃)₂]_n with only EO-azide (Mautner *et al.*, 1997) and 2.404 (3) to 2.474 (3) Å in [Cd(N₃)(4-aba)(H₂O)]_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 [Cd₂(N₃)₂] four-membered metallacycle. The neighboring metallacycles have a common Cd^{II} atom and form a one-dimensional inorganic zigzag chain [Cd(N₃)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(N₃)₂]_n chain point in four different directions (Fig. 3) binding to adjacent [Cd(N₃)₂]_n chain and generating a three-dimensional network (Fig. 4).

Experimental

An aqueous (20 mL) solution of $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ (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 $\text{C}_8\text{H}_{10}\text{CdN}_{10}$: C, 26.79; H, 2.81; N, 39.06%. Found: C, 26.68; H, 2.72; N, 38.98%.

Refinement

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

Computing details

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear* (Rigaku, 2000); data reduction: *CrystalClear* (Rigaku, 2000); 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* (Sheldrick, 2008).

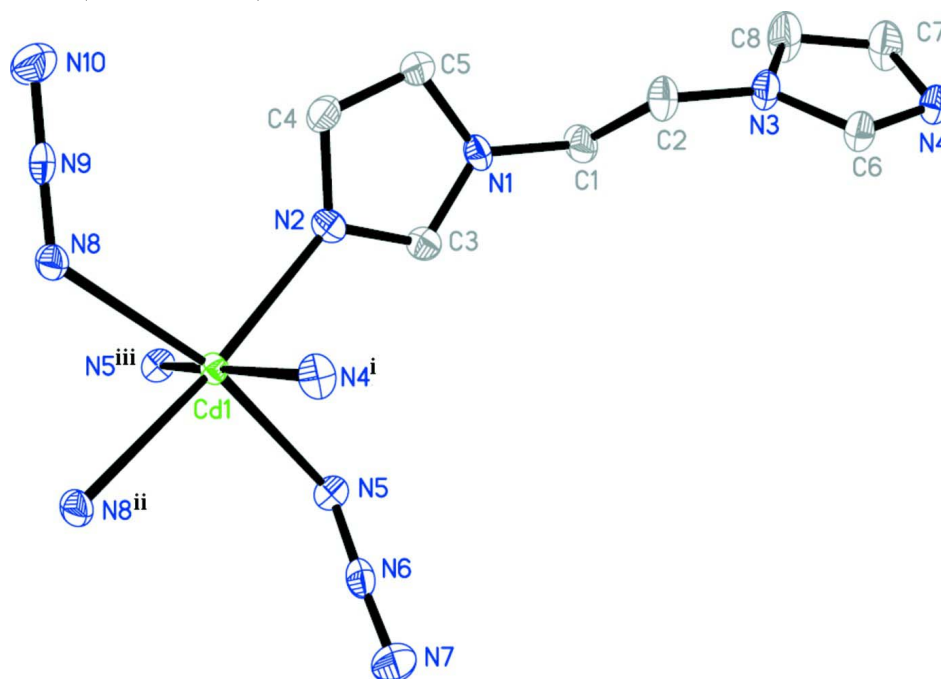


Figure 1

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) $-x + 1, -y + 1, -z + 1$].

