Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Dichloridobis[*N*-(2-pyridylmethyl)-benzamide-κ^2N,O]cadmium(II)

Shu-Fang Zhang,[a,b]* Xiao-Gang Yang,[a,b] Zhi Liu,[c] Feng-Ling Xu[a] and Bao-Rong Hou[a]

[a]Institute of Oceanology, Chinese Academy of Sciences, Qingdao 266071, People's Republic of China, [b]Graduate School of the Chinese Academy of Sciences, Beijing 100039, People's Republic of China, and [c]College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China
Correspondence e-mail: zhangshufangzsf@yahoo.com.cn

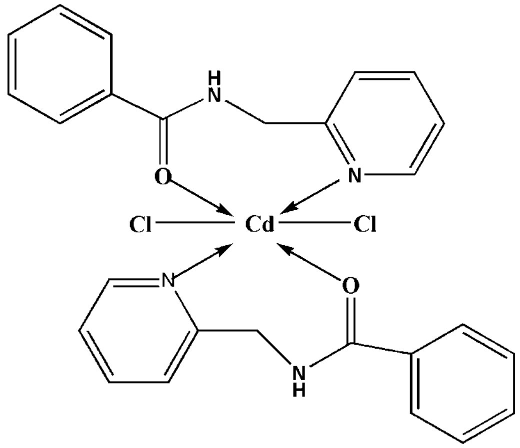
Received 20 June 2007; accepted 25 June 2007

Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.066; data-to-parameter ratio = 17.4.

In the title compound, [$\mathrm{CdCl_2(C_{13}H_{12}N_2O)_2}$], the $\mathrm{Cd^{II}}$ ion is situated on an inversion centre, coordinated by two O atoms [Cd—O = 2.3878 (17) Å] and two N atoms [Cd—N = 2.3404 (15) Å] from two *N*-(2-pyridylmethyl)benzamide ligands, and two Cl atoms [Cd—Cl = 2.5566 (6) Å], in a distorted octahedral geometry. In the crystal structure, intermolecular N—H⋯Cl hydrogen bonds [N⋯Cl = 3.1705 (18) Å] and π–π interactions, with a distance of 3.868 (3) Å between the centroids of the phenyl and pyridyl rings of neighbouring molecules, lead to the formation of two-dimensional layers parallel to the *bc* plane.

Related literature

For a related crystal structure, see: Zhang *et al.* (2006). For general background, see: MacDonald *et al.* (2000); Noverson *et al.* (2002); Fekner *et al.* (2004).



Experimental

Crystal data

[$\mathrm{CdCl_2(C_{13}H_{12}N_2O)_2}$]
M_r = 607.80
Monoclinic, $P2_1/c$
a = 11.800 (2) Å
b = 8.5536 (17) Å
c = 12.909 (3) Å
β = 105.60 (3)°
V = 1254.9 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.12 mm^{-1}
T = 153 (2) K
0.42 × 0.34 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.642, T_{max} = 0.762
11378 measured reflections
2876 independent reflections
2620 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.066
S = 1.01
2876 reflections
165 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\mathrm{max}}$ = 0.69 e Å^{-3}
$\Delta\rho_{\mathrm{min}}$ = −0.76 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N2—H2B⋯Cl1$^{\mathrm{i}}$	0.83 (3)	2.39 (3)	3.1705 (18)	158 (2)

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

Data collection: *RAPID-AUTO* (Rigaku, 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

The authors thank the International Cooperation Bureau of the Chinese Academy of Sciences (project No. GJHZ0527).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2267).

