

Poly[(2,2'-bipyridine- κ^2N,N')-(μ_3 -2,4,6-trimethylisophthalato- $\kappa^5O^1,O^1':O^1:O^3,O^3'$)cadmium]

Shao-Gang Hou and Mei-Fang Jin*

College of Chemical and Environmental Engineering, Anyang Institute of Technology, Anyang 455000, People's Republic of China

Correspondence e-mail: aymeifangjin@163.com

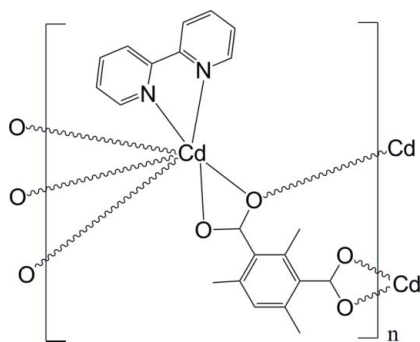
Received 23 November 2011; accepted 16 December 2011

 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.007$ Å; R factor = 0.045; wR factor = 0.098; data-to-parameter ratio = 17.0.

In the crystal structure of the polymeric title complex, $[Cd(C_{11}H_{10}O_4)(C_{10}H_8N_2)]_n$, the Cd^{II} cation is chelated by one 2,2'-bipyridine ligand and two carboxyl groups from two trimethylisophthalate (TMIPA) anions, and is further coordinated by one carboxylate O atom from a third TMIPA anion, forming a distorted pentagonal-bipyramidal geometry. Each TMIPA anion bridges three Cd^{II} cations, forming polymeric complex sheets parallel to (001). Weak $C-H \cdots O$ hydrogen bonding occurs between adjacent sheets.

Related literature

For applications of functional metal-organic frameworks, see: Evans & Lin (2002); Chen *et al.* (2010); Leong & Vittal (2011); Sun *et al.* (2011). For related structures, see: Ma *et al.* (2008); Zhang *et al.* (2008); Zhou *et al.* (2003); Zhang *et al.* (2003); He *et al.* (2010); Liu *et al.* (2008). For our previous work, see: Dai *et al.* (2008, 2009); Zhao *et al.* (2009).



Experimental

Crystal data

$[Cd(C_{11}H_{10}O_4)(C_{10}H_8N_2)]$
 $M_r = 474.77$
 Orthorhombic, *Pbca*

$a = 13.1985$ (8) Å
 $b = 15.5714$ (9) Å
 $c = 18.1926$ (11) Å

$V = 3738.9$ (4) Å³
 $Z = 8$
 Mo $K\alpha$ radiation

$\mu = 1.20$ mm⁻¹
 $T = 298$ K
 $0.15 \times 0.10 \times 0.10$ mm

Data collection

Bruker SMART APEXII CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
 $T_{min} = 0.841$, $T_{max} = 0.890$

14349 measured reflections
 4299 independent reflections
 2454 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.054$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.098$
 $S = 0.99$
 4299 reflections

253 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.51$ e Å⁻³
 $\Delta\rho_{min} = -0.63$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cd1—N1	2.393 (4)	Cd1—O2	2.372 (3)
Cd1—N2	2.334 (4)	Cd1—O3 ⁱⁱ	2.347 (3)
Cd1—O1	2.607 (3)	Cd1—O4 ⁱⁱ	2.396 (3)
Cd1—O2 ⁱ	2.317 (3)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C4—H4A \cdots O1 ⁱⁱⁱ	0.93	2.32	3.240 (6)	169
C8—H8A \cdots O3 ⁱⁱⁱ	0.93	2.39	3.251 (6)	155

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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, 2008); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

This work was supported financially by Anyang Institute of Technology, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5394).

