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Poly[[[(2,2′-bipyridine)cadmium(II)]-μ_3-pyridine-2,4-dicarboxylato] monohydrate]

Xiu-Mei Li,[a]* Qing-Wei Wang[b] and Bo Liu[b]

[a]Department of Chemistry, Tonghua Teachers' College, Tonghua 134002, People's Republic of China, and [b]Department of Chemistry, Jilin Normal University, Siping 136000, People's Republic of China
Correspondence e-mail: lixm20032006@163.com

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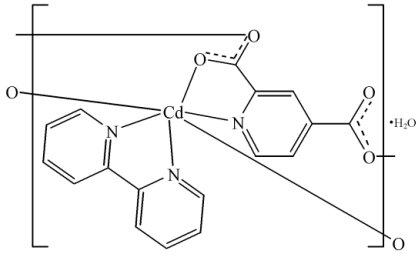
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; R factor = 0.023; wR factor = 0.061; data-to-parameter ratio = 13.7.

In the title compound, $\{[Cd(C_7H_3NO_4)(C_{10}H_8N_2)]\cdot H_2O\}_n$, each Cd^{II} atom is octahedrally coordinated by one *N*,*N*-bidentate 2,2′-bipyridine (bpy) molecule and three pyridine-2,4-dicarboxylate ($pydc^{2-}$) dianions (one *N*,*O*-bidentate and two *O*-monodentate). The pydc species serve as bridges in a layered polymeric network. The crystal structure features π–π stacking interactions between the bpy molecules [closest atomic separation = 3.721 (4) Å] and probable O—H···O hydrogen bonds between the solvent water molecule and the uncoordinated carboxylate O atoms of the $pydc^{2-}$ dianions.

Related literature

For related literature, see: Gu *et al.* (2004); Wang *et al.* (2004); Zhang & Chen (2003).



Experimental

Crystal data

$[Cd(C_7H_3NO_4)(C_{10}H_8N_2)]\cdot H_2O$
M_r = 451.70
Monoclinic, $P2_1/c$
a = 12.0969 (6) Å
b = 14.4457 (7) Å
c = 10.1629 (5) Å
β = 111.045 (1)°
V = 1657.49 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.35 mm^{-1}
T = 292 (2) K
0.43 × 0.33 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.591, T_{max} = 0.731
13935 measured reflections
3249 independent reflections
2842 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.061
S = 1.04
3249 reflections
237 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O2	2.2742 (16)	Cd1—N1	2.3446 (18)
Cd1—N3^{i}	2.3030 (17)	Cd1—N2	2.346 (2)
Cd1—O4^{ii}	2.3042 (14)	Cd1—O3^{i}	2.4125 (15)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O1	0.81	2.06	2.783 (4)	149
O5—H2W···O2^{iii}	1.06	2.38	3.308 (4)	145
O5—H2W···O1^{iii}	1.06	2.57	3.333 (4)	129

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: HB2513).

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supplementary materials

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Poly[[[(2,2'-bipyridine)cadmium(II)]-μ_3-pyridine-2,4-dicarboxylato] monohydrate]

X.-M. Li, Q.-W. Wang and B. Liu

Comment

In the title compound, (I), each Cd^{II} atom is six-coordinated in an octahedral geometry (Table 1) by two N atom from the 2,2'-bipyridine (bpy) ligand, and one N atom and three O atoms from three pyridine-2,4-dicarboxylate ($pydc^{2-}$) dianions (one N,*O*-bidentate, two O-monodentate) (Fig. 1). The bridging $pydc^{2-}$ species result in a layered, polymeric network propagating in (100). Aromatic π–π interactions between the bpy molecules, with a shortest atom-to-atom distance of 3.721 (4) Å, and probable O—H···O hydrogen bonds (Fig. 2 and Table 2) complete the structure.

For related structures, see: Gu *et al.* (2004); Wang *et al.* (2004); Zhang & Chen (2003).

