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Di-μ-chlorido-bis{chlorido[2-(2-pyridyl)-1*H*-benzimidazole]cadmium(II)}

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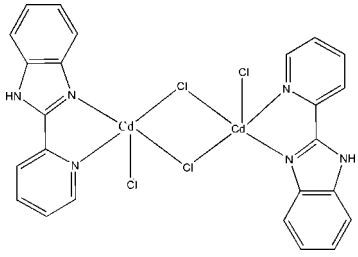
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.023; wR factor = 0.062; data-to-parameter ratio = 17.0.

The title compound, $[Cd_2Cl_4(C_{12}H_9N_3)_2]$, was prepared under hydrothermal conditions. In the centrosymmetric dimeric molecule, two Cd^{II} atoms are bridged by two Cl atoms. One terminal Cl atom and two N atoms from a bidentate chelating 2-(2-pyridyl)benzimidazole ligand complete a distorted square-pyramidal geometry around each Cd^{II} atom. A three-dimensional network is constructed *via* intermolecular N—H···Cl and weak C—H···Cl hydrogen bonds, as well as π–π interactions between adjacent ligands with a centroid-to-centroid distance of 3.49 (1) Å between the benzimidazolyl and pyridyl groups and a centroid-to-centroid distance of 3.54 (1) Å between the imidazolyl rings.

Related literature

For related literature, see: Alcade *et al.* (1992); Dave & Czernuszewicz (1994); Muller-Buschbaum & Quitmann (2003); Tangoulis *et al.* (1996).



Experimental

Crystal data

$[Cd_2Cl_4(C_{12}H_9N_3)_2]$
M_r = 757.04
Triclinic, $P\overline{1}$
a = 7.852 (2) Å
b = 8.971 (2) Å
c = 9.466 (3) Å
α = 103.224 (1)°
β = 101.050 (2)°
γ = 100.665 (4)°
V = 618.5 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.18 mm^{-1}
T = 293 (2) K
0.40 × 0.25 × 0.15 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
T_{min} = 0.525, T_{max} = 0.718
4683 measured reflections
2765 independent reflections
2646 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.062
S = 1.05
2765 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N2	2.2956 (17)	Cd1—Cl1	2.5852 (7)
Cd1—N1	2.3581 (17)	Cd1—Cl1^{i}	2.5782 (7)
Cd1—Cl2	2.4657 (8)		
N2—Cd1—N1	71.68 (6)	Cl2—Cd1—Cl1^{i}	115.34 (2)
N2—Cd1—Cl2	101.94 (5)	N2—Cd1—Cl1	95.34 (4)
N1—Cd1—Cl2	101.14 (5)	N1—Cd1—Cl1	151.59 (5)
N2—Cd1—Cl1^{i}	141.01 (5)	Cl2—Cd1—Cl1	106.34 (3)
N1—Cd1—Cl1^{i}	89.60 (5)	Cl1^{i}—Cd1—Cl1	85.21 (2)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···Cl2^{ii}	0.86	2.45	3.2708 (18)	160
C4—H4A···Cl2^{ii}	0.93	2.83	3.690 (2)	155

Symmetry code: (ii) $-x+2, -y+1, -z+2$.

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2099).

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supplementary materials

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Di-μ-chlorido-bis{chlorido[2-(2-pyridyl)-1*H*-benzimidazole]cadmium(II)}

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Comment

The 2-(2-pyridyl)benzimidazole ligand is often used to act as bidentate chelating ligand in metal complexes and those complexes can be mononuclear (Muller-Buschbaum & Quitmann, 2003), dinuclear (Dave & Czernuszewicz, 1994) or trinuclear (Tangoulis *et al.*, 1996). The noncoordinating N—H group of the ligand acts as hydrogen bond donor for the formation of robust heteromeric hydrogen bonds, contributing to the crystal packing. Herein we report the synthesis and structure of the title compound with the 2-(2-pyridyl)benzimidazole ligand.