References

Bruker (1999). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Fekner, T., Gallucci, J. & Chan, M. K. (2004). *J. Am. Chem. Soc.* **126**, 223–236.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
MacDonald, J. C., Dorrestein, P. C., Pilley, M. M., Foote, M. M., Lundburg, J. L., Henning, R. W., Shultz, A. J. & Manson, A. L. (2000). *J. Am. Chem. Soc.* **122**, 11692–11702.
Noverson, J. C., Lah, L. S., Del Sesto, R. E., Miller, A. M., Miller, J. S. & Stang, P. J. (2002). *J. Am. Chem. Soc.* **124**, 6613–6625.
Rigaku (2001). *RAPID-AUTO*. Rigaku Corporation, Takyo, Japan.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, X.-R., Jia, J.-L., Li, X.-M. & Zhang, S.-S. (2006). *Acta Cryst.* E**62**, m185–m187.

doi:10.1107/S1600536807031054

supplementary materials

Acta Cryst. (2007). E**63**, m2058 [**doi:10.1107/S1600536807031054**]

Dichloridobis[*N*-(2-pyridylmethyl)benzamide-κ^2N,O]cadmium(II)

S.-F. Zhang, X.-G. Yang, Z. Liu, F.-L. Xu and **B.-R. Hou**

Comment

It is known that some 2-pyridylmethyl benzamide derivatives as N– or O-donors exhibit excellent coordination capability to form supramolecular frameworks. Self-assembly by H-bonding, π–π stacking, and van der Waals interactions is also an important process in the formation of noncovalent supramolecular frameworks (MacDonald *et al.*, 2000; Noverson *et al.*, 2002). The title compound, (I), was separated by employing 2-pyridylmethyl benzamide as ligand. Here we present its crystal structure.

The Cd(II) atom is coordinated by two O atoms and two N atoms from two benzamide ligands, and bonded to two Cl atoms with the Cd–O distance of 2.388 Å, Cd–N distance of 2.340 Å, and Cd–Cl distance of 2.557 Å, respectively (Fig. 1). The phenyl ring and pyridyl ring in the 2-pyridylmethyl benzamide molecule are rigid, and possess of typical bond lengths and angles. The amide C–N bond is known to possess a partial double-bond character due to donation of the non-bonding electron pair on the nitrogen (Fekner *et al.*, 2004).

In the crystal structure, the N atoms on the pyridyl rings act as donors to form N–H···Cl hydrogen bonds (Table 1), which link the $[(C_{13}H_{12}N_2O)_2CdCl_2]$ molecules into two-dimensional layers with four-membered ring $\{Cd_4\}$ extending along the *bc* plane (Fig. 2). The packing of adjacent layers is also stabilized by intermolecular π–π stacking interactions (Fig. 3), with relatively short distance $Cg1\cdots Cg2^{i}$ 3.868 (3) Å, where *Cg*1 and *Cg*2 are centroids of C1–C6 and N1/C8–C12 rings, respectively [symmetry code: (i) $-x + 2, y + 1/2, -z + 3/2$].

Experimental

To a cold solution of 2-(2-aminomethyl)pyridine (2 ml, 19 mmol) and triethylamine (2.63 ml, 19 mmol) in anhydrous CH_2Cl_2 (25 ml) was added dropwise a solution of benzyl chloride (2 ml, 17.2 mmol) in anhydrous CH_2Cl_2 (15 ml). Stirring was continued at room temperature for 1 h, then at 333 K for 5 h. After filtering, the filtrate was washed with water, dried over anhydrous Na_2SO_4, and then evaporated to give *N*-(pyridin-2-ylmethyl)benzamide as a yellow oil.

To a solution of the oil (0.16 g, 0.75 mmol) in ethyl acetate (10 ml), 0.114 g (0.5 mmol) $CdCl_2$ powder was slowly added. After stirring for four hours, the solution was filtered to remove the precipitate and placed in a desiccator filled with phosphorus pentaoxide. Colourless crystals were obtained about one month later.

Refinement

The H2B atom (attached to N2) was located on a difference Fourier map and isotropically refined. The C-bound H-atoms were geometrically positioned (C—H 0.93–0.97 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

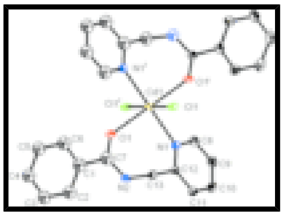


Fig. 1. View of the title compound, with displacement ellipsoids drawn at the 30% probability level [symmetry code: (i) $-x + 2$, $-y$, $-z + 1$].

