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Crystal structure and fluorescence properties of *catena*-poly[[(2,2′-bi-1*H*-imidazole-κ^2N,N')-cadmium]-di-μ-chlorido]

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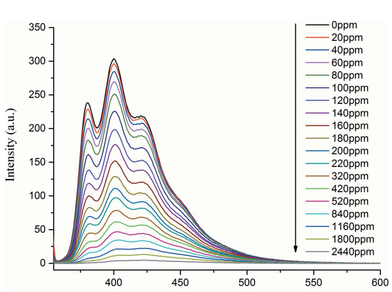
In the polymeric title compound, $[CdCl_2(C_6H_6N_4)]_n$, the central Cd^{II} atom is coordinated by four chloride ligands and two N atoms from a chelating 2,2′-bi-1*H*-imidazole molecule, leading to a distorted octahedral Cl_4N_2 coordination set. As a result of the μ_2-bridging character of the Cl ligands, chains parallel to the *c* axis are formed, with the chelating 2,2′-bi-1*H*-imidazole ligands decorated on both sides of the chain. The luminescence properties of the complex dispersed in dimethylformamide shows that the emission intensities are significantly quenched by nitrobenzene.



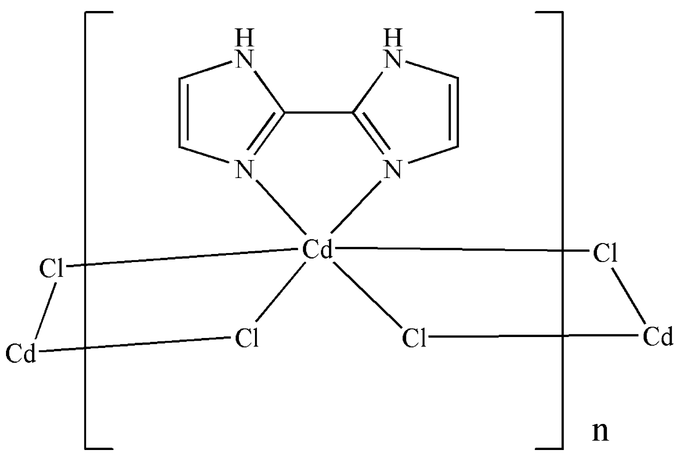
1. Chemical context

In recent years, great efforts have been devoted to the design and assembly of coordination polymers, not only because of the aesthetic beauty of their structures but also their potential applications in the fields of gas storage, separation, magnetism or their optical properties (Thangavelu *et al.*, 2015; Zhao *et al.*, 2014; Erer *et al.*, 2015; Eddaoudi *et al.*, 2015; O'Keeffe, 2009). The structural chemistry of transition metal halides with neutral N-donor co-ligands has been investigated thoroughly, leading to a multitude of complexes with new topologies and functionalities. Such N-donor ligands include, for example, tethering ligands such as bis(4-pyridylmethyl)piperazine (Low & LaDuca, 2015), 4,4′-dipyridylamine (Brown *et al.*, 2008) or 4,4′-bipyridine (Lyons *et al.*, 2008). We are also interested in conjugated terminal *N*-heterocyclic molecules as ligands, which can endow the resulting structures with photoluminescent properties. 2,2′-Bi-1*H*-imidazole is used as such an important terminal N-donor co-ligand, which can not only direct the structural properties with hydrogen-bonding networks, but also can be used as a suitable fragment for π–π interactions through the imidazole rings.

We have explored the self-assembly of $CdCl_2$ and 2,2′-bi-1*H*-imidazole in the presence of 2,2-dimethylsuccinic acid and obtained a new polymeric cadmium complex, $[Cd(2,2'\text{-bi-}1H\text{-imidazole})Cl_2]_n$. Its crystal structure and luminescence sensing of solvent molecules are reported in this communication.