The title compound is a centrosymmetric dimeric complex. The Cd^{II} atom is five-coordinated in an N_2Cl_3 environment with a distorted square-pyramidal geometry (Fig. 1). Two Cd^{II} atoms are bridged by two Cl atoms, forming a coplanar Cd_2Cl_2 unit. The coordination geometry is completed by one terminal Cl atom and two N atoms from the chelating 2-(2-pyridyl)benzimidazole ligand (Table 1). Intermolecular N—H···Cl and C—H···Cl hydrogen bonds, as well as π–π interactions between the pyridyl and benzimidazole groups of two adjacent dinuclear units, with a centroid-to-centroid distance of 3.49 (1) Å, lead to a one-dimensional chain (Fig. 2). The individual chains are associated with each other through π–π interactions between the imidazole rings of the neighboring chains, with a centroid-to-centroid distance of 3.54 (1) Å, forming a two-dimensional layer structure. The layers are further connected into a three-dimensional network through weak C—H···Cl interactions [$H2A\cdots Cl2^{i}$ = 2.92 Å, $C2\cdots Cl2^{i}$ = 3.600 (2) Å, $C2—H2A\cdots Cl2^{i}$ = 131°; symmetry code: (i) $x, y-1, z$](Fig. 3).

Experimental

A solution of $CdCl_2·2.5H_2O$ (0.14 g, 0.61 mmol), 2-(2-pyridyl)benzimidazole (0.08 g, 0.41 mmol) (Alcade *et al.*, 1992) and H_2O (15 ml) was stirred under ambient condition, then sealed in a 25 ml Teflon-lined stainless steel vessel, heated at 383 K for 3 d and cooled to room temperature. The resulting product was collected by filtration, washed with distilled water and dried in air (yield 80%).

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 and N—H = 0.86Å and $U_{iso}(H) = 1.2U_{eq}(C, N)$.

Figures

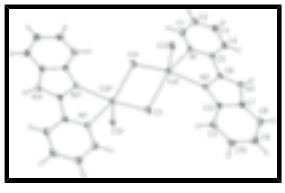

Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

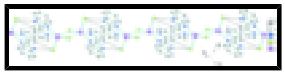

Fig. 2. A view of the one-dimensional chain in the title compound. H atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

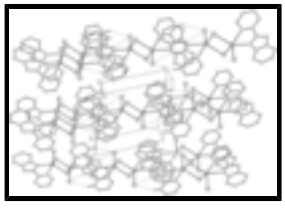

Fig. 3. The crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

Di-μ-chlorido-bis[chlorido[2-(2-pyridyl)-1*H*-benzimidazole]cadmium(II)]

Crystal data

$[Cd_2Cl_4(C_{12}H_9N_3)_2]$	$Z = 1$
$M_r = 757.04$	$F_{000} = 368$
Triclinic, $P\bar{1}$	$D_x = 2.032$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.852$ (2) Å	Cell parameters from 1784 reflections
$b = 8.971$ (2) Å	$\theta = 3.2$–27.5º
$c = 9.466$ (3) Å	$\mu = 2.18$ mm^{-1}
$\alpha = 103.224$ (1)º	$T = 293$ (2) K
$\beta = 101.050$ (2)º	Prism, colorless
$\gamma = 100.665$ (4)º	0.40 × 0.25 × 0.15 mm
$V = 618.5$ (3) Å^3	

