

catena-Poly[[bis[2-(2-pyridyl)-1-*H*-imidazole- κ^2N^2,N^3]cadmium]- μ -benzene-1,3-dicarboxylato- $\kappa^2O^1:O^3$]

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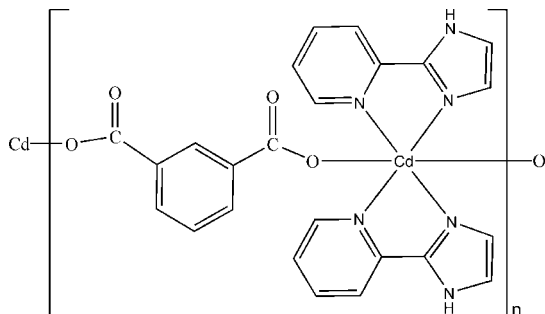
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.034; wR factor = 0.100; data-to-parameter ratio = 14.2.

In the title coordination polymer, $[\text{Cd}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_8\text{H}_7\text{N}_3)_2]_n$, the Cd^{II} atom, lying on a twofold rotation axis, is six-coordinated by two carboxylate O atoms from two benzene-1,3-dicarboxylate (*m*-BDC) ligands and four N atoms from two chelating 2-(2-pyridyl)imidazole molecules, forming a slightly distorted octahedral geometry. The *m*-BDC ligand is located over a twofold rotation axis. The Cd^{II} atoms are bridged by the *m*-BDC ligands, leading to a wave-shaped chain structure along [010]. $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds connect the chains.

Related literature

For general background to metal-organic frameworks, see: Chen *et al.* (2009); Rosi *et al.* (2003); Su *et al.* (2004); Xiao *et al.* (2006). For compounds based on benzene-1,3-dicarboxylate ligands, see: Banerjee *et al.* (2008); Che *et al.* (2009); Clegg & Russo (2009); Li *et al.* (2008); Su *et al.* (2009); Zhao (2008).



Experimental

Crystal data

$[\text{Cd}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_8\text{H}_7\text{N}_3)_2]$
 $M_r = 566.85$
 Orthorhombic, *Pnna*
 $a = 8.720$ (5) Å
 $b = 20.102$ (4) Å
 $c = 13.483$ (5) Å
 $V = 2363.4$ (17) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.97$ mm⁻¹
 $T = 293$ K
 $0.10 \times 0.08 \times 0.06$ mm

Data collection

Bruker APEX CCD diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.911$, $T_{\text{max}} = 0.944$
 11996 measured reflections
 2330 independent reflections
 1298 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.060$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.100$
 $S = 1.00$
 2330 reflections
 164 parameters
 75 restraints
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.39$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.69$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cd1—O1	2.257 (3)	Cd1—N3	2.461 (4)
Cd1—N1	2.288 (4)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H1N \cdots O2 ⁱ	0.95 (5)	1.80 (5)	2.741 (5)	166 (5)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2397).

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supplementary materials

Acta Cryst. (2011). E67, m269-m270 [doi:10.1107/S1600536811001243]

catena-Poly[[bis[2-(2-pyridyl)-1-*H*-imidazole- κ^2N^2,N^3]cadmium]- μ -benzene-1,3-dicarboxylato- $\kappa^2O^1:O^3$]

C.-J. Li, J.-M. Lu, F. Tu, J.-Y. Chen and Y.-J. Li

Comment

Currently, the design and synthesis of metal-organic frameworks (MOFs) are of great interest owing to their intriguing variety of architectures and their tremendous potential applications in many fields (Chen *et al.*, 2009; Rosi *et al.*, 2003; Su *et al.*, 2004; Xiao *et al.*, 2006). As a multidentate ligand, benzene-1,3-dicarboxylic acid (*m*-H₂BDC) has two carboxyl groups and, therefore, has been widely reported as a good candidate not only in the construction of various coordination polymers but also in the construction of MOFs with multi-dimension (Banerjee *et al.*, 2008; Che *et al.*, 2009; Clegg & Russo, 2009; Li *et al.*, 2008; Su *et al.*, 2009; Zhao, 2008).

In the title coordination polymer (Fig. 1), the central Cd^{II} ion is six-coordinated by two carboxylate O atoms from two *m*-BDC ligands and four N atoms from two 2-(2-pyridyl)imidazole (2-PyIM) molecules (Table 1), forming a slightly distorted octahedral geometry. The Cd^{II} ions are bridged by the *m*-BDC ligands, leading to a wave-shaped chain structure, as shown in Fig. 2. N—H...O hydrogen bonds connect the chains (Table 2).