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supplementary materials

Acta Cryst. (2012). E68, m84-m85 [doi:10.1107/S1600536811054183]

Poly[(2,2'-bipyridine- κ^2N,N')(μ_3 -2,4,6-trimethylisophthalato- $\kappa^5O^1,O^1':O^3,O^3'$)cadmium]

S.-G. Hou and M.-F. Jin

Comment

The rational design and synthesis of functional metal-organic frameworks (MOFs) is a more and more fascinating field in recent years due to their interesting topologies and potential applications in gas adsorption, nonlinear optics, magnetism, molecular recognition, etc (Evans & Lin, 2002; Chen, *et al.*, 2010; Leong & Vittal, 2011; Sun *et al.*, 2011). As we know, the construction of MOFs mainly depends on the coordination geometry of metal ions and the nature of ligands. Besides, some secondary interactions, such as aromatic $\pi\cdots\pi$ interactions, classical hydrogen bonds (such as O-H \cdots O and N-H \cdots O hydrogen bonds), and non-classical hydrogen bonds (such as C-H \cdots O hydrogen bond) often influence the packing of molecules from discrete subunits or low-dimensional entities to high-dimensional supramolecular frameworks. One of the most effective strategies to assemble MOFs is to use carboxylates as linkers because of their diverse conformations and coordination modes observed in the coordination process (Ma *et al.*, 2008; Zhang *et al.*, 2008). In spite of isophthalate-based MOFs (Zhou *et al.*, 2003; Zhang *et al.*, 2003) have been widely reported, to the best of our knowledge, only one MOF based on 2,4,6-trimethylisophthalic acid (H₂TMIPA) has been documented until now (He *et al.*, 2010). Based on our previous work (Dai *et al.*, 2008; Dai *et al.*, 2009; Zhao *et al.*, 2009) and consideration the steric hindrance effects of additional three methyl groups on isophthalate, herein, we choose the H₂TMIPA as a bridging ligand to construct a novel Cd^{II} coordination polymer (**I**), which is a 2D (4,4) net incorporating [Cd₂(COO)₄N₂] SBUs.

The asymmetric unit of (**I**) contains one crystallographically independent Cd^{II} center, one TMIPA ligand and one bpy ligand. The Cd^{II} ion is in a slightly distorted pentagonal bipyramidal geometry, completed by five O atoms from three different TMIPA ligands and two N atoms from the same bpy ligand (Fig. 1). The equatorial plane of pentagonal bipyramid is defined by O2ⁱ, O3ⁱⁱ, O4ⁱⁱ, N2 atoms, while the axial positions are occupied N1, O1 atoms. [symmetry codes: (i) -x+1, -y+1, -z+1; (ii) -x+3/2, y+1/2, z]. Two carboxyl groups on TMIPA ligand adopt two different coordination patterns, μ_1 - η^1 : η^1 chelating and μ_2 - η^2 : η^1 bridging, respectively. The Cd-N bond lengths are 2.393 (4) and 2.334 (4) Å, while the Cd-O bond lengths vary from 2.317 (3) to 2.607 (3) Å (Table). The average Cd-N and Cd-O distances in (**I**) are comparable with those reported for Cd-based MOFs (Liu *et al.*, 2008). Two crystallographically equivalent Cd^{II} anions are bridged by two tridentate bridging carboxyl groups to form a binuclear SBU with a Cd \cdots Cd contact of 3.7886 (6) Å. Because of the steric hindrance between the methyl and the carboxyl groups, the two carboxyl groups of H₂TMIPA are not coplanar with the central benzene ring, generating two dihedral angles of 55.1 (2) and 85.3 (2)^o, respectively. The [Cd₂(COO)₄N₂] SBUs are joined by TMIPA ligands to form an infinite 1D zigzag chain. Furthermore, TMIPA ligands connect the zigzag chain to a 2D layer (Fig. 2) which is consolidated by the intrasheet weak face-to-face $\pi\cdots\pi$ interaction between bpy and TMIPA with Cg1 \cdots Cg2ⁱ separation of 3.725 (3) Å (Cg1 and Cg2 are the centroids of the N1/C1-C5 and C12-C17 rings, respectively; symmetry code: (i) -x+1, -y+1, -z+1). The bpy ligand acts as a terminal group to occupy the remaining coordinate sites, which prevents the structure from higher dimensionalities. The adjacent 2D layers are further extended to a 3D supramolecular framework by virtue of non-classical C-H \cdots O hydrogen bonds (Table 2).