Experimental

A mixture of $Cd(NO_3)_2{\cdot}4H_2O$ (0.150 g, 0.5 mmol), H_2pydc (0.167 g, 1.0 mmol), bpy (0.156 g, 1.0 mmol) and H_2O (18 ml) in a 30 ml Teflon-lined autoclave were heated under autogenous pressure at 413 K for five days. After cooling to room temperature, colorless blocks of (I) were obtained. Elemental analysis calculated for $C_{17}H_{13}N_3O_5Cd$: C 45.2, H 2.9, N 9.3%; found: C 45.0, H 2.8, N 9.2%.

Refinement

All the C-bound H atoms were generated geometrically (C—H = 0.93 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of the water molecule were located in a difference Fourier map and refined as riding in their as-found relative positions with free refinement of U_{iso}. The water H-atom positions reported here should be regarded as tentative.

Figures

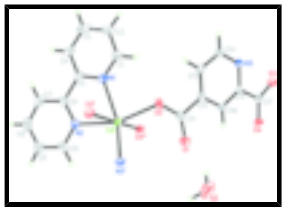

Fig. 1. The asymmetric unit of (I), expanded to show the Cd coordination, with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms). Symmetry codes: (i) −*x*, 1/2 + *y*, 3/2 − *z*; (ii) −*x*, −*y*, 1 − *z*.

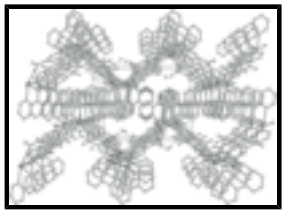

Fig. 2. The packing for (I), viewed along the *c* axis. Dashed lines indicate hydrogen bonds.

Poly[[[(2,2'-bipyridine)cadmium(II)]-μ$_3$-pyridine-2,4-dicarboxylato] monohydrate]

Crystal data

$[Cd(C_7H_3NO_4)(C_{10}H_8N_2)]\cdot H_2O$	$F_{000} = 896$
$M_r = 451.70$	$D_x = 1.810$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3238 reflections
$a = 12.0969$ (6) Å	$\theta = 2.3$–26.0º
$b = 14.4457$ (7) Å	$\mu = 1.35$ mm^{-1}
$c = 10.1629$ (5) Å	$T = 292$ (2) K
$\beta = 111.045$ (1)º	Block, colourless
$V = 1657.49$ (14) Å^3	0.43 × 0.33 × 0.23 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3249 independent reflections
Radiation source: fine-focus sealed tube	2842 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.060$
$T = 292$(2) K	$\theta_{max} = 26.0$º
ω scans	$\theta_{min} = 2.3$º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -14\rightarrow14$
$T_{min} = 0.591$, $T_{max} = 0.731$	$k = -17\rightarrow17$
13935 measured reflections	$l = -12\rightarrow12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)] = 0.023$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.061$	$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
3249 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
237 parameters	$\Delta\rho_{min} = -0.72$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.244494 (14)	0.182255 (10)	0.898812 (16)	0.02916 (8)
C14	−0.0973 (2)	−0.14669 (16)	0.7861 (2)	0.0343 (5)
H14A	−0.0901	−0.1872	0.8599	0.041*
C4	0.5261 (3)	0.00825 (19)	1.2185 (3)	0.0503 (7)
H4A	0.6083	0.0115	1.2572	0.060*
C10	0.4989 (3)	0.27229 (19)	0.9184 (3)	0.0485 (7)
H10A	0.4496	0.3112	0.8492	0.058*
O2	0.07129 (15)	0.10789 (11)	0.86810 (16)	0.0410 (4)
N3	−0.16050 (18)	−0.17299 (11)	0.65473 (19)	0.0296 (4)
N2	0.44967 (18)	0.20406 (14)	0.9674 (2)	0.0361 (4)
N1	0.34439 (18)	0.06681 (13)	1.05976 (19)	0.0362 (5)
C15	−0.16857 (18)	−0.11471 (14)	0.5488 (2)	0.0262 (4)
O1	−0.0301 (2)	0.15522 (13)	0.6491 (2)	0.0621 (6)
C9	0.6189 (3)	0.2877 (2)	0.9654 (3)	0.0604 (8)
H9A	0.6498	0.3359	0.9286	0.072*
C5	0.4627 (2)	0.07151 (16)	1.1180 (2)	0.0338 (5)
C12	−0.05572 (19)	0.00095 (14)	0.7100 (2)	0.0286 (5)
C2	0.3452 (3)	−0.0643 (2)	1.2019 (3)	0.0607 (8)
H2A	0.3030	−0.1094	1.2294	0.073*
C16	−0.11956 (19)	−0.02688 (15)	0.5725 (2)	0.0294 (5)
H16A	−0.1292	0.0130	0.4974	0.035*
C13	−0.0424 (2)	−0.06178 (15)	0.8165 (2)	0.0334 (5)
H13A	0.0036	−0.0468	0.9090	0.040*
C6	0.5212 (2)	0.14681 (17)	1.0671 (2)	0.0354 (5)
C11	−0.0009 (2)	0.09652 (16)	0.7424 (2)	0.0358 (5)
C1	0.2879 (3)	0.00001 (19)	1.1009 (3)	0.0474 (6)
H1A	0.2058	−0.0032	1.0593	0.057*
C7	0.6434 (3)	0.1597 (2)	1.1185 (3)	0.0546 (7)
H7A	0.6921	0.1202	1.1874	0.066*
C3	0.4659 (3)	−0.0600 (2)	1.2609 (3)	0.0645 (9)
H3A	0.5073	−0.1028	1.3291	0.077*
C8	0.6921 (3)	0.2310 (3)	1.0671 (3)	0.0645 (9)
H8A	0.7736	0.2404	1.1013	0.077*

