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catena-Poly[cadmium-μ-[1,3-bis(imidazol-1-yl)propane]-di-μ-chlorido]

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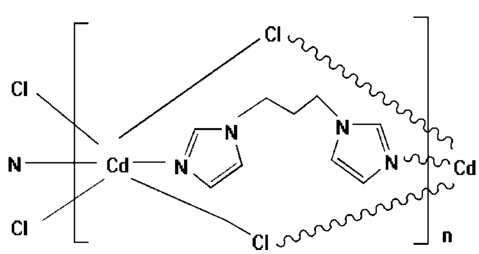
Key indicators: single-crystal X-ray study; *T* = 296 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.013; *wR* factor = 0.037; data-to-parameter ratio = 18.5.

The title complex, $[CdCl_2(C_9H_{12}N_4)]_n$, is characterized by the formation of a zigzag chain structure parallel to [001]. In the chain, the Cd^{2+} cation is coordinated by four bridging Cl^- ligands in equatorial positions and two N atoms from symmetry-related and likewise bridging 1,3-bis(imidazol-1-yl)propane ligands in axial positions, forming a distorted $CdCl_4N_2$ octahedron.

Related literature

For related structures, see: Carlucci *et al.* (1997); Wang *et al.* (2011); Yang *et al.* (2010).



Experimental

Crystal data

$[CdCl_2(C_9H_{12}N_4)]$
M_r = 359.54
Orthorhombic, $P2_12_12_1$
a = 15.1617 (16) Å
b = 9.9810 (11) Å
c = 7.8022 (8) Å
V = 1180.7 (2) Å^3
Z = 4
Mo *K*α radiation
μ = 2.28 mm^{-1}
T = 296 K
0.31 × 0.20 × 0.12 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.585, T_{max} = 0.761
18692 measured reflections
2707 independent reflections
2645 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.013
$wR(F^2)$ = 0.037
S = 1.00
2707 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Absolute structure: Flack (1983), 1109 Friedel pairs
Flack parameter: 0.294 (18)

Table 1
Selected bond lengths (Å).

Cd—N2	2.2836 (12)	Cd—Cl2	2.6800 (4)
Cd—N1^{i}	2.2911 (13)	Cd—Cl1^{ii}	2.7010 (4)
Cd—Cl1	2.6370 (4)	Cd—Cl2^{i}	2.7409 (5)

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2624).

References

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2006). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Carlucci, L., Ciani, G., Gudenberg, D. W. V. & Proserpio, D. M. (1997). *Inorg. Chem.* **36**, 3812–3813.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, X. J., Zhan, C. H., Feng, Y. L., Lan, Y. Z., Yin, J. L. & Cheng, J. W. (2011). *CrystEngComm*, **13**, 684–689.
Yang, G. P., Wang, Y. Y., Liu, P., Fu, A. Y., Zhang, Y. N., Jin, J. C. & Shi, Q. Z. (2010). *Cryst. Growth Des.* **10**, 1443–1450.

supporting information

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Qiao-Lian Shen and Hong Lin

S1. Comment

In the past few years, complexes based on the 1,3-bi-4-pyridylpropane (bpp) ligand, such as $[Ni_2(C_{10}H_8O_4S_2)_2(bpp)_2(H_2O)]_n$ (Wang *et al.*, 2011), $[Ag(C_8H_9O_4)(bpp)]_n$ (Yang *et al.*, 2010), $[Ag(bpp)]_nn(CF_3SO_3)$ (Carlucci *et al.*, 1997), have been reported. However, complexes with 1,3-bis(imidazol-1′-yl)propane (bip) as ligand are scarce. Herein, we report the synthesis and structure of a new complex, $[Cd(bip)Cl_2]_n$ (I).

A perspective view of the molecular entities of compound (I) is presented in Fig.1. The asymmetric unit consists of one Cd^{2+} ion, one 1,3-bis(imidazol-1′-yl)propane ligand, and two chlorine atoms. The Cd^{2+} ion is six-coordinate and has a slightly distorted octahedral coordination environment, defined by four chlorine atoms and two nitrogen atoms from two symmetry-related 1,3-bis(imidazol-1′-yl)propane ligands. As shown in Fig. 2, the adjacent Cd(II) ions are bridged by one 1,3-bis(imidazol-1′-yl)propane ligand and two chlorine atoms to generate a zigzag-chain structure running along [001].

It should be noted that there are no remarkable hydrogen bonding interactions in the crystal.