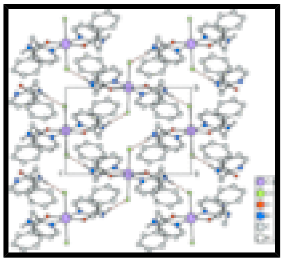


Fig. 2. Two-dimensional layers parallel to *bc* plane in (I).

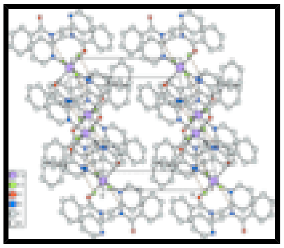


Fig. 3. Packing diagram for (I) viewed down the *b* axis.

Dichloridobis[*N*-(2-pyridylmethyl)benzamide-κ^2*N*,*O*]cadmium(II)

Crystal data

$[CdCl_2(C_{13}H_{12}N_2O)_2]$

$M_r = 607.80$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.800$ (2) Å

$b = 8.5536$ (17) Å

$c = 12.909$ (3) Å

$\beta = 105.60$ (3)°

$V = 1254.9$ (5) Å^3

$Z = 2$

$F_{000} = 612.0$

$D_x = 1.609$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 5099 reflections

$\theta = 3.2$–27.5°

$\mu = 1.12$ mm^{-1}

$T = 153$ (2) K

Block, colourless

0.42 × 0.34 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 153(2)$ K

2876 independent reflections

2620 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 27.5$°

ω scans	θ_{min} = 3.2°
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -15 \rightarrow 15$
T_{min} = 0.642, T_{max} = 0.762	$k = -11 \rightarrow 11$
11378 measured reflections	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.025$	$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2 + 0.9904P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.066$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max}$ = 0.69 e Å^{-3}
2876 reflections	$\Delta\rho_{min}$ = −0.75 e Å^{-3}
165 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0144 (10)
Secondary atom site location: difference Fourier map	

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*	$U_{iso}*/U_{eq}$
Cd1	1.0000	0.0000	0.5000	0.01528 (9)
Cl1	0.93804 (4)	−0.28494 (5)	0.50928 (3)	0.02087 (12)
N1	0.88328 (14)	0.07711 (18)	0.61167 (12)	0.0176 (3)
N2	1.11051 (14)	0.0398 (2)	0.79049 (13)	0.0183 (3)
C9	0.71170 (17)	0.2170 (2)	0.62332 (16)	0.0245 (4)
H9A	0.6497	0.2834	0.5914	0.029*
C13	1.00864 (16)	−0.0644 (2)	0.76345 (14)	0.0180 (4)
H13A	1.0008	−0.1162	0.8280	0.022*
H13B	1.0199	−0.1439	0.7135	0.022*
C8	0.79178 (17)	0.1707 (2)	0.56796 (15)	0.0218 (4)