O3	−0.26657 (15)	−0.23395 (12)	0.38788 (15)	0.0384 (4)
C17	−0.22854 (19)	−0.15273 (16)	0.4008 (2)	0.0282 (5)
O4	−0.23259 (15)	−0.10070 (10)	0.30068 (15)	0.0363 (4)
O5	−0.1177 (3)	0.2292 (3)	0.3783 (3)	0.1224 (12)
H1W	−0.1044	0.1901	0.4386	0.088 (15)*
H2W	−0.0417	0.2560	0.3627	0.23 (3)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03122 (11)	0.02280 (10)	0.02797 (11)	0.00096 (6)	0.00396 (8)	0.00026 (6)
C14	0.0464 (14)	0.0303 (11)	0.0239 (11)	−0.0063 (11)	0.0099 (10)	0.0006 (9)
C4	0.0481 (16)	0.0513 (16)	0.0446 (15)	0.0176 (13)	0.0083 (13)	0.0086 (12)
C10	0.0527 (17)	0.0474 (16)	0.0425 (14)	−0.0086 (13)	0.0137 (13)	0.0044 (12)
O2	0.0447 (10)	0.0408 (10)	0.0343 (9)	−0.0184 (8)	0.0104 (8)	−0.0086 (7)
N3	0.0367 (11)	0.0245 (9)	0.0250 (9)	−0.0024 (8)	0.0081 (9)	−0.0014 (7)
N2	0.0361 (11)	0.0383 (11)	0.0307 (10)	−0.0022 (9)	0.0079 (9)	−0.0018 (9)
N1	0.0407 (12)	0.0317 (11)	0.0358 (10)	0.0073 (9)	0.0131 (9)	0.0051 (8)
C15	0.0253 (11)	0.0279 (11)	0.0241 (10)	0.0024 (9)	0.0073 (9)	0.0005 (8)
O1	0.0675 (14)	0.0331 (10)	0.0621 (13)	−0.0128 (10)	−0.0054 (11)	0.0116 (9)
C9	0.0538 (19)	0.078 (2)	0.0511 (17)	−0.0243 (17)	0.0214 (16)	−0.0022 (16)
C5	0.0372 (13)	0.0360 (13)	0.0264 (11)	0.0118 (10)	0.0094 (10)	−0.0012 (9)
C12	0.0287 (11)	0.0256 (11)	0.0315 (11)	−0.0033 (9)	0.0110 (10)	−0.0045 (9)
C2	0.071 (2)	0.0491 (17)	0.0670 (19)	0.0080 (15)	0.0302 (17)	0.0243 (14)
C16	0.0313 (12)	0.0271 (11)	0.0291 (11)	−0.0004 (9)	0.0100 (10)	0.0011 (9)
C13	0.0413 (13)	0.0340 (12)	0.0233 (10)	−0.0068 (10)	0.0096 (10)	−0.0058 (9)
C6	0.0350 (13)	0.0419 (13)	0.0271 (11)	0.0042 (11)	0.0086 (10)	−0.0054 (10)
C11	0.0358 (13)	0.0285 (12)	0.0432 (14)	−0.0055 (10)	0.0143 (11)	−0.0033 (10)
C1	0.0473 (15)	0.0411 (15)	0.0562 (16)	0.0039 (12)	0.0217 (13)	0.0124 (12)
C7	0.0381 (15)	0.082 (2)	0.0386 (15)	0.0047 (15)	0.0078 (13)	0.0008 (14)
C3	0.077 (2)	0.0557 (19)	0.0583 (19)	0.0268 (16)	0.0206 (17)	0.0266 (15)
C8	0.0436 (17)	0.099 (3)	0.0504 (17)	−0.0219 (18)	0.0163 (15)	−0.0099 (18)
O3	0.0495 (11)	0.0301 (9)	0.0281 (8)	−0.0037 (7)	0.0049 (8)	−0.0044 (6)
C17	0.0250 (11)	0.0291 (12)	0.0285 (11)	0.0052 (9)	0.0072 (9)	−0.0023 (9)
O4	0.0456 (10)	0.0368 (9)	0.0232 (7)	−0.0004 (7)	0.0084 (7)	0.0026 (7)
O5	0.0634 (18)	0.224 (4)	0.0726 (18)	−0.003 (2)	0.0149 (15)	0.053 (2)