S2. Experimental

A mixture of 1,3-bis(imidazol-1′-yl)propane (0.088 g, 0.5 mmol), $CdCl_2·2.5H_2O$ (0.342 g, 1.5 mmol), and Na_2CO_3 (0.060 g, 0.5 mmol) in H_2O (16 ml)/C_2H_5OH (2 ml) was placed in a 25 ml Teflon-lined stainless steel vessel and heated at 433 K for 72 h, then cooled to room temperature over 3 days. Colourless crystals suitable for X-ray analysis were obtained.

S3. Refinement

The carbon-bound H-atoms were positioned geometrically and included in the refinement using a riding model [aromatic C—H 0.93 Å and aliphatic C—H 0.97 Å, $U_{iso}(H) = 1.2U_{eq}(C)$]. The used intensity data originates from an inversion-twinned crystal.

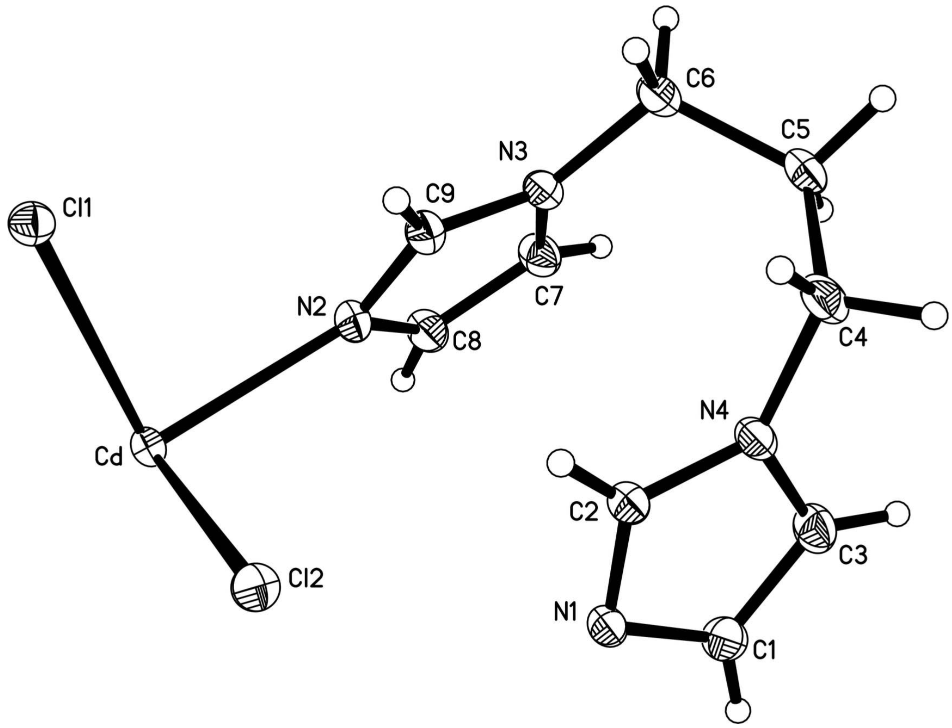

Figure 1

The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability elevl.