H8A	0.7816	0.2058	0.4979	0.026*
C12	0.89841 (17)	0.0275 (2)	0.71330 (15)	0.0164 (3)
C11	0.82046 (17)	0.0666 (2)	0.77302 (15)	0.0208 (4)
H11A	0.8317	0.0289	0.8426	0.025*
C10	0.72589 (17)	0.1625 (3)	0.72706 (17)	0.0257 (4)
H10A	0.6725	0.1900	0.7654	0.031*
H2B	1.116 (2)	0.097 (3)	0.843 (2)	0.022 (6)*
O1	1.17479 (13)	−0.01963 (15)	0.64476 (11)	0.0197 (3)
C6	1.34268 (17)	0.2209 (2)	0.69617 (16)	0.0240 (4)
H6A	1.3150	0.1940	0.6240	0.029*
C5	1.43790 (18)	0.3211 (3)	0.72918 (19)	0.0311 (5)
H5A	1.4734	0.3619	0.6789	0.037*
C3	1.42620 (19)	0.3022 (3)	0.91142 (19)	0.0335 (5)
H3A	1.4541	0.3297	0.9835	0.040*
C7	1.18598 (16)	0.0533 (2)	0.73064 (14)	0.0174 (3)
C1	1.28839 (16)	0.1604 (2)	0.77084 (15)	0.0200 (4)
C4	1.48055 (19)	0.3610 (3)	0.8368 (2)	0.0337 (5)
H4A	1.5453	0.4269	0.8588	0.040*
C2	1.33055 (18)	0.2026 (3)	0.87908 (16)	0.0265 (4)
H2A	1.2943	0.1637	0.9294	0.032*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02031 (12)	0.01474 (12)	0.01195 (12)	0.00114 (6)	0.00633 (7)	−0.00019 (6)
Cl1	0.0316 (2)	0.0164 (2)	0.0165 (2)	−0.00131 (17)	0.00967 (17)	0.00081 (16)
N1	0.0205 (7)	0.0162 (7)	0.0173 (7)	0.0004 (6)	0.0071 (6)	−0.0016 (6)
N2	0.0201 (8)	0.0204 (7)	0.0142 (7)	0.0013 (6)	0.0042 (6)	−0.0038 (7)
C9	0.0184 (9)	0.0256 (10)	0.0281 (10)	0.0027 (8)	0.0039 (7)	−0.0051 (8)
C13	0.0233 (9)	0.0157 (9)	0.0161 (8)	0.0007 (7)	0.0073 (7)	0.0011 (7)
C8	0.0230 (9)	0.0221 (9)	0.0195 (8)	0.0016 (8)	0.0045 (7)	−0.0009 (8)
C12	0.0191 (8)	0.0146 (8)	0.0162 (8)	−0.0041 (7)	0.0059 (7)	−0.0030 (7)
C11	0.0225 (9)	0.0237 (10)	0.0186 (8)	−0.0056 (8)	0.0096 (7)	−0.0038 (8)
C10	0.0202 (9)	0.0305 (11)	0.0298 (10)	−0.0030 (8)	0.0123 (8)	−0.0091 (9)
O1	0.0237 (7)	0.0218 (7)	0.0140 (6)	0.0028 (5)	0.0056 (5)	−0.0017 (5)
C6	0.0225 (9)	0.0260 (10)	0.0249 (9)	0.0052 (8)	0.0087 (7)	−0.0001 (8)
C5	0.0235 (10)	0.0315 (11)	0.0417 (12)	0.0021 (8)	0.0149 (9)	0.0018 (10)
C3	0.0261 (10)	0.0389 (12)	0.0314 (11)	−0.0028 (9)	0.0008 (8)	−0.0083 (10)
C7	0.0198 (8)	0.0174 (9)	0.0141 (8)	0.0053 (7)	0.0031 (6)	0.0020 (7)
C1	0.0180 (8)	0.0203 (9)	0.0213 (9)	0.0047 (7)	0.0045 (7)	−0.0010 (7)
C4	0.0207 (9)	0.0312 (11)	0.0485 (13)	−0.0027 (9)	0.0081 (9)	−0.0071 (10)
C2	0.0241 (9)	0.0329 (11)	0.0216 (9)	−0.0002 (9)	0.0043 (7)	−0.0026 (8)

Geometric parameters (Å, °)

Cd1—N1^{i}	2.3404 (15)	C12—C11	1.391 (3)
Cd1—N1	2.3404 (15)	C11—C10	1.384 (3)
Cd1—O1	2.3878 (17)	C11—H11A	0.9300

Cd1—O1^{i}	2.3878 (17)	C10—H10A	0.9300
Cd1—Cl1^{i}	2.5566 (6)	O1—C7	1.248 (2)
Cd1—Cl1	2.5566 (6)	C6—C5	1.386 (3)
N1—C8	1.340 (3)	C6—C1	1.393 (3)
N1—C12	1.344 (2)	C6—H6A	0.9300
N2—C7	1.332 (2)	C5—C4	1.387 (3)
N2—C13	1.461 (2)	C5—H5A	0.9300
N2—H2B	0.83 (3)	C3—C2	1.386 (3)
C9—C10	1.385 (3)	C3—C4	1.387 (3)
C9—C8	1.387 (3)	C3—H3A	0.9300
C9—H9A	0.9300	C7—C1	1.494 (3)
C13—C12	1.508 (3)	C1—C2	1.399 (3)
C13—H13A	0.9700	C4—H4A	0.9300
C13—H13B	0.9700	C2—H2A	0.9300
C8—H8A	0.9300		