Experimental

All chemicals were purchased from commercial sources and used without further purification. CdSO₄·8H₂O (0.033 mmol), *m*-H₂BDC (0.1 mmol) and 2-PyIM (0.2 mmol) were dissolved in 15 ml of water. The mixture was stirred for 2 h at room temperature and then heated in a 30 ml Teflon-lined stainless steel autoclave for 3 d at 323 K. After the autoclave was cooled to room temperature, colorless block crystals were harvested.

Refinement

C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atom on imidazole N2 was located from a difference Fourier map and refined isotropically.

Figures

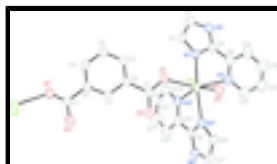


Fig. 1. The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $-x+5/2, -y+1, z$; (ii) $x, -y+1/2, -z+3/2$.]

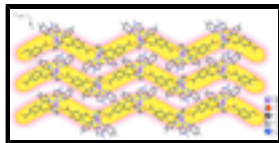


Fig. 2. View of the one-dimensional chain structure of the title compound.

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Crystal data

[Cd(C₈H₄O₄)(C₈H₇N₃)₂]

$M_r = 566.85$

Orthorhombic, *Pnna*

Hall symbol: -P 2a 2bc

$a = 8.720$ (5) Å

$b = 20.102$ (4) Å

$c = 13.483$ (5) Å

$V = 2363.4$ (17) Å³

$Z = 4$

$F(000) = 1136$

$D_x = 1.593$ Mg m⁻³

$D_m = 1.593$ Mg m⁻³

D_m measured by not measured

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

Cell parameters from 2329 reflections

$\theta = 2.0$ – 52.0°

$\mu = 0.97$ mm⁻¹

$T = 293$ K

Block, colorless

$0.10 \times 0.08 \times 0.06$ mm

Data collection

Bruker APEX CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.911$, $T_{\max} = 0.944$

11996 measured reflections

2330 independent reflections

1298 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.060$

$\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 1.8^\circ$

$h = -10 \rightarrow 10$

$k = -21 \rightarrow 24$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.100$

$S = 1.00$

2330 reflections

164 parameters

75 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.051P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.39$ e Å⁻³