Geometric parameters (Å, °)

Cd1—O2	2.2742 (16)	C9—C8	1.366 (5)
Cd1—N3^{i}	2.3030 (17)	C9—H9A	0.9300
Cd1—O4^{ii}	2.3042 (14)	C5—C6	1.488 (3)
Cd1—N1	2.3446 (18)	C12—C13	1.376 (3)
Cd1—N2	2.346 (2)	C12—C16	1.391 (3)
Cd1—O3^{i}	2.4125 (15)	C12—C11	1.516 (3)
C14—N3	1.333 (3)	C2—C3	1.366 (4)
C14—C13	1.376 (3)	C2—C1	1.373 (4)
C14—H14A	0.9300	C2—H2A	0.9300

C4—C5	1.379 (3)	C16—H16A	0.9300
C4—C3	1.384 (4)	C13—H13A	0.9300
C4—H4A	0.9300	C6—C7	1.392 (4)
C10—N2	1.337 (3)	C1—H1A	0.9300
C10—C9	1.374 (4)	C7—C8	1.379 (4)
C10—H10A	0.9300	C7—H7A	0.9300
O2—C11	1.273 (3)	C3—H3A	0.9300
N3—C15	1.342 (3)	C8—H8A	0.9300
N3—Cd1^{iii}	2.3030 (17)	O3—C17	1.250 (3)
N2—C6	1.353 (3)	O3—Cd1^{iii}	2.4125 (15)
N1—C1	1.334 (3)	C17—O4	1.252 (3)
N1—C5	1.340 (3)	O4—Cd1^{ii}	2.3042 (14)
C15—C16	1.384 (3)	O5—H1W	0.8068
C15—C17	1.519 (3)	O5—H2W	1.0603
O1—C11	1.226 (3)		
O2—Cd1—N3^{i}	95.16 (7)	N1—C5—C4	121.0 (2)
O2—Cd1—O4^{ii}	82.78 (6)	N1—C5—C6	116.69 (19)
N3^{i}—Cd1—O4^{ii}	111.93 (6)	C4—C5—C6	122.3 (2)
O2—Cd1—N1	88.76 (7)	C13—C12—C16	117.74 (19)
N3^{i}—Cd1—N1	152.10 (6)	C13—C12—C11	120.72 (19)
O4^{ii}—Cd1—N1	95.96 (6)	C16—C12—C11	121.54 (19)
O2—Cd1—N2	158.22 (7)	C3—C2—C1	118.0 (3)
N3^{i}—Cd1—N2	106.15 (7)	C3—C2—H2A	121.0
O4^{ii}—Cd1—N2	93.16 (6)	C1—C2—H2A	121.0
N1—Cd1—N2	70.31 (7)	C15—C16—C12	119.22 (19)
O2—Cd1—O3^{i}	99.18 (6)	C15—C16—H16A	120.4
N3^{i}—Cd1—O3^{i}	69.74 (6)	C12—C16—H16A	120.4
O4^{ii}—Cd1—O3^{i}	177.36 (6)	C12—C13—C14	120.0 (2)
N1—Cd1—O3^{i}	82.36 (6)	C12—C13—H13A	120.0
N2—Cd1—O3^{i}	84.37 (6)	C14—C13—H13A	120.0
N3—C14—C13	122.4 (2)	N2—C6—C7	120.5 (2)