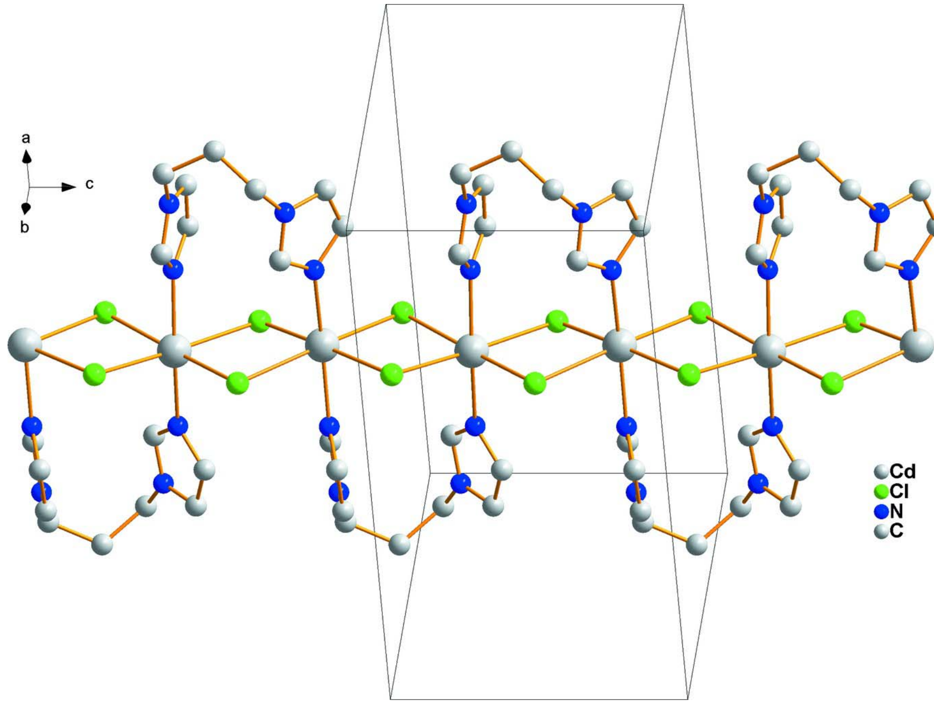

Figure 2

A view of the one-dimensional chain structure of (I).

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Crystal data

$[CdCl_2(C_9H_{12}N_4)]$
M_r = 359.54
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 15.1617 (16) Å
b = 9.9810 (11) Å
c = 7.8022 (8) Å
V = 1180.7 (2) Å^3
Z = 4
F(000) = 704
D_x = 2.023 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9933 reflections
θ = 2.4–27.5°
μ = 2.28 mm^{-1}
T = 296 K
Block, colourless
0.31 × 0.20 × 0.12 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.585, T_{max} = 0.761
18692 measured reflections
2707 independent reflections
2645 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.5°, θ_{min} = 2.4°
$h = -19 \rightarrow 19$
$k = -12 \rightarrow 12$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.013
$wR(F^2)$ = 0.037
S = 1.00
2707 reflections
146 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
$w = 1/[\sigma^2(F_o^2) + (0.024P)^2 + 0.1705P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Absolute structure: Flack (1983), 1109 Friedel pairs
Absolute structure parameter: 0.294 (18)

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_{iso}*/U_{eq}
Cd	0.743239 (6)	0.998451 (13)	0.383812 (14)	0.02486 (4)
Cl1	0.77859 (3)	1.17683 (4)	0.14414 (5)	0.02759 (8)
Cl2	0.76493 (3)	1.18680 (4)	0.62497 (5)	0.02915 (8)

N1	0.90723 (8)	0.98124 (13)	0.87595 (17)	0.0275 (3)
N2	0.88887 (8)	0.94055 (13)	0.39339 (19)	0.0275 (3)
N3	1.03373 (9)	0.95040 (13)	0.40284 (19)	0.0272 (3)
N4	1.04570 (8)	1.01445 (15)	0.80238 (17)	0.0283 (3)
C1	0.96006 (11)	0.89687 (17)	0.9691 (2)	0.0325 (4)
H1B	0.9401	0.8358	1.0504	0.039*
C2	0.96144 (10)	1.05139 (16)	0.7788 (2)	0.0278 (3)
H2A	0.9435	1.1182	0.7034	0.033*
C3	1.04561 (12)	0.91557 (17)	0.9251 (2)	0.0348 (4)
H3A	1.0944	0.8707	0.9691	0.042*
C4	1.12411 (11)	1.07572 (18)	0.7238 (2)	0.0360 (4)
H4A	1.1676	1.0905	0.8129	0.043*
H4B	1.1076	1.1627	0.6787	0.043*
C5	1.16718 (9)	0.99572 (18)	0.5806 (2)	0.0339 (3)
H5B	1.1687	0.9023	0.6148	0.041*
H5A	1.2278	1.0256	0.5692	0.041*
C6	1.12330 (9)	1.00460 (18)	0.4051 (2)	0.0325 (3)
H6A	1.1215	1.0977	0.3696	0.039*
H6B	1.1589	0.9561	0.3225	0.039*
C7	1.01061 (11)	0.81997 (16)	0.4383 (2)	0.0321 (3)
H7A	1.0485	0.7491	0.4622	0.039*
C8	0.92134 (11)	0.81612 (16)	0.4312 (2)	0.0317 (3)
H8A	0.8872	0.7401	0.4494	0.038*
C9	0.95856 (10)	1.01840 (16)	0.3763 (2)	0.0282 (3)
H9A	0.9560	1.1091	0.3492	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd	0.01757 (6)	0.03157 (7)	0.02543 (7)	0.00113 (4)	−0.00088 (3)	0.00122 (5)
Cl1	0.02733 (19)	0.02735 (16)	0.02807 (19)	−0.00186 (15)	0.00135 (14)	0.00086 (14)
Cl2	0.02980 (16)	0.02852 (17)	0.02914 (19)	−0.00164 (16)	0.00014 (17)	−0.00060 (15)
N1	0.0205 (6)	0.0341 (6)	0.0280 (7)	0.0008 (5)	0.0000 (5)	−0.0041 (7)
N2	0.0214 (6)	0.0324 (6)	0.0287 (7)	0.0032 (5)	−0.0016 (6)	0.0004 (6)
N3	0.0210 (6)	0.0315 (6)	0.0289 (7)	−0.0002 (5)	0.0016 (6)	0.0026 (6)
N4	0.0197 (6)	0.0333 (7)	0.0318 (7)	−0.0011 (6)	0.0018 (5)	−0.0040 (6)
C1	0.0314 (9)	0.0337 (8)	0.0323 (9)	0.0030 (7)	0.0015 (7)	0.0042 (7)
C2	0.0222 (7)	0.0335 (8)	0.0278 (8)	0.0012 (6)	0.0009 (6)	−0.0016 (6)
C3	0.0269 (8)	0.0385 (9)	0.0391 (10)	0.0065 (7)	−0.0032 (7)	0.0002 (8)
C4	0.0226 (8)	0.0414 (9)	0.0439 (10)	−0.0091 (7)	0.0029 (7)	−0.0063 (8)
C5	0.0174 (6)	0.0446 (9)	0.0396 (8)	−0.0008 (7)	0.0019 (6)	−0.0008 (9)
C6	0.0217 (7)	0.0387 (8)	0.0370 (8)	−0.0024 (7)	0.0029 (6)	0.0043 (9)
C7	0.0265 (8)	0.0308 (8)	0.0390 (9)	0.0062 (7)	0.0018 (7)	0.0044 (7)
C8	0.0262 (8)	0.0321 (7)	0.0369 (9)	−0.0003 (7)	0.0009 (6)	0.0025 (7)
C9	0.0235 (7)	0.0312 (7)	0.0301 (8)	0.0025 (6)	−0.0012 (6)	0.0023 (8)