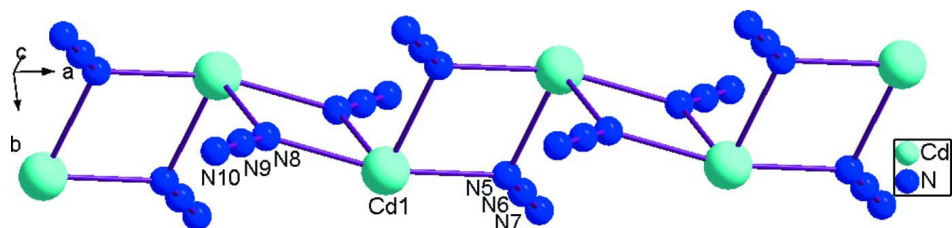


Figure 2

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

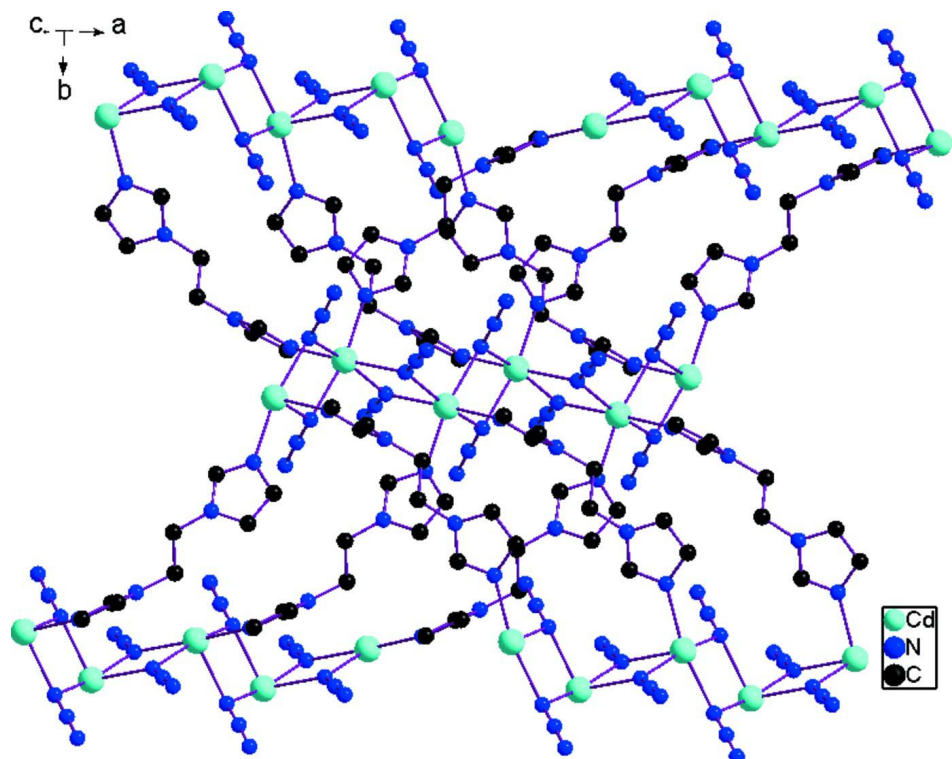
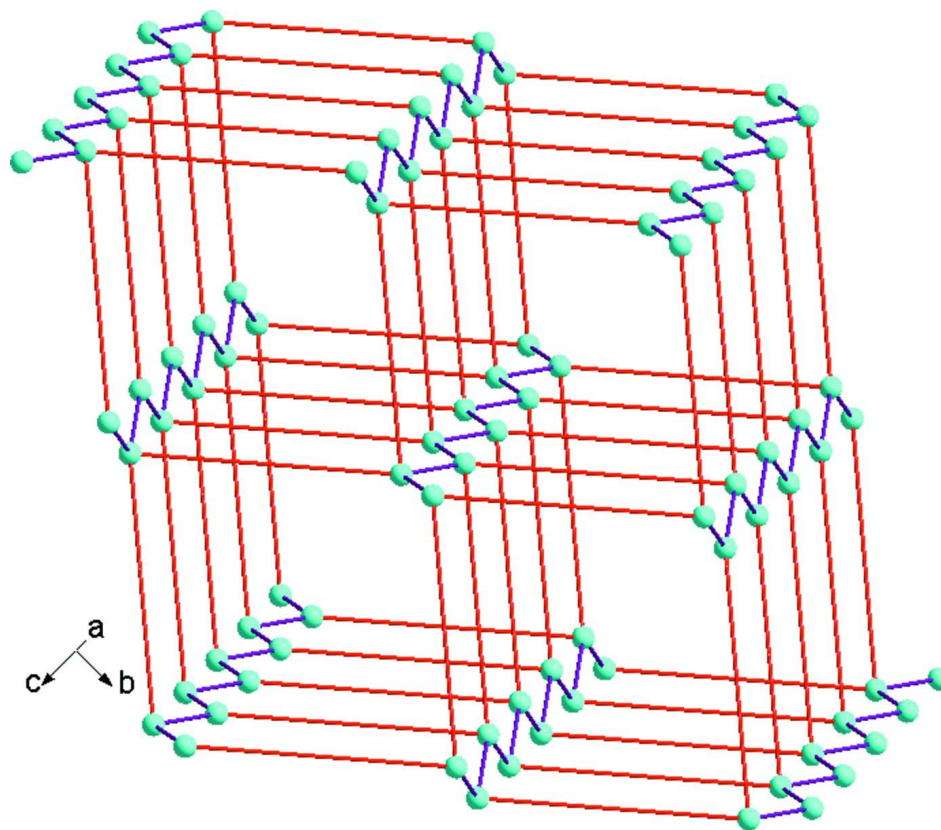


Figure 3

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- $\kappa^2N^1:N^1$)[μ -1,2-bis(imidazol-1-yl)ethane- $\kappa^2N^3:N^3$]cadmium]

Crystal data

[Cd(N₃)₂(C₈H₁₀N₄)]

$M_r = 358.66$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 6.4565$ (14) Å

$b = 18.874$ (4) Å

$c = 10.449$ (2) Å

$\beta = 90.485$ (5)°

$V = 1273.2$ (5) Å³

$Z = 4$

$F(000) = 704$

$D_x = 1.871$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å

Cell parameters from 4950 reflections

$\theta = 3.2$ – 25.4 °

$\mu = 1.72$ mm⁻¹

$T = 153$ K

Block, colourless

$0.36 \times 0.17 \times 0.15$ 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 $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 25.3$ °, $\theta_{\min} = 3.2$ °

$h = -7 \rightarrow 7$

$k = -22 \rightarrow 21$

$l = -12 \rightarrow 12$

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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.68 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.39 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|---------------|----------------------------------|
| 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 (\AA^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 (\AA , $^\circ$)

| | | | |
|------------------------|-----------|--------------------------|------------|
| 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) $x+1, -y+3/2, z-1/2$.