2. Structural commentary

The asymmetric unit of the title compound is shown in Fig. 1. The central Cd^{II} atom is coordinated by four chloride ligands and two nitrogen atoms from a chelating 2,2′-bi-1*H*-imidazole ligand, forming a distorted Cl_4N_2 octahedral coordination set (Fig. 2). The Cd—Cl and Cd—N bond lengths range from 2.5271 (11)–2.8150 (14) and 2.323 (3)–2.342 (4) Å, respectively. The five-membered Cd1/N1/C1/C2/N2 chelate ring is characterized by a bite angle of 72.6 (1)°. The two imidazole rings of the 2,2′-bi-1*H*-imidazole ligand are nearly parallel to each other, making a dihedral angle of 0.8 (5)°. The μ_2-bridging character of the four Cl ligands leads to the formation of a chain expanding parallel to the *c* axis (Fig. 2).



3. Supramolecular features

In the presence of the chelating 2,2′-bi-1*H*-imidazole ligands that decorate the chains on both sides, the chains are directed by weak π–π interactions into zipper-like double-stranded chains with centroid-to-centroid distances of 3.6538 (15) and 3.9452 (14) Å, respectively. In addition, there are intermolecular hydrogen bonds between the imidazole N atoms and coordinating Cl atoms of neighboring chains (Table 1). The π–π stacking interactions together with N—H···Cl hydrogen-bonding interactions expand the $[CdCl_{4/2}]_n$ chains to supramolecular sheets parallel to the *bc* plane (Fig. 2).

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H7···Cl2^{i}	0.86	2.32	3.174 (4)	172
N4—H8···Cl1^{i}	0.86	2.63	3.237 (4)	129

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

4. Luminescence properties

Coordination polymers based on d^{10} metal ions and conjugated organic ligands are promising candidates for potential photoactive materials with applications in chemical sensoring or in photochemistry. In particular, solvent-dependent quenching behaviour is of interest for the development of luminescent probes for chemical species (Liu *et al.*, 2015). Hence the luminescence properties of the title compound in different solvent emulsions were investigated. The luminescent intensities had no distinct differences if dichloromethane, acetonitrile, ethanol, ethyl acetate or benzene were selected as dispersing agents. However, the intensity had an abrupt decrease when the powdered samples of the title compound were dispersed in nitrobenzene. When the nitrobenzene solvent was gradually and increasingly added to the standard emulsions, the fluorescence intensities of the standard emulsions gradually decreased with increasing addition of nitrobenzene (Fig. 3). The fluorescence decrease was nearly proportional to the nitrobenzene concentration and intensity ultimately was found to be negligible. The efficient quenching of nitrobenzene in this system can be ascribed to the physical interaction of the solute and solvent, which induces the elec-

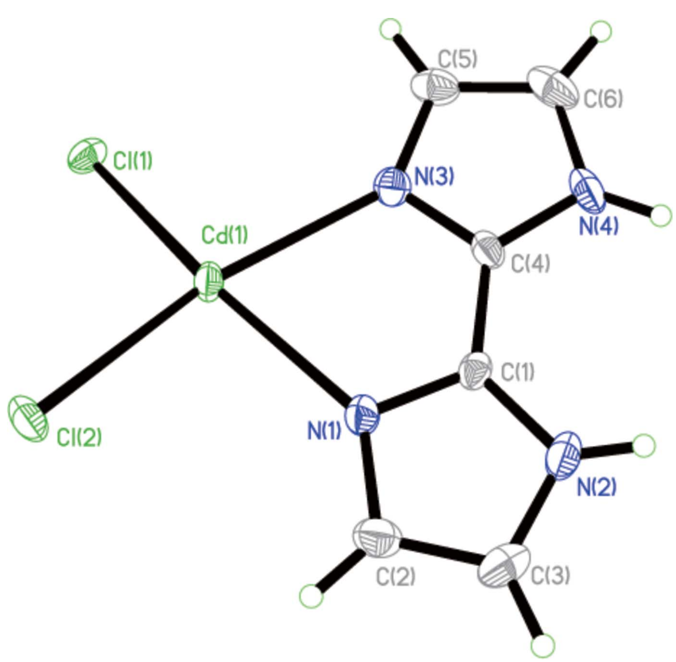


Figure 1
The asymmetric unit of the title compound, with anisotropic displacement parameters drawn at the 30% probability level.