Experimental

A mixture of Cd(NO₃)₂·6H₂O (30 mg, 0.12 mmol), 2,4,6-trimethylisophthalic acid (H₂TMIPA) (20 mg, 0.12 mmol) and bipyridine (10 mg, 0.06 mmol) was suspended in 15 mL mixed solvents of N,N'-dimethylformamide, ethanol and H₂O (*v/v* = 1:1:1), and heated in a Teflon-lined steel bomb at 373 K for 4 days. After cooling to room temperature, colorless crystals were collected, washed with ethanol several times, and dried in the air (yield: 47%, based on H₂TMIPA).

Refinement

H atoms were generated geometrically and were allowed to ride on their parent atoms in the riding model approximations with C—H = 0.93 (aromatic) and 0.96 Å (methyl), U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms and 1.5U_{eq}(C) for methyl H atoms.

Figures

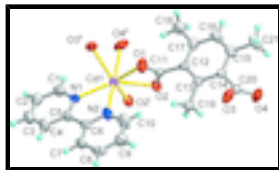


Fig. 1. The structure of (**I**), showing the atom-numbering scheme and the coordination environment around the Cd^{II} centre. Displacement ellipsoids are drawn at 50% probability level and H atoms are shown as small spheres of arbitrary radii. (symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+3/2, y+1/2, z$)

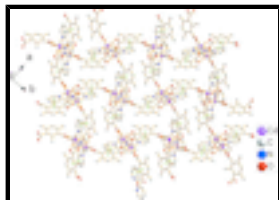


Fig. 2. A ball-and-stick perspective view of the 2D sheet incorporating weak face-to-face $\pi \cdots \pi$ interaction (green dashed lines). Hydrogen atoms are omitted for clarity.

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Crystal data

[Cd(C₁₁H₁₀O₄)(C₁₀H₈N₂)]

$M_r = 474.77$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 13.1985$ (8) Å

$b = 15.5714$ (9) Å

$c = 18.1926$ (11) Å

$V = 3738.9$ (4) Å³

$Z = 8$

$F(000) = 1904$

$D_x = 1.687$ Mg m⁻³

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

Cell parameters from 5089 reflections

$\theta = 2.2$ – 27.8°

$\mu = 1.20$ mm⁻¹

$T = 298$ K

Block, colorless

$0.15 \times 0.10 \times 0.10$ mm

Data collection

Bruker SMART APEXII CCD
diffractometer

4299 independent reflections

Radiation source: fine-focus sealed tube graphite	2454 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.054$
ω and φ scans	$\theta_{\text{max}} = 27.6^\circ$, $\theta_{\text{min}} = 2.2^\circ$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2001)	$h = -17 \rightarrow 11$
$T_{\text{min}} = 0.841$, $T_{\text{max}} = 0.890$	$k = -17 \rightarrow 20$
14349 measured reflections	$l = -15 \rightarrow 23$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.045$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.098$	H-atom parameters constrained
$S = 0.99$	$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2]$
4299 reflections	where $P = (F_o^2 + 2F_c^2)/3$
253 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.51 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.63 \text{ e } \text{\AA}^{-3}$

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.50573 (2)	0.584163 (18)	0.575068 (16)	0.03177 (11)
C1	0.3060 (4)	0.7000 (3)	0.6257 (3)	0.0496 (14)
H1A	0.3218	0.7291	0.5826	0.060*
C2	0.2259 (4)	0.7293 (3)	0.6667 (3)	0.0569 (15)
H2A	0.1873	0.7758	0.6512	0.068*
C3	0.2046 (4)	0.6877 (3)	0.7314 (3)	0.0634 (16)
H3A	0.1518	0.7064	0.7613	0.076*
C4	0.2620 (4)	0.6187 (3)	0.7511 (3)	0.0586 (15)
H4A	0.2489	0.5903	0.7951	0.070*
C5	0.3391 (3)	0.5909 (3)	0.7063 (2)	0.0385 (11)
C6	0.4024 (4)	0.5140 (3)	0.7238 (2)	0.0396 (11)