N1^{i}—Cd1—N1	180.0	C9—C8—H8A	118.8
N1^{i}—Cd1—O1	86.26 (5)	N1—C12—C11	122.07 (18)
N1—Cd1—O1	93.74 (5)	N1—C12—C13	117.14 (16)
N1^{i}—Cd1—O1^{i}	93.74 (5)	C11—C12—C13	120.66 (17)
N1—Cd1—O1^{i}	86.26 (5)	C10—C11—C12	118.84 (18)
O1—Cd1—O1^{i}	180.000 (1)	C10—C11—H11A	120.6
N1^{i}—Cd1—Cl1^{i}	90.96 (4)	C12—C11—H11A	120.6
N1—Cd1—Cl1^{i}	89.04 (4)	C11—C10—C9	119.22 (17)
O1—Cd1—Cl1^{i}	84.61 (3)	C11—C10—H10A	120.4
O1^{i}—Cd1—Cl1^{i}	95.39 (3)	C9—C10—H10A	120.4
N1^{i}—Cd1—Cl1	89.04 (4)	C7—O1—Cd1	121.53 (12)
N1—Cd1—Cl1	90.96 (4)	C5—C6—C1	120.18 (19)
O1—Cd1—Cl1	95.39 (3)	C5—C6—H6A	119.9
O1^{i}—Cd1—Cl1	84.61 (3)	C1—C6—H6A	119.9
Cl1^{i}—Cd1—Cl1	180.0	C6—C5—C4	120.4 (2)
C8—N1—C12	118.68 (16)	C6—C5—H5A	119.8
C8—N1—Cd1	116.73 (12)	C4—C5—H5A	119.8
C12—N1—Cd1	124.50 (12)	C2—C3—C4	120.3 (2)
C7—N2—C13	123.35 (16)	C2—C3—H3A	119.8
C7—N2—H2B	120.5 (17)	C4—C3—H3A	119.8
C13—N2—H2B	116.0 (16)	O1—C7—N2	122.99 (18)
C10—C9—C8	118.67 (18)	O1—C7—C1	119.86 (16)
C10—C9—H9A	120.7	N2—C7—C1	117.15 (16)
C8—C9—H9A	120.7	C6—C1—C2	119.30 (18)
N2—C13—C12	110.11 (15)	C6—C1—C7	117.84 (17)
N2—C13—H13A	109.6	C2—C1—C7	122.85 (17)
C12—C13—H13A	109.6	C5—C4—C3	119.7 (2)
N2—C13—H13B	109.6	C5—C4—H4A	120.2
C12—C13—H13B	109.6	C3—C4—H4A	120.2
H13A—C13—H13B	108.2	C3—C2—C1	120.1 (2)
N1—C8—C9	122.48 (18)	C3—C2—H2A	120.0

N1—C8—H8A	118.8	C1—C2—H2A	120.0

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···Cl1^{ii}	0.83 (3)	2.39 (3)	3.1705 (18)	158 (2)

Symmetry codes: (ii) −*x*+2, *y*+1/2, −*z*+3/2.