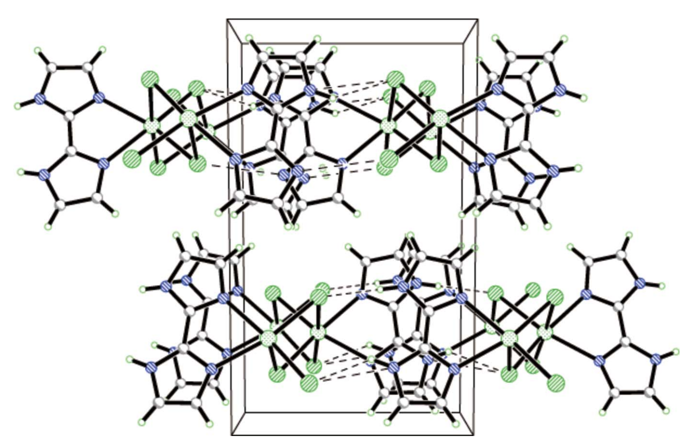


Figure 2
The supramolecular structure showing the interactions between neighbouring chains. N—H···Cl hydrogen bonds are shown as dashed lines.

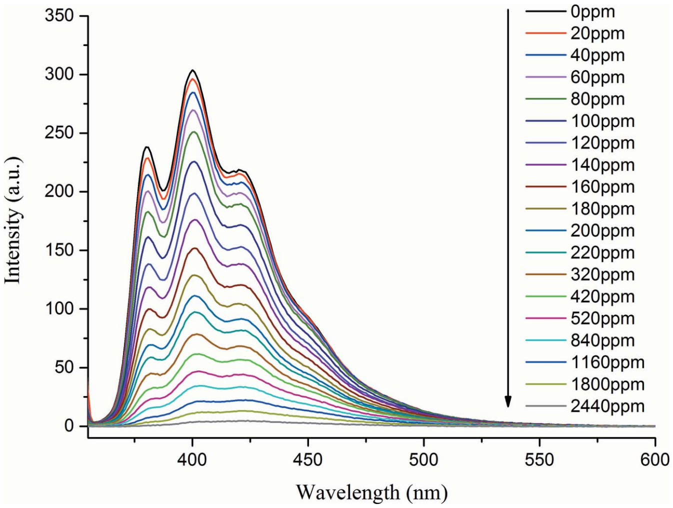


Figure 3
Fluorescence intensity of the title complex at different nitrobenzene concentrations in DMF.

tron transfer from the excited title compound to the electron-deficient nitrobenzene (Hao *et al.*, 2013). These results have given us the impetus to carry out more detailed investigations on the sensing behaviour of the title compound.

5. Database survey

A search of the Cambridge Structure Database (Version 5.35; last update May 2015; Groom *et al.*, 2016) for related Cd-based complexes with 2,2′-bi-1*H*-imidazole gave 41 hits. In most cases, 2,2′-bi-1*H*-imidazole serves as an ancillary ligand to be incorporated in carboxylate coordination polymer systems. $[Cd(2,2'\text{-bi-}1H\text{-imidazole})Br_2]_n$ has a very similar composition to the title compound and also shows an arrangement of polymeric chains constructed from the bridging behaviour of the Br ligand (Hester *et al.*, 1996); however, the space group is different ($C2/c$).