Data collection

Rigaku Mercury CCD diffractometer	2765 independent reflections
Radiation source: fine-focus sealed tube	2646 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.015$
$T = 293$(2) K	$\theta_{max} = 27.5$º
ω scan	$\theta_{min} = 3.2$º
Absorption correction: multi-scan (CrystalClear; Rigaku, 2002)	$h = -10 \rightarrow 7$
$T_{min} = 0.525$, $T_{max} = 0.718$	$k = -11 \rightarrow 11$
4683 measured reflections	$l = -12 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.023$	H-atom parameters constrained
$wR(F^2) = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2 + 0.1317P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.05	$(\Delta/\sigma)_{max}$ = 0.002
2765 reflections	$\Delta\rho_{max}$ = 0.48 e Å^{-3}
163 parameters	$\Delta\rho_{min}$ = −1.04 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.702580 (19)	0.513530 (16)	0.653164 (14)	0.02650 (7)
Cl1	0.46761 (8)	0.67515 (7)	0.60517 (6)	0.03671 (13)
Cl2	0.99264 (7)	0.68125 (6)	0.66049 (6)	0.03132 (12)
C1	0.8247 (3)	0.1778 (3)	0.6348 (2)	0.0313 (4)
H1A	0.8154	0.1761	0.5350	0.038*
C2	0.8710 (3)	0.0522 (3)	0.6827 (3)	0.0343 (5)
H2A	0.8920	−0.0322	0.6161	0.041*
C3	0.8851 (3)	0.0548 (3)	0.8302 (3)	0.0338 (5)
H3A	0.9153	−0.0283	0.8646	0.041*
C4	0.8540 (3)	0.1826 (3)	0.9277 (2)	0.0305 (4)
H4A	0.8635	0.1870	1.0281	0.037*
C5	0.8084 (3)	0.3032 (2)	0.8712 (2)	0.0226 (4)
C6	0.7681 (3)	0.4433 (2)	0.9627 (2)	0.0219 (4)
C7	0.7286 (3)	0.6161 (2)	1.1522 (2)	0.0247 (4)
C8	0.7131 (3)	0.7043 (3)	1.2898 (2)	0.0321 (4)
H8A	0.7399	0.6726	1.3768	0.039*
C9	0.6561 (3)	0.8398 (3)	1.2894 (3)	0.0367 (5)
H9A	0.6423	0.9007	1.3783	0.044*
C10	0.6179 (3)	0.8898 (3)	1.1581 (3)	0.0358 (5)
H10A	0.5826	0.9839	1.1632	0.043*
C11	0.6318 (3)	0.8019 (3)	1.0226 (3)	0.0311 (4)
H11A	0.6053	0.8341	0.9360	0.037*
C12	0.6873 (3)	0.6625 (2)	1.0208 (2)	0.0239 (4)
N1	0.7931 (2)	0.3006 (2)	0.72678 (19)	0.0250 (3)
N2	0.7126 (2)	0.55058 (19)	0.90301 (18)	0.0237 (3)
N3	0.7801 (2)	0.4761 (2)	1.11117 (19)	0.0250 (3)
H3B	0.8134	0.4205	1.1694	0.030*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02836 (11)	0.03118 (10)	0.02066 (10)	0.00903 (7)	0.00083 (7)	0.01128 (7)
Cl1	0.0397 (3)	0.0401 (3)	0.0265 (3)	0.0207 (2)	−0.0043 (2)	0.0030 (2)
Cl2	0.0294 (3)	0.0367 (3)	0.0305 (3)	0.0082 (2)	0.0051 (2)	0.0162 (2)
C1	0.0372 (12)	0.0334 (10)	0.0232 (10)	0.0104 (9)	0.0057 (9)	0.0074 (8)
C2	0.0384 (12)	0.0284 (10)	0.0327 (11)	0.0120 (9)	0.0038 (9)	0.0028 (9)
C3	0.0371 (12)	0.0297 (10)	0.0356 (12)	0.0138 (9)	0.0019 (9)	0.0123 (9)
C4	0.0363 (11)	0.0319 (10)	0.0242 (10)	0.0113 (9)	0.0022 (8)	0.0115 (8)
C5	0.0192 (9)	0.0256 (9)	0.0223 (9)	0.0050 (7)	0.0014 (7)	0.0084 (7)