Geometric parameters (Å, º)

Cd—N2	2.2836 (12)	N4—C4	1.471 (2)
Cd—N1^{i}	2.2911 (13)	C1—C3	1.355 (2)
Cd—Cl1	2.6370 (4)	C1—H1B	0.9300
Cd—Cl2	2.6800 (4)	C2—H2A	0.9300
Cd—Cl1^{ii}	2.7010 (4)	C3—H3A	0.9300
Cd—Cl2^{i}	2.7409 (5)	C4—C5	1.521 (2)
Cl1—Cd^{i}	2.7010 (4)	C4—H4A	0.9700
Cl2—Cd^{ii}	2.7409 (5)	C4—H4B	0.9700
N1—C2	1.319 (2)	C5—C6	1.525 (2)
N1—C1	1.371 (2)	C5—H5B	0.9700
N1—Cd^{ii}	2.2911 (13)	C5—H5A	0.9700
N2—C9	1.318 (2)	C6—H6A	0.9700
N2—C8	1.368 (2)	C6—H6B	0.9700
N3—C9	1.3425 (19)	C7—C8	1.355 (2)
N3—C7	1.376 (2)	C7—H7A	0.9300
N3—C6	1.4618 (19)	C8—H8A	0.9300
N4—C2	1.3423 (19)	C9—H9A	0.9300
N4—C3	1.375 (2)		
N2—Cd—N1^{i}	170.41 (4)	N1—C2—H2A	124.2
N2—Cd—Cl1	89.86 (4)	N4—C2—H2A	124.2
N1^{i}—Cd—Cl1	97.10 (3)	C1—C3—N4	106.03 (14)
N2—Cd—Cl2	92.06 (4)	C1—C3—H3A	127.0
N1^{i}—Cd—Cl2	94.53 (3)	N4—C3—H3A	127.0
Cl1—Cd—Cl2	89.962 (15)	N4—C4—C5	115.79 (14)
N2—Cd—Cl1^{ii}	85.98 (4)	N4—C4—H4A	108.3
N1^{i}—Cd—Cl1^{ii}	87.45 (3)	C5—C4—H4A	108.3
Cl1—Cd—Cl1^{ii}	174.530 (8)	N4—C4—H4B	108.3
Cl2—Cd—Cl1^{ii}	86.642 (15)	C5—C4—H4B	108.3
N2—Cd—Cl2^{i}	84.09 (4)	H4A—C4—H4B	107.4
N1^{i}—Cd—Cl2^{i}	89.71 (3)	C4—C5—C6	116.23 (14)
Cl1—Cd—Cl2^{i}	86.682 (15)	C4—C5—H5B	108.2
Cl2—Cd—Cl2^{i}	174.893 (8)	C6—C5—H5B	108.2
Cl1^{ii}—Cd—Cl2^{i}	96.408 (14)	C4—C5—H5A	108.2
Cd—Cl1—Cd^{i}	94.075 (14)	C6—C5—H5A	108.2
Cd—Cl2—Cd^{ii}	92.210 (15)	H5B—C5—H5A	107.4
C2—N1—C1	105.45 (14)	N3—C6—C5	113.23 (13)
C2—N1—Cd^{ii}	126.08 (10)	N3—C6—H6A	108.9
C1—N1—Cd^{ii}	128.47 (11)	C5—C6—H6A	108.9
C9—N2—C8	105.57 (13)	N3—C6—H6B	108.9
C9—N2—Cd	128.50 (11)	C5—C6—H6B	108.9
C8—N2—Cd	125.78 (10)	H6A—C6—H6B	107.7
C9—N3—C7	107.04 (13)	C8—C7—N3	105.85 (14)
C9—N3—C6	127.11 (13)	C8—C7—H7A	127.1
C7—N3—C6	125.75 (14)	N3—C7—H7A	127.1
C2—N4—C3	106.95 (13)	C7—C8—N2	110.02 (15)