6. Synthesis and crystallization

A mixture of $CdCl_2 \cdot 2.5H_2O$ (0.5 mmol, 0.114 g), 2,2-dimethylsuccinic acid (0.5 mmol, 0.073 g), 2,2′-bi-1*H*-imidazole (0.5 mmol, 0.067 g) in water (8 ml) was stirred vigorously for 1 h at 333 K. Slow evaporation of the clear solution resulted in the separation of block-like colorless crystals as a pure phase. The crystals were washed with ethanol, and dried at room temperature. Calculated: C, 22.70; H, 1.90; N, 17.65; found: C, 22.51; H, 2.58; N, 17.49%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were positioned geometrically and constrained using a riding-model approximation, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms attached to the N atoms were found from difference maps but constrained with N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(N)$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[CdCl_2(C_6H_6N_4)]$
M_r	317.45
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	14.977 (5), 8.777 (3), 7.160 (3)
β (°)	97.900 (5)
V (Å^3)	932.3 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.87
Crystal size (mm)	0.26 × 0.21 × 0.17
Data collection	
Diffractometer	Bruker APEXII CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.523, 0.641
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5643, 2229, 1997
R_{int}	0.042
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.113, 1.10
No. of reflections	2229
No. of parameters	119
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.50, −1.62

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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Crystal structure and fluorescence properties of *catena*-poly[[(2,2′-bi-1*H*-imidazole-κ^2N,N')cadmium]-di-μ-chlorido]

Yang Liu and Hai-Hui Liu

Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); 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).

catena-Poly[[(2,2′-bi-1*H*-imidazole-κ^2N,N')cadmium]-di-μ-chlorido]

Crystal data

$[CdCl_2(C_6H_6N_4)]$
M_r = 317.45
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 14.977 (5) Å
b = 8.777 (3) Å
c = 7.160 (3) Å
β = 97.900 (5)°
V = 932.3 (6) Å^3
Z = 4
$F(000)$ = 608
D_x = 2.262 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3238 reflections
θ = 2.7–28.3°
μ = 2.87 mm^{-1}
T = 296 K
Block, colorless
0.26 × 0.21 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.523, T_{max} = 0.641
5643 measured reflections
2229 independent reflections
1997 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 28.3°, θ_{min} = 2.7°
h = −12→19
k = −11→11
l = −9→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.113
S = 1.10
2229 reflections
119 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
$w = 1/[\sigma^2(F_o^2) + (0.0676P)^2 + 0.4551P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.50$ e Å^{-3}
$\Delta\rho_{min} = -1.62$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.044 (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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.23613 (2)	−0.15121 (3)	0.09150 (4)	0.02900 (17)
Cl1	0.13506 (7)	−0.32441 (12)	−0.12634 (15)	0.0334 (2)
Cl2	0.33418 (8)	−0.35735 (11)	0.28324 (18)	0.0385 (3)
N1	0.3334 (2)	0.0418 (4)	0.2122 (5)	0.0313 (7)
N2	0.3617 (3)	0.2854 (4)	0.2529 (6)	0.0381 (8)
H7	0.3545	0.3826	0.2492	0.046*
N3	0.1636 (2)	0.0810 (4)	0.0127 (5)	0.0317 (7)
N4	0.1669 (3)	0.3302 (4)	0.0271 (6)	0.0403 (9)
H8	0.1863	0.4213	0.0515	0.048*
C1	0.3014 (3)	0.1809 (4)	0.1799 (6)	0.0271 (8)
C2	0.4183 (3)	0.0601 (6)	0.3068 (7)	0.0415 (10)
H2	0.4577	−0.0189	0.3468	0.050*
C3	0.4364 (3)	0.2096 (6)	0.3338 (7)	0.0455 (11)
H3	0.4893	0.2522	0.3952	0.055*
C4	0.2120 (3)	0.2008 (5)	0.0758 (6)	0.0297 (8)
C5	0.0842 (3)	0.1383 (6)	−0.0763 (7)	0.0410 (11)
H5	0.0365	0.0801	−0.1346	0.049*
C6	0.0854 (3)	0.2916 (7)	−0.0671 (7)	0.0489 (13)
H6	0.0395	0.3577	−0.1157	0.059*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0339 (2)	0.0185 (2)	0.0330 (2)	−0.00127 (9)	−0.00124 (13)	−0.00016 (9)
Cl1	0.0291 (5)	0.0343 (5)	0.0368 (5)	−0.0095 (4)	0.0048 (4)	−0.0071 (4)
Cl2	0.0386 (6)	0.0319 (5)	0.0468 (6)	0.0149 (4)	0.0129 (5)	0.0112 (4)
N1	0.0334 (17)	0.0234 (15)	0.0358 (18)	−0.0003 (13)	0.0009 (13)	−0.0044 (13)
N2	0.044 (2)	0.0264 (18)	0.047 (2)	−0.0092 (15)	0.0150 (16)	−0.0079 (16)
N3	0.0334 (17)	0.0297 (17)	0.0320 (17)	0.0002 (14)	0.0049 (13)	0.0043 (14)
N4	0.048 (2)	0.0257 (17)	0.052 (2)	0.0143 (15)	0.0236 (19)	0.0099 (16)
C1	0.0300 (18)	0.0227 (16)	0.031 (2)	−0.0048 (15)	0.0129 (15)	−0.0025 (15)
C2	0.031 (2)	0.047 (3)	0.044 (2)	0.0051 (19)	−0.0024 (17)	−0.008 (2)