Fig. 1

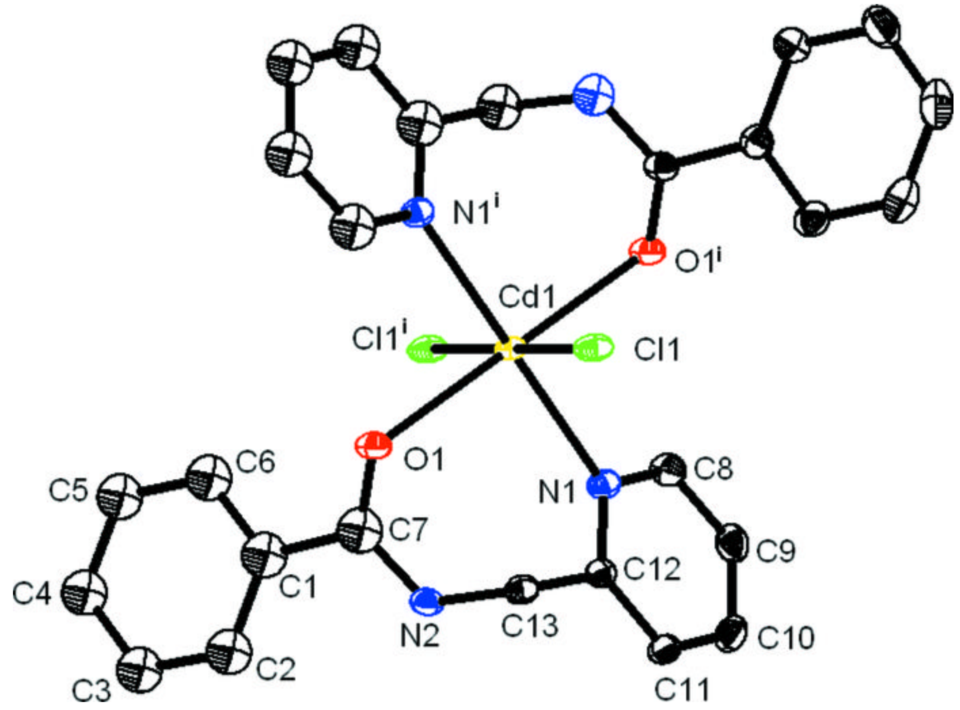

N1i
O1i
Cd1
Cl1i
Cl1
O1
N1
C8
C6
C5
C7
C9
C12
C4
C1
N2
C13
C10
C3
C2
C11

Fig. 2

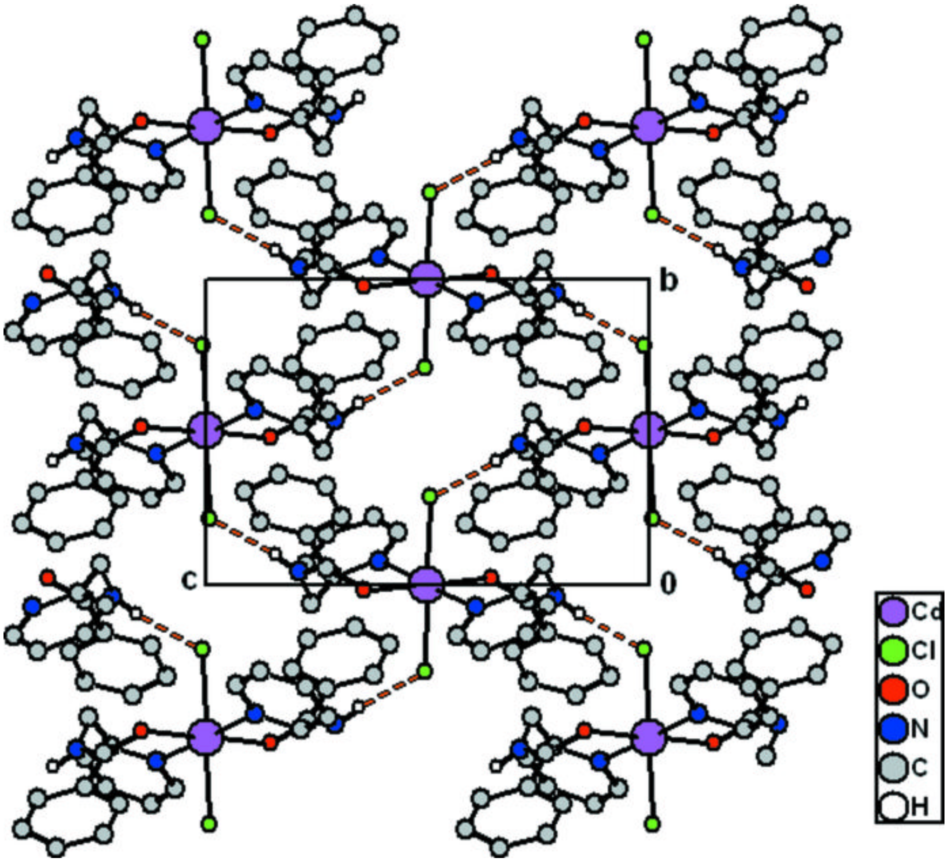


Fig. 3