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C7	0.3857 (4)	0.4630 (3)	0.7852 (3)	0.0471 (13)
H7A	0.3346	0.4768	0.8183	0.057*
C8	0.4453 (4)	0.3916 (3)	0.7965 (3)	0.0541 (15)
H8A	0.4352	0.3573	0.8377	0.065*
C9	0.5189 (4)	0.3718 (3)	0.7472 (3)	0.0622 (16)
H9A	0.5590	0.3232	0.7533	0.075*
C10	0.5323 (5)	0.4249 (4)	0.6888 (3)	0.082 (2)
H10A	0.5835	0.4116	0.6555	0.098*
C11	0.6847 (3)	0.4899 (3)	0.5399 (2)	0.0311 (10)
C12	0.7761 (3)	0.4466 (3)	0.5081 (2)	0.0335 (11)
C13	0.8065 (3)	0.3639 (3)	0.5314 (2)	0.0344 (11)
C14	0.8932 (3)	0.3269 (3)	0.5012 (3)	0.0387 (12)
C15	0.9490 (4)	0.3712 (3)	0.4471 (3)	0.0581 (16)
C16	0.9164 (4)	0.4521 (3)	0.4247 (3)	0.0699 (18)
H16A	0.9529	0.4813	0.3888	0.084*
C17	0.8299 (4)	0.4907 (3)	0.4549 (3)	0.0543 (15)
C18	0.7974 (5)	0.5776 (3)	0.4262 (3)	0.078 (2)
H18A	0.7381	0.5964	0.4522	0.117*
H18B	0.7823	0.5733	0.3747	0.117*
H18C	0.8511	0.6183	0.4334	0.117*
C19	0.7417 (4)	0.3160 (3)	0.5853 (3)	0.0456 (13)
H19A	0.7717	0.2611	0.5955	0.068*
H19B	0.6753	0.3078	0.5648	0.068*
H19C	0.7365	0.3483	0.6301	0.068*
C20	0.9284 (3)	0.2395 (3)	0.5264 (3)	0.0417 (12)
C21	1.0421 (5)	0.3344 (4)	0.4112 (4)	0.097 (3)
H21A	1.0683	0.3748	0.3761	0.146*
H21B	1.0249	0.2819	0.3866	0.146*
H21C	1.0926	0.3232	0.4479	0.146*
N1	0.3624 (3)	0.6324 (2)	0.64418 (19)	0.0367 (9)
N2	0.4764 (3)	0.4950 (3)	0.6760 (2)	0.0532 (12)
O1	0.6951 (3)	0.5405 (2)	0.59115 (17)	0.0536 (9)
O2	0.5988 (2)	0.47532 (18)	0.51372 (16)	0.0412 (8)
O3	0.9433 (3)	0.2269 (2)	0.5937 (2)	0.0580 (10)
O4	0.9409 (3)	0.18136 (19)	0.48063 (19)	0.0618 (11)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0381 (2)	0.02748 (17)	0.02972 (17)	-0.00141 (17)	0.00347 (18)	-0.00099 (13)
C1	0.059 (4)	0.047 (3)	0.043 (3)	0.003 (3)	0.007 (3)	0.009 (2)
C2	0.056 (4)	0.048 (3)	0.067 (4)	0.008 (3)	0.011 (3)	0.005 (3)
C3	0.061 (4)	0.063 (4)	0.066 (4)	0.016 (3)	0.021 (3)	0.002 (3)
C4	0.063 (4)	0.059 (3)	0.054 (3)	0.017 (3)	0.019 (3)	0.017 (3)
C5	0.040 (3)	0.041 (3)	0.035 (3)	-0.001 (3)	0.006 (2)	-0.001 (2)
C6	0.044 (3)	0.038 (3)	0.038 (3)	-0.001 (2)	0.002 (2)	0.002 (2)
C7	0.051 (3)	0.047 (3)	0.044 (3)	0.004 (3)	0.015 (3)	0.011 (2)
C8	0.060 (4)	0.047 (3)	0.054 (4)	-0.011 (3)	0.002 (3)	0.021 (3)