C3	0.037 (2)	0.053 (3)	0.046 (3)	−0.015 (2)	0.0044 (18)	−0.010 (2)
C4	0.0311 (19)	0.0236 (19)	0.037 (2)	0.0067 (16)	0.0151 (15)	0.0047 (16)
C5	0.030 (2)	0.054 (3)	0.038 (2)	0.0056 (18)	0.0020 (17)	0.0118 (19)
C6	0.043 (3)	0.057 (3)	0.048 (3)	0.023 (2)	0.013 (2)	0.019 (2)

Geometric parameters (Å, º)

Cd1—N1	2.323 (3)	N3—C5	1.365 (5)
Cd1—N3	2.342 (4)	N4—C4	1.343 (5)
Cd1—Cl1	2.5271 (11)	N4—C6	1.354 (7)
Cd1—Cl2	2.6001 (12)	N4—H8	0.8600
Cd1—Cl1^{i}	2.6944 (13)	C1—C4	1.450 (6)
Cd1—Cl2^{ii}	2.8150 (14)	C2—C3	1.348 (8)
N1—C1	1.320 (5)	C2—H2	0.9300
N1—C2	1.365 (5)	C3—H3	0.9300
N2—C1	1.342 (5)	C5—C6	1.348 (7)
N2—C3	1.360 (7)	C5—H5	0.9300
N2—H7	0.8600	C6—H6	0.9300
N3—C4	1.321 (6)		
N1—Cd1—N3	72.61 (11)	C4—N3—Cd1	113.3 (3)
N1—Cd1—Cl1	163.82 (9)	C5—N3—Cd1	141.1 (3)
N3—Cd1—Cl1	98.98 (9)	C4—N4—C6	107.8 (4)
N1—Cd1—Cl2	91.80 (9)	C4—N4—H8	126.1
N3—Cd1—Cl2	160.47 (9)	C6—N4—H8	126.1
Cl1—Cd1—Cl2	98.87 (5)	N1—C1—N2	110.7 (4)
N1—Cd1—Cl1^{i}	99.64 (9)	N1—C1—C4	119.3 (3)
N3—Cd1—Cl1^{i}	87.70 (8)	N2—C1—C4	130.0 (4)
Cl1—Cd1—Cl1^{i}	93.69 (4)	C3—C2—N1	109.9 (4)
Cl2—Cd1—Cl1^{i}	83.31 (4)	C3—C2—H2	125.0
N1—Cd1—Cl2^{ii}	84.49 (9)	N1—C2—H2	125.0
N3—Cd1—Cl2^{ii}	93.59 (8)	C2—C3—N2	106.1 (4)
Cl1—Cd1—Cl2^{ii}	82.24 (4)	C2—C3—H3	127.0
Cl2—Cd1—Cl2^{ii}	96.60 (4)	N2—C3—H3	127.0
Cl1^{i}—Cd1—Cl2^{ii}	175.87 (3)	N3—C4—N4	110.5 (4)
Cd1—Cl1—Cd1^{ii}	99.20 (4)	N3—C4—C1	120.3 (3)
Cd1—Cl2—Cd1^{i}	94.46 (4)	N4—C4—C1	129.1 (4)
C1—N1—C2	105.6 (4)	C6—C5—N3	109.9 (5)
C1—N1—Cd1	114.5 (3)	C6—C5—H5	125.1
C2—N1—Cd1	139.8 (3)	N3—C5—H5	125.1
C1—N2—C3	107.6 (4)	C5—C6—N4	106.2 (4)
C1—N2—H7	126.2	C5—C6—H6	126.9
C3—N2—H7	126.2	N4—C6—H6	126.9
C4—N3—C5	105.6 (4)		
N1—Cd1—Cl1—Cd1^{ii}	41.8 (3)	Cl2—Cd1—N3—C5	−140.3 (4)
N3—Cd1—Cl1—Cd1^{ii}	99.06 (9)	Cl1^{i}—Cd1—N3—C5	−77.8 (4)
Cl2—Cd1—Cl1—Cd1^{ii}	−88.90 (4)	Cl2^{ii}—Cd1—N3—C5	98.2 (4)