$\Delta\rho_{\min} = -0.69$ e Å⁻³

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.96428 (5)	0.2500	0.7500	0.05598 (19)
O1	1.1284 (4)	0.33138 (14)	0.7049 (2)	0.0738 (8)
C2	1.2020 (5)	0.44358 (18)	0.6952 (3)	0.0589 (10)
O2	1.1291 (4)	0.39000 (15)	0.8440 (2)	0.0883 (10)
C9	0.7428 (5)	0.1504 (2)	0.6230 (4)	0.0691 (12)
C3	1.2500	0.5000	0.7444 (4)	0.0549 (13)
H3	1.2500	0.5000	0.8133	0.066*
N3	0.7725 (5)	0.16257 (19)	0.7191 (3)	0.0692 (10)
N2	0.7945 (5)	0.1991 (2)	0.4546 (3)	0.0759 (12)
C13	0.7096 (7)	0.1223 (3)	0.7857 (4)	0.0919 (16)
H13	0.7293	0.1300	0.8525	0.110*
N1	0.9098 (5)	0.24430 (17)	0.5842 (3)	0.0673 (10)
C8	0.8139 (5)	0.1966 (2)	0.5556 (3)	0.0621 (11)
C6	0.9516 (6)	0.2781 (3)	0.4998 (4)	0.0769 (15)
H6	1.0177	0.3144	0.4980	0.092*
C1	1.1489 (6)	0.3835 (2)	0.7533 (3)	0.0630 (9)
C4	1.2024 (6)	0.4443 (2)	0.5936 (3)	0.0934 (15)
H4	1.1702	0.4070	0.5587	0.112*
C10	0.6521 (6)	0.0978 (3)	0.5917 (4)	0.0947 (16)
H10	0.6344	0.0903	0.5246	0.114*
C11	0.5901 (6)	0.0577 (3)	0.6615 (5)	0.1110 (17)
H11	0.5292	0.0218	0.6429	0.133*
C12	0.6178 (8)	0.0702 (3)	0.7606 (4)	0.1049 (17)
H12	0.5744	0.0435	0.8094	0.126*
C7	0.8821 (8)	0.2507 (3)	0.4193 (4)	0.0852 (15)
H7	0.8919	0.2642	0.3537	0.102*
C5	1.2500	0.5000	0.5431 (5)	0.158 (5)
H5	1.2500	0.5000	0.4741	0.189*
H1N	0.735 (6)	0.174 (3)	0.409 (4)	0.14 (2)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0763 (3)	0.0434 (3)	0.0482 (3)	0.000	0.000	0.0039 (2)
O1	0.0959 (19)	0.0469 (15)	0.0786 (16)	-0.0127 (15)	0.0124 (16)	-0.0040 (14)
C2	0.086 (3)	0.041 (2)	0.0496 (19)	-0.006 (2)	0.000 (2)	-0.0011 (18)
O2	0.139 (3)	0.064 (2)	0.061 (2)	-0.016 (2)	0.000 (2)	0.0127 (16)
C9	0.062 (3)	0.063 (3)	0.083 (3)	0.002 (2)	0.001 (3)	-0.001 (3)
C3	0.075 (3)	0.046 (3)	0.045 (3)	0.000 (3)	0.000	0.000
N3	0.076 (3)	0.066 (2)	0.066 (2)	-0.011 (2)	0.007 (2)	0.0065 (19)
N2	0.094 (3)	0.072 (3)	0.062 (3)	0.005 (2)	-0.018 (2)	-0.010 (2)
C13	0.101 (4)	0.100 (4)	0.075 (3)	-0.020 (4)	0.006 (3)	0.007 (3)
N1	0.088 (3)	0.060 (2)	0.054 (2)	-0.007 (2)	-0.008 (2)	0.0039 (19)
C8	0.074 (3)	0.056 (3)	0.057 (3)	0.006 (2)	-0.009 (2)	-0.002 (2)

supplementary materials

C6	0.106 (4)	0.061 (3)	0.064 (3)	-0.011 (3)	-0.004 (3)	0.012 (3)
C1	0.083 (2)	0.0461 (18)	0.0602 (19)	-0.0035 (17)	0.000 (2)	-0.0019 (19)
C4	0.152 (4)	0.071 (3)	0.057 (2)	-0.041 (3)	0.001 (3)	-0.010 (2)
C10	0.090 (4)	0.099 (4)	0.095 (4)	-0.028 (3)	0.000 (3)	-0.003 (3)
C11	0.100 (4)	0.125 (4)	0.108 (3)	-0.033 (3)	0.004 (3)	-0.001 (3)
C12	0.105 (4)	0.114 (4)	0.096 (3)	-0.033 (4)	0.005 (3)	0.009 (3)
C7	0.121 (4)	0.082 (4)	0.052 (3)	0.004 (4)	-0.007 (3)	0.014 (3)
C5	0.319 (13)	0.108 (6)	0.046 (4)	-0.116 (8)	0.000	0.000

Geometric parameters (\AA , $^\circ$)