C2—N4—C4	126.73 (15)	C7—C8—H8A	125.0
C3—N4—C4	126.12 (14)	N2—C8—H8A	125.0
C3—C1—N1	109.92 (15)	N2—C9—N3	111.52 (14)
C3—C1—H1B	125.0	N2—C9—H9A	124.2
N1—C1—H1B	125.0	N3—C9—H9A	124.2
N1—C2—N4	111.63 (15)		

N2—Cd—Cl1—Cd^{i}	88.81 (4)	C3—N4—C2—N1	−1.12 (19)
N1^{i}—Cd—Cl1—Cd^{i}	−84.57 (3)	C4—N4—C2—N1	−176.17 (14)
Cl2—Cd—Cl1—Cd^{i}	−179.129 (15)	N1—C1—C3—N4	0.3 (2)
Cl2^{i}—Cd—Cl1—Cd^{i}	4.723 (13)	C2—N4—C3—C1	0.47 (18)
N2—Cd—Cl2—Cd^{ii}	−81.21 (4)	C4—N4—C3—C1	175.56 (16)
N1^{i}—Cd—Cl2—Cd^{ii}	91.81 (3)	C2—N4—C4—C5	−105.45 (19)
Cl1—Cd—Cl2—Cd^{ii}	−171.071 (13)	C3—N4—C4—C5	80.4 (2)
Cl1^{ii}—Cd—Cl2—Cd^{ii}	4.639 (13)	N4—C4—C5—C6	79.6 (2)
Cl1—Cd—N2—C9	36.26 (14)	C9—N3—C6—C5	114.19 (19)
Cl2—Cd—N2—C9	−53.70 (14)	C7—N3—C6—C5	−61.6 (2)
Cl1^{ii}—Cd—N2—C9	−140.18 (14)	C4—C5—C6—N3	−63.3 (2)
Cl2^{i}—Cd—N2—C9	122.94 (14)	C9—N3—C7—C8	−0.01 (19)
Cl1—Cd—N2—C8	−148.84 (13)	C6—N3—C7—C8	176.46 (15)
Cl2—Cd—N2—C8	121.21 (13)	N3—C7—C8—N2	−0.34 (19)
Cl1^{ii}—Cd—N2—C8	34.72 (13)	C9—N2—C8—C7	0.57 (19)
Cl2^{i}—Cd—N2—C8	−62.16 (13)	Cd—N2—C8—C7	−175.29 (11)
C2—N1—C1—C3	−0.95 (19)	C8—N2—C9—N3	−0.58 (19)
Cd^{ii}—N1—C1—C3	179.52 (12)	Cd—N2—C9—N3	175.12 (11)
C1—N1—C2—N4	1.27 (18)	C7—N3—C9—N2	0.4 (2)
Cd^{ii}—N1—C2—N4	−179.18 (10)	C6—N3—C9—N2	−176.03 (14)

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