C6	0.0179 (8)	0.0261 (9)	0.0212 (9)	0.0049 (7)	0.0010 (7)	0.0089 (7)
C7	0.0201 (9)	0.0286 (9)	0.0231 (9)	0.0034 (7)	0.0022 (7)	0.0073 (8)
C8	0.0308 (11)	0.0391 (11)	0.0216 (10)	0.0040 (9)	0.0031 (8)	0.0051 (8)
C9	0.0337 (12)	0.0399 (12)	0.0292 (11)	0.0073 (10)	0.0063 (9)	−0.0022 (9)
C10	0.0332 (12)	0.0334 (11)	0.0384 (12)	0.0143 (9)	0.0048 (10)	0.0034 (9)
C11	0.0294 (11)	0.0333 (10)	0.0329 (11)	0.0124 (9)	0.0045 (9)	0.0121 (9)
C12	0.0204 (9)	0.0274 (9)	0.0221 (9)	0.0045 (7)	0.0028 (7)	0.0062 (7)
N1	0.0270 (9)	0.0257 (8)	0.0219 (8)	0.0059 (7)	0.0032 (7)	0.0081 (6)
N2	0.0241 (8)	0.0286 (8)	0.0203 (8)	0.0091 (7)	0.0038 (6)	0.0096 (6)
N3	0.0267 (9)	0.0279 (8)	0.0205 (8)	0.0068 (7)	0.0013 (6)	0.0101 (6)

Geometric parameters (Å, °)

Cd1—N2	2.2956 (17)	C6—N2	1.321 (2)
Cd1—N1	2.3581 (17)	C6—N3	1.350 (3)
Cd1—Cl2	2.4657 (8)	C7—N3	1.385 (3)
Cd1—Cl1	2.5852 (7)	C7—C12	1.399 (3)
Cd1—Cl1^{i}	2.5782 (7)	C7—C8	1.401 (3)
C1—N1	1.334 (3)	C8—C9	1.371 (3)
C1—C2	1.389 (3)	C8—H8A	0.9300
C1—H1A	0.9300	C9—C10	1.413 (4)
C2—C3	1.374 (3)	C9—H9A	0.9300
C2—H2A	0.9300	C10—C11	1.379 (3)
C3—C4	1.390 (3)	C10—H10A	0.9300
C3—H3A	0.9300	C11—C12	1.396 (3)
C4—C5	1.385 (3)	C11—H11A	0.9300
C4—Cl2^{ii}	3.690 (2)	C12—N2	1.392 (3)
C4—H4A	0.9300	N3—Cl2^{ii}	3.2708 (18)
C5—N1	1.344 (3)	N3—H3B	0.8600
C5—C6	1.477 (3)		
N2—Cd1—N1	71.68 (6)	N3—C6—C5	125.53 (17)
N2—Cd1—Cl2	101.94 (5)	N3—C7—C12	105.75 (17)
N1—Cd1—Cl2	101.14 (5)	N3—C7—C8	132.14 (19)
N2—Cd1—Cl1^{i}	141.01 (5)	C12—C7—C8	122.10 (19)
N1—Cd1—Cl1^{i}	89.60 (5)	C9—C8—C7	116.4 (2)
Cl2—Cd1—Cl1^{i}	115.34 (2)	C9—C8—H8A	121.8
N2—Cd1—Cl1	95.34 (4)	C7—C8—H8A	121.8
N1—Cd1—Cl1	151.59 (5)	C8—C9—C10	122.1 (2)
Cl2—Cd1—Cl1	106.34 (3)	C8—C9—H9A	119.0
Cl1^{i}—Cd1—Cl1	85.21 (2)	C10—C9—H9A	119.0
Cd1^{i}—Cl1—Cd1	94.79 (2)	C11—C10—C9	121.3 (2)
N1—C1—C2	122.4 (2)	C11—C10—H10A	119.3
N1—C1—H1A	118.8	C9—C10—H10A	119.3
C2—C1—H1A	118.8	C10—C11—C12	117.3 (2)
C3—C2—C1	118.7 (2)	C10—C11—H11A	121.3
C3—C2—H2A	120.6	C12—C11—H11A	121.3
C1—C2—H2A	120.6	N2—C12—C11	130.41 (19)