Cd1—O1	2.257 (3)	C13—C12	1.360 (8)
Cd1—N1	2.288 (4)	C13—H13	0.9300
Cd1—N3	2.461 (4)	N1—C8	1.330 (5)
O1—C1	1.246 (5)	N1—C6	1.376 (6)
C2—C4	1.370 (5)	C6—C7	1.359 (7)
C2—C3	1.378 (4)	C6—H6	0.9300
C2—C1	1.512 (6)	C4—C5	1.374 (5)
O2—C1	1.243 (4)	C4—H4	0.9300
C9—N3	1.343 (5)	C10—C11	1.352 (7)
C9—C10	1.388 (6)	C10—H10	0.9300
C9—C8	1.439 (6)	C11—C12	1.380 (6)
C3—C2 ⁱ	1.378 (4)	C11—H11	0.9300
C3—H3	0.9300	C12—H12	0.9300
N3—C13	1.328 (6)	C7—H7	0.9300
N2—C7	1.373 (6)	C5—C4 ⁱ	1.374 (5)
N2—C8	1.374 (5)	C5—H5	0.9300
N2—H1N	0.95 (5)		
O1 ⁱⁱ —Cd1—O1	101.29 (17)	N3—C13—H13	118.5
O1 ⁱⁱ —Cd1—N1 ⁱⁱ	84.54 (13)	C12—C13—H13	118.5
O1—Cd1—N1 ⁱⁱ	111.01 (12)	C8—N1—C6	106.5 (4)
O1 ⁱⁱ —Cd1—N1	111.01 (12)	C8—N1—Cd1	116.8 (3)
O1—Cd1—N1	84.54 (13)	C6—N1—Cd1	136.8 (3)
N1 ⁱⁱ —Cd1—N1	156.0 (2)	N1—C8—N2	109.7 (4)
O1 ⁱⁱ —Cd1—N3	87.64 (13)	N1—C8—C9	123.5 (4)
O1—Cd1—N3	154.52 (13)	N2—C8—C9	126.7 (5)
N1 ⁱⁱ —Cd1—N3	93.45 (13)	C7—C6—N1	110.0 (4)
N1—Cd1—N3	69.99 (13)	C7—C6—H6	125.0
O1 ⁱⁱ —Cd1—N3 ⁱⁱ	154.52 (13)	N1—C6—H6	125.0
O1—Cd1—N3 ⁱⁱ	87.64 (13)	O2—C1—O1	125.7 (4)
N1 ⁱⁱ —Cd1—N3 ⁱⁱ	69.99 (13)	O2—C1—C2	117.9 (4)
N1—Cd1—N3 ⁱⁱ	93.45 (13)	O1—C1—C2	116.4 (4)
N3—Cd1—N3 ⁱⁱ	94.41 (19)	C2—C4—C5	120.4 (5)
C1—O1—Cd1	124.0 (3)	C2—C4—H4	119.8
C4—C2—C3	118.1 (4)	C5—C4—H4	119.8
C4—C2—C1	121.8 (4)	C11—C10—C9	118.1 (5)

C3—C2—C1	120.1 (4)	C11—C10—H10	121.0
N3—C9—C10	122.9 (4)	C9—C10—H10	121.0
N3—C9—C8	114.1 (4)	C10—C11—C12	119.7 (6)
C10—C9—C8	123.0 (5)	C10—C11—H11	120.2
C2—C3—C2 ⁱ	122.6 (5)	C12—C11—H11	120.2
C2—C3—H3	118.7	C13—C12—C11	119.0 (5)
C2 ⁱ —C3—H3	118.7	C13—C12—H12	120.5
C13—N3—C9	117.5 (4)	C11—C12—H12	120.5
C13—N3—Cd1	127.0 (4)	C6—C7—N2	106.2 (4)
C9—N3—Cd1	115.1 (3)	C6—C7—H7	126.9
C7—N2—C8	107.7 (4)	N2—C7—H7	126.9
C7—N2—H1N	119 (3)	C4 ⁱ —C5—C4	120.5 (6)
C8—N2—H1N	133 (3)	C4 ⁱ —C5—H5	119.7
N3—C13—C12	123.0 (5)	C4—C5—H5	119.7
O1 ⁱⁱ —Cd1—O1—C1	-109.2 (4)	N3—Cd1—N1—C6	177.0 (5)
N1 ⁱⁱ —Cd1—O1—C1	-20.8 (4)	N3 ⁱⁱ —Cd1—N1—C6	83.6 (5)
N1—Cd1—O1—C1	140.4 (4)	C6—N1—C8—N2	0.4 (5)
N3—Cd1—O1—C1	142.1 (4)	Cd1—N1—C8—N2	-179.2 (3)
N3 ⁱⁱ —Cd1—O1—C1	46.7 (4)	C6—N1—C8—C9	-179.4 (4)
C4—C2—C3—C2 ⁱ	-0.1 (3)	Cd1—N1—C8—C9	1.1 (6)
C1—C2—C3—C2 ⁱ	-179.3 (4)	C7—N2—C8—N1	-0.1 (6)
C10—C9—N3—C13	-0.8 (7)	C7—N2—C8—C9	179.6 (4)
C8—C9—N3—C13	179.5 (4)	N3—C9—C8—N1	4.8 (6)
C10—C9—N3—Cd1	172.1 (4)	C10—C9—C8—N1	-175.0 (4)
C8—C9—N3—Cd1	-7.6 (5)	N3—C9—C8—N2	-174.9 (4)
O1 ⁱⁱ —Cd1—N3—C13	64.9 (4)	C10—C9—C8—N2	5.3 (7)
O1—Cd1—N3—C13	176.6 (4)	C8—N1—C6—C7	-0.5 (6)
N1 ⁱⁱ —Cd1—N3—C13	-19.4 (4)	Cd1—N1—C6—C7	178.9 (4)
N1—Cd1—N3—C13	178.3 (4)	Cd1—O1—C1—O2	26.3 (7)
N3 ⁱⁱ —Cd1—N3—C13	-89.6 (4)	Cd1—O1—C1—C2	-153.4 (3)
O1 ⁱⁱ —Cd1—N3—C9	-107.2 (3)	C4—C2—C1—O2	-168.9 (5)
O1—Cd1—N3—C9	4.5 (5)	C3—C2—C1—O2	10.2 (6)
N1 ⁱⁱ —Cd1—N3—C9	168.4 (3)	C4—C2—C1—O1	10.9 (7)
N1—Cd1—N3—C9	6.2 (3)	C3—C2—C1—O1	-170.0 (4)
N3 ⁱⁱ —Cd1—N3—C9	98.2 (3)	C3—C2—C4—C5	0.3 (7)
C9—N3—C13—C12	-0.1 (8)	C1—C2—C4—C5	179.4 (4)
Cd1—N3—C13—C12	-172.1 (5)	N3—C9—C10—C11	0.7 (8)
O1 ⁱⁱ —Cd1—N1—C8	75.6 (3)	C8—C9—C10—C11	-179.6 (5)
O1—Cd1—N1—C8	175.6 (3)	C9—C10—C11—C12	0.3 (9)
N1 ⁱⁱ —Cd1—N1—C8	-52.2 (3)	N3—C13—C12—C11	1.1 (10)
N3—Cd1—N1—C8	-3.6 (3)	C10—C11—C12—C13	-1.2 (9)
N3 ⁱⁱ —Cd1—N1—C8	-97.1 (3)	N1—C6—C7—N2	0.4 (6)
O1 ⁱⁱ —Cd1—N1—C6	-103.8 (5)	C8—N2—C7—C6	-0.2 (6)
O1—Cd1—N1—C6	-3.7 (5)	C2—C4—C5—C4 ⁱ	-0.1 (3)