C9	0.068 (4)	0.048 (3)	0.070 (4)	0.019 (3)	0.009 (3)	0.022 (3)
C10	0.098 (5)	0.065 (4)	0.082 (5)	0.040 (4)	0.044 (4)	0.033 (3)
C11	0.029 (3)	0.026 (2)	0.038 (3)	0.004 (2)	0.002 (2)	0.007 (2)
C12	0.033 (3)	0.027 (2)	0.040 (3)	0.000 (2)	-0.003 (2)	0.005 (2)
C13	0.025 (3)	0.031 (2)	0.047 (3)	-0.004 (2)	-0.006 (2)	0.001 (2)
C14	0.026 (3)	0.030 (2)	0.061 (3)	0.003 (2)	0.003 (2)	0.001 (2)
C15	0.041 (3)	0.044 (3)	0.089 (4)	0.010 (3)	0.021 (3)	0.010 (3)
C16	0.055 (4)	0.048 (3)	0.106 (5)	0.014 (3)	0.040 (4)	0.034 (3)
C17	0.045 (3)	0.039 (3)	0.079 (4)	0.014 (3)	0.015 (3)	0.009 (3)
C18	0.084 (5)	0.049 (3)	0.102 (5)	0.020 (3)	0.036 (4)	0.029 (3)
C19	0.035 (3)	0.038 (3)	0.064 (3)	0.000 (2)	0.000 (3)	0.008 (2)
C20	0.034 (3)	0.027 (3)	0.064 (4)	0.002 (2)	-0.002 (3)	0.004 (3)
C21	0.069 (4)	0.071 (4)	0.152 (7)	0.034 (4)	0.063 (5)	0.032 (4)
N1	0.044 (3)	0.030 (2)	0.036 (2)	-0.002 (2)	0.0083 (19)	0.0022 (17)
N2	0.065 (3)	0.046 (2)	0.048 (3)	0.019 (2)	0.022 (2)	0.016 (2)
O1	0.049 (2)	0.061 (2)	0.051 (2)	0.0074 (19)	-0.0078 (18)	-0.0182 (18)
O2	0.0239 (18)	0.0478 (19)	0.052 (2)	0.0033 (16)	-0.0045 (16)	-0.0085 (15)
O3	0.072 (3)	0.038 (2)	0.064 (3)	0.0192 (19)	-0.023 (2)	-0.0055 (17)
O4	0.092 (3)	0.0328 (19)	0.061 (2)	0.017 (2)	0.010 (2)	-0.0006 (17)

Geometric parameters (Å, °)

Cd1—N1	2.393 (4)	C11—O2	1.250 (5)
Cd1—N2	2.334 (4)	C11—C12	1.499 (6)
Cd1—O1	2.607 (3)	C12—C17	1.382 (6)
Cd1—O2 ⁱ	2.317 (3)	C12—C13	1.414 (5)
Cd1—O2	2.372 (3)	C13—C14	1.394 (6)
Cd1—O3 ⁱⁱ	2.347 (3)	C13—C19	1.500 (6)
Cd1—O4 ⁱⁱ	2.396 (3)	C14—C15	1.409 (6)
C1—N1	1.333 (5)	C14—C20	1.510 (6)
C1—C2	1.371 (6)	C15—C16	1.392 (7)
C1—H1A	0.9300	C15—C21	1.505 (7)
C2—C3	1.372 (6)	C16—C17	1.402 (7)
C2—H2A	0.9300	C16—H16A	0.9300
C3—C4	1.363 (7)	C17—C18	1.514 (6)
C3—H3A	0.9300	C18—H18A	0.9600
C4—C5	1.374 (6)	C18—H18B	0.9600
C4—H4A	0.9300	C18—H18C	0.9600
C5—N1	1.338 (5)	C19—H19A	0.9600
C5—C6	1.494 (6)	C19—H19B	0.9600
C6—N2	1.341 (5)	C19—H19C	0.9600
C6—C7	1.388 (6)	C20—O4	1.241 (5)
C7—C8	1.377 (6)	C20—O3	1.255 (5)
C7—H7A	0.9300	C20—Cd1 ⁱⁱⁱ	2.718 (4)
C8—C9	1.357 (7)	C21—H21A	0.9600
C8—H8A	0.9300	C21—H21B	0.9600
C9—C10	1.359 (7)	C21—H21C	0.9600
C9—H9A	0.9300	O2—Cd1 ⁱ	2.317 (3)