C2—C3—C4	119.5 (2)	N2—C12—C7	108.79 (17)
C2—C3—H3A	120.2	C11—C12—C7	120.80 (19)
C4—C3—H3A	120.2	C1—N1—C5	118.60 (17)
C5—C4—C3	118.2 (2)	C1—N1—Cd1	124.66 (14)
C5—C4—Cl2^{ii}	110.35 (14)	C5—N1—Cd1	116.71 (13)
C3—C4—Cl2^{ii}	128.49 (14)	C6—N2—C12	105.63 (16)
C5—C4—H4A	120.9	C6—N2—Cd1	115.58 (13)
C3—C4—H4A	120.9	C12—N2—Cd1	138.63 (13)
N1—C5—C4	122.49 (19)	C6—N3—C7	107.08 (16)
N1—C5—C6	114.19 (16)	C6—N3—Cl2^{ii}	124.62 (12)
C4—C5—C6	123.30 (18)	C7—N3—Cl2^{ii}	125.61 (12)
N2—C6—N3	112.74 (17)	C6—N3—H3B	126.5
N2—C6—C5	121.72 (17)	C7—N3—H3B	126.5
N2—Cd1—Cl1—Cd1^{i}	−140.85 (5)	N2—Cd1—N1—C1	177.38 (19)
N1—Cd1—Cl1—Cd1^{i}	−80.23 (9)	Cl2—Cd1—N1—C1	−83.59 (18)
Cl2—Cd1—Cl1—Cd1^{i}	115.02 (2)	Cl1^{i}—Cd1—N1—C1	32.19 (17)
Cl1^{i}—Cd1—Cl1—Cd1^{i}	0.0	Cl1—Cd1—N1—C1	111.32 (17)
N1—C1—C2—C3	−0.1 (4)	N2—Cd1—N1—C5	−0.68 (14)
C1—C2—C3—C4	−0.4 (4)	Cl2—Cd1—N1—C5	98.35 (14)
C2—C3—C4—C5	0.4 (4)	Cl1^{i}—Cd1—N1—C5	−145.87 (14)
C2—C3—C4—Cl2^{ii}	−158.16 (17)	Cl1—Cd1—N1—C5	−66.74 (18)
C3—C4—C5—N1	0.1 (3)	N3—C6—N2—C12	0.4 (2)
Cl2^{ii}—C4—C5—N1	162.33 (15)	C5—C6—N2—C12	179.52 (18)
C3—C4—C5—C6	178.6 (2)	N3—C6—N2—Cd1	176.70 (13)
Cl2^{ii}—C4—C5—C6	−19.2 (2)	C5—C6—N2—Cd1	−4.2 (2)
N1—C5—C6—N2	3.5 (3)	C11—C12—N2—C6	179.2 (2)
C4—C5—C6—N2	−175.0 (2)	C7—C12—N2—C6	−0.5 (2)
N1—C5—C6—N3	−177.46 (19)	C11—C12—N2—Cd1	4.2 (4)
C4—C5—C6—N3	4.0 (3)	C7—C12—N2—Cd1	−175.48 (15)
N3—C7—C8—C9	−179.7 (2)	N1—Cd1—N2—C6	2.49 (14)
C12—C7—C8—C9	−0.4 (3)	Cl2—Cd1—N2—C6	−95.44 (14)
C7—C8—C9—C10	−1.0 (4)	Cl1^{i}—Cd1—N2—C6	67.61 (16)
C8—C9—C10—C11	1.7 (4)	Cl1—Cd1—N2—C6	156.59 (14)
C9—C10—C11—C12	−0.7 (4)	N1—Cd1—N2—C12	177.1 (2)
C10—C11—C12—N2	179.6 (2)	Cl2—Cd1—N2—C12	79.2 (2)
C10—C11—C12—C7	−0.7 (3)	Cl1^{i}—Cd1—N2—C12	−117.76 (19)
N3—C7—C12—N2	0.5 (2)	Cl1—Cd1—N2—C12	−28.8 (2)
C8—C7—C12—N2	−178.94 (19)	N2—C6—N3—C7	−0.1 (2)
N3—C7—C12—C11	−179.27 (19)	C5—C6—N3—C7	−179.20 (18)
C8—C7—C12—C11	1.3 (3)	N2—C6—N3—Cl2^{ii}	−162.33 (12)
C2—C1—N1—C5	0.6 (3)	C5—C6—N3—Cl2^{ii}	18.6 (3)
C2—C1—N1—Cd1	−177.40 (18)	C12—C7—N3—C6	−0.2 (2)
C4—C5—N1—C1	−0.6 (3)	C8—C7—N3—C6	179.1 (2)
C6—C5—N1—C1	−179.19 (19)	C12—C7—N3—Cl2^{ii}	161.78 (12)
C4—C5—N1—Cd1	177.57 (16)	C8—C7—N3—Cl2^{ii}	−18.9 (3)