Cl1^{i}—Cd1—Cl1—Cd1^{ii}	−172.70 (4)	C2—N1—C1—N2	−1.1 (5)
Cl2^{ii}—Cd1—Cl1—Cd1^{ii}	6.62 (3)	Cd1—N1—C1—N2	−179.6 (2)
N1—Cd1—Cl2—Cd1^{i}	93.14 (9)	C2—N1—C1—C4	178.4 (4)
N3—Cd1—Cl2—Cd1^{i}	56.8 (3)	Cd1—N1—C1—C4	−0.2 (4)
Cl1—Cd1—Cl2—Cd1^{i}	−99.06 (4)	C3—N2—C1—N1	0.8 (5)
Cl1^{i}—Cd1—Cl2—Cd1^{i}	−6.35 (3)	C3—N2—C1—C4	−178.6 (4)
Cl2^{ii}—Cd1—Cl2—Cd1^{i}	177.80 (3)	C1—N1—C2—C3	1.0 (5)
N3—Cd1—N1—C1	0.5 (3)	Cd1—N1—C2—C3	178.9 (3)
Cl1—Cd1—N1—C1	61.0 (5)	N1—C2—C3—N2	−0.5 (5)
Cl2—Cd1—N1—C1	−167.6 (3)	C1—N2—C3—C2	−0.1 (5)
Cl1^{i}—Cd1—N1—C1	−84.0 (3)	C5—N3—C4—N4	−1.1 (4)
Cl2^{ii}—Cd1—N1—C1	96.0 (3)	Cd1—N3—C4—N4	−179.7 (3)
N3—Cd1—N1—C2	−177.4 (5)	C5—N3—C4—C1	179.6 (4)
Cl1—Cd1—N1—C2	−116.8 (4)	Cd1—N3—C4—C1	0.9 (4)
Cl2—Cd1—N1—C2	14.6 (4)	C6—N4—C4—N3	1.5 (5)
Cl1^{i}—Cd1—N1—C2	98.1 (4)	C6—N4—C4—C1	−179.2 (4)
Cl2^{ii}—Cd1—N1—C2	−81.9 (4)	N1—C1—C4—N3	−0.5 (6)
N1—Cd1—N3—C4	−0.7 (2)	N2—C1—C4—N3	178.8 (4)
Cl1—Cd1—N3—C4	−166.5 (2)	N1—C1—C4—N4	−179.8 (4)
Cl2—Cd1—N3—C4	37.6 (4)	N2—C1—C4—N4	−0.5 (7)
Cl1^{i}—Cd1—N3—C4	100.1 (3)	C4—N3—C5—C6	0.3 (5)
Cl2^{ii}—Cd1—N3—C4	−83.8 (3)	Cd1—N3—C5—C6	178.3 (3)
N1—Cd1—N3—C5	−178.7 (5)	N3—C5—C6—N4	0.6 (6)
Cl1—Cd1—N3—C5	15.5 (5)	C4—N4—C6—C5	−1.2 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H7···Cl2^{iii}	0.86	2.32	3.174 (4)	172
N4—H8···Cl1^{iii}	0.86	2.63	3.237 (4)	129

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