supplementary materials

C10—N2	1.339 (6)	O3—Cd1 ⁱⁱⁱ	2.347 (3)
C10—H10A	0.9300	O4—Cd1 ⁱⁱⁱ	2.396 (3)
C11—O1	1.228 (5)		
O2 ⁱ —Cd1—N2	102.23 (14)	O1—C11—O2	120.5 (4)
O2 ⁱ —Cd1—O3 ⁱⁱ	130.54 (12)	O1—C11—C12	119.5 (4)
N2—Cd1—O3 ⁱⁱ	119.81 (14)	O2—C11—C12	120.0 (4)
O2 ⁱ —Cd1—O2	72.22 (12)	C17—C12—C13	121.1 (4)
N2—Cd1—O2	91.79 (12)	C17—C12—C11	117.4 (4)
O3 ⁱⁱ —Cd1—O2	126.60 (12)	C13—C12—C11	121.5 (4)
O2 ⁱ —Cd1—N1	91.21 (11)	C14—C13—C12	119.4 (4)
N2—Cd1—N1	69.02 (13)	C14—C13—C19	121.4 (4)
O3 ⁱⁱ —Cd1—N1	81.58 (12)	C12—C13—C19	119.1 (4)
O2—Cd1—N1	151.76 (11)	C13—C14—C15	120.2 (4)
O2 ⁱ —Cd1—O4 ⁱⁱ	85.85 (11)	C13—C14—C20	120.3 (4)
N2—Cd1—O4 ⁱⁱ	171.39 (14)	C15—C14—C20	119.5 (4)
O3 ⁱⁱ —Cd1—O4 ⁱⁱ	54.62 (11)	C16—C15—C14	119.0 (5)
O2—Cd1—O4 ⁱⁱ	87.81 (12)	C16—C15—C21	118.0 (5)
N1—Cd1—O4 ⁱⁱ	114.27 (12)	C14—C15—C21	123.0 (5)
O2 ⁱ —Cd1—O1	123.00 (10)	C15—C16—C17	121.6 (5)
N2—Cd1—O1	85.17 (13)	C15—C16—H16A	119.2
O3 ⁱⁱ —Cd1—O1	87.47 (12)	C17—C16—H16A	119.2
O2—Cd1—O1	50.95 (10)	C12—C17—C16	118.7 (4)
N1—Cd1—O1	141.36 (11)	C12—C17—C18	122.7 (4)
O4 ⁱⁱ —Cd1—O1	87.91 (12)	C16—C17—C18	118.6 (5)
O2 ⁱ —Cd1—C20 ⁱⁱ	108.60 (14)	C17—C18—H18A	109.5
N2—Cd1—C20 ⁱⁱ	146.97 (16)	C17—C18—H18B	109.5
O3 ⁱⁱ —Cd1—C20 ⁱⁱ	27.47 (12)	H18A—C18—H18B	109.5
O2—Cd1—C20 ⁱⁱ	108.48 (13)	C17—C18—H18C	109.5
N1—Cd1—C20 ⁱⁱ	98.32 (13)	H18A—C18—H18C	109.5
O4 ⁱⁱ —Cd1—C20 ⁱⁱ	27.16 (12)	H18B—C18—H18C	109.5
O1—Cd1—C20 ⁱⁱ	87.82 (12)	C13—C19—H19A	109.5
N1—C1—C2	123.8 (4)	C13—C19—H19B	109.5
N1—C1—H1A	118.1	H19A—C19—H19B	109.5
C2—C1—H1A	118.1	C13—C19—H19C	109.5
C1—C2—C3	117.9 (5)	H19A—C19—H19C	109.5
C1—C2—H2A	121.1	H19B—C19—H19C	109.5
C3—C2—H2A	121.1	O4—C20—O3	121.3 (4)
C4—C3—C2	118.9 (5)	O4—C20—C14	119.6 (5)
C4—C3—H3A	120.5	O3—C20—C14	119.0 (4)
C2—C3—H3A	120.5	O4—C20—Cd1 ⁱⁱⁱ	61.8 (2)
C3—C4—C5	120.3 (5)	O3—C20—Cd1 ⁱⁱⁱ	59.6 (2)
C3—C4—H4A	119.9	C14—C20—Cd1 ⁱⁱⁱ	178.4 (4)
C5—C4—H4A	119.9	C15—C21—H21A	109.5