C6—C5—N1—Cd1	−1.0 (2)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3B···Cl2^{ii}	0.86	2.45	3.2708 (18)	160
C4—H4A···Cl2^{ii}	0.93	2.83	3.690 (2)	155

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

Fig. 1

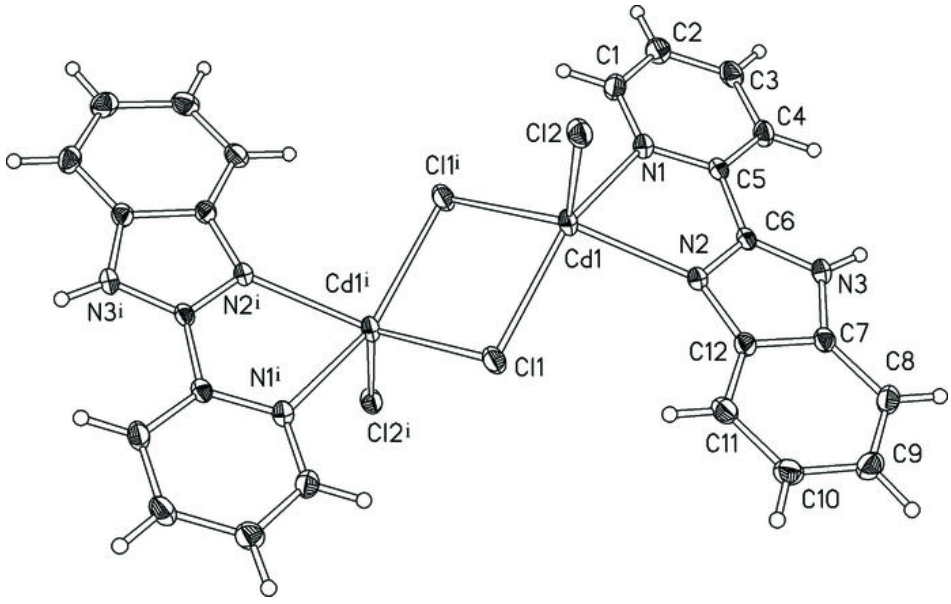
C2
C1
C3
C4
Cl2
Cl1i
N1
C5
C6
N2
Cd1
Cd1i
N3
N3i
N2i
C7
C12
C8
Cl1
N1i
Cl2i
C11
C9
C10

Fig. 2

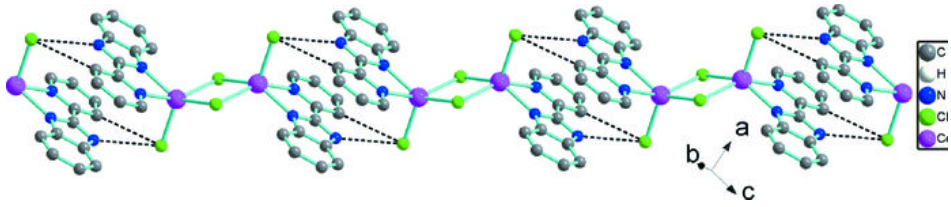

Fig. 3