supplementary materials

$\text{N1}^{\text{ii}}-\text{Cd1}-\text{N1}-\text{C6}$ 128.4 (5)

Symmetry codes: (i) $-x+5/2, -y+1, z$; (ii) $x, -y+1/2, -z+3/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H1N}\cdots\text{O2}^{\text{iii}}$	0.95 (5)	1.80 (5)	2.741 (5)	166 (5)

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

Fig. 1

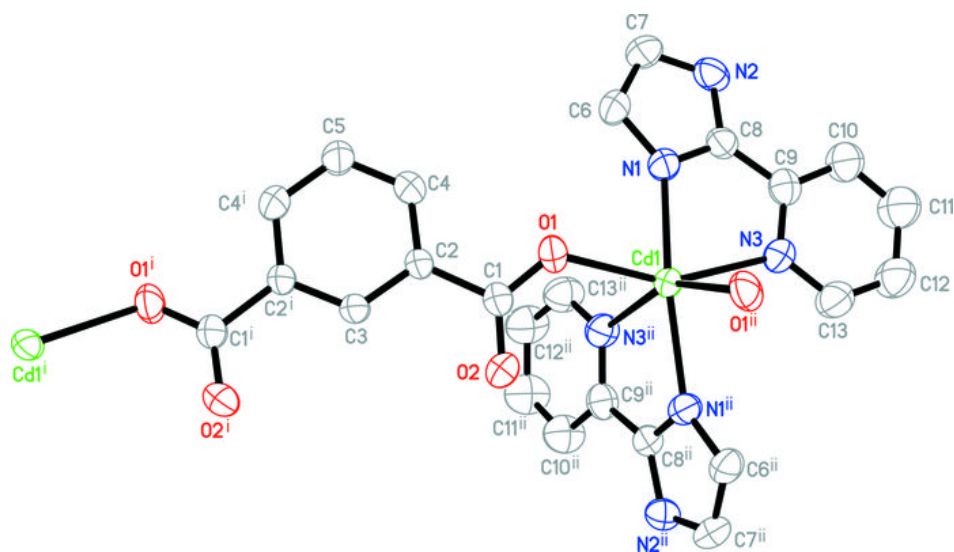


Fig. 2