N1—C5—C4	121.2 (4)	C15—C21—H21B	109.5
N1—C5—C6	116.1 (4)	H21A—C21—H21B	109.5
C4—C5—C6	122.7 (4)	C15—C21—H21C	109.5
N2—C6—C7	120.8 (4)	H21A—C21—H21C	109.5
N2—C6—C5	116.4 (4)	H21B—C21—H21C	109.5
C7—C6—C5	122.8 (4)	C1—N1—C5	117.8 (4)
C8—C7—C6	119.4 (5)	C1—N1—Cd1	123.9 (3)
C8—C7—H7A	120.3	C5—N1—Cd1	118.3 (3)
C6—C7—H7A	120.3	C10—N2—C6	117.9 (4)
C9—C8—C7	119.6 (5)	C10—N2—Cd1	122.0 (3)
C9—C8—H8A	120.2	C6—N2—Cd1	120.0 (3)
C7—C8—H8A	120.2	C11—O1—Cd1	88.5 (3)
C10—C9—C8	118.1 (5)	C11—O2—Cd1 ⁱ	151.4 (3)
C10—C9—H9A	120.9	C11—O2—Cd1	99.2 (3)
C8—C9—H9A	120.9	Cd1 ⁱ —O2—Cd1	107.78 (12)
N2—C10—C9	124.1 (5)	C20—O3—Cd1 ⁱⁱⁱ	93.0 (3)
N2—C10—H10A	118.0	C20—O4—Cd1 ⁱⁱⁱ	91.1 (3)
C9—C10—H10A	118.0		

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

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>
C4—H4A \cdots O1 ^{iv}	0.93	2.32	3.240 (6)	169
C8—H8A \cdots O3 ^{iv}	0.93	2.39	3.251 (6)	155

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

Fig. 1

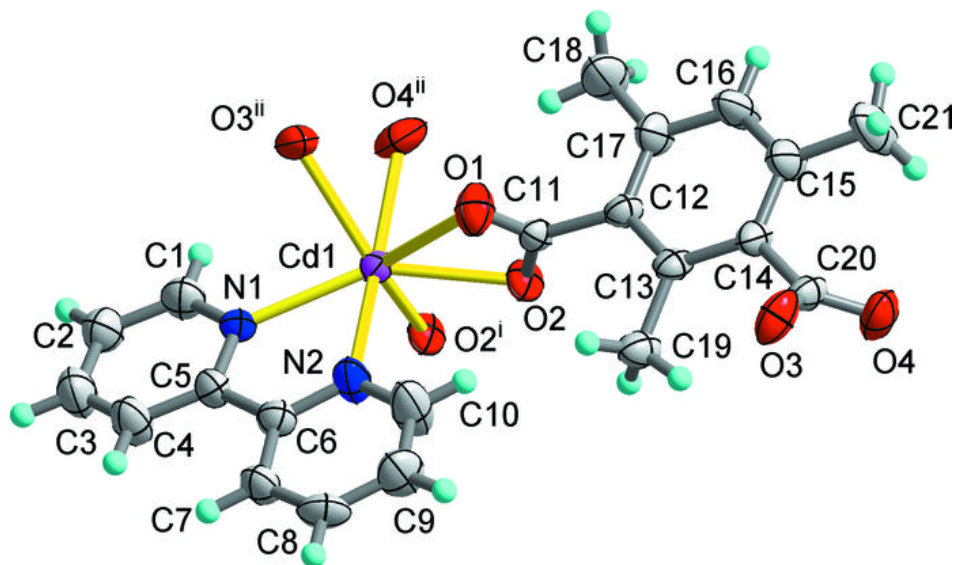


Fig. 2