N3—C14—H14A	118.8	N2—C6—C5	116.8 (2)
C13—C14—H14A	118.8	C7—C6—C5	122.7 (2)
C5—C4—C3	119.2 (3)	O1—C11—O2	126.2 (2)
C5—C4—H4A	120.4	O1—C11—C12	118.7 (2)
C3—C4—H4A	120.4	O2—C11—C12	115.1 (2)
N2—C10—C9	123.1 (3)	N1—C1—C2	123.1 (3)
N2—C10—H10A	118.4	N1—C1—H1A	118.5
C9—C10—H10A	118.4	C2—C1—H1A	118.5
C11—O2—Cd1	117.70 (14)	C8—C7—C6	119.9 (3)
C14—N3—C15	118.34 (18)	C8—C7—H7A	120.1
C14—N3—Cd1^{iii}	122.74 (14)	C6—C7—H7A	120.1
C15—N3—Cd1^{iii}	118.76 (13)	C2—C3—C4	119.7 (3)
C10—N2—C6	118.6 (2)	C2—C3—H3A	120.2
C10—N2—Cd1	123.63 (17)	C4—C3—H3A	120.2

C6—N2—Cd1	117.67 (16)	C9—C8—C7	119.1 (3)
C1—N1—C5	119.0 (2)	C9—C8—H8A	120.5
C1—N1—Cd1	122.66 (17)	C7—C8—H8A	120.5
C5—N1—Cd1	118.26 (15)	C17—O3—Cd1^{iii}	117.30 (12)
N3—C15—C16	122.14 (18)	O3—C17—O4	124.93 (19)
N3—C15—C17	116.02 (18)	O3—C17—C15	118.07 (18)
C16—C15—C17	121.75 (18)	O4—C17—C15	117.0 (2)
C8—C9—C10	118.9 (3)	C17—O4—Cd1^{ii}	112.35 (14)
C8—C9—H9A	120.6	H1W—O5—H2W	115.0
C10—C9—H9A	120.6		
N3^{i}—Cd1—O2—C11	73.72 (17)	C3—C4—C5—C6	−179.9 (2)
O4^{ii}—Cd1—O2—C11	−37.78 (17)	N3—C15—C16—C12	2.6 (3)
N1—Cd1—O2—C11	−133.95 (17)	C17—C15—C16—C12	−173.8 (2)
N2—Cd1—O2—C11	−118.2 (2)	C13—C12—C16—C15	1.3 (3)
O3^{i}—Cd1—O2—C11	144.00 (17)	C11—C12—C16—C15	−179.5 (2)
C13—C14—N3—C15	1.2 (3)	C16—C12—C13—C14	−3.8 (3)
C13—C14—N3—Cd1^{iii}	176.65 (18)	C11—C12—C13—C14	177.0 (2)
C9—C10—N2—C6	−0.6 (4)	N3—C14—C13—C12	2.7 (4)
C9—C10—N2—Cd1	176.1 (2)	C10—N2—C6—C7	0.8 (3)
O2—Cd1—N2—C10	162.49 (18)	Cd1—N2—C6—C7	−176.09 (18)
N3^{i}—Cd1—N2—C10	−29.8 (2)	C10—N2—C6—C5	−179.7 (2)
O4^{ii}—Cd1—N2—C10	84.1 (2)	Cd1—N2—C6—C5	3.5 (3)
N1—Cd1—N2—C10	179.3 (2)	N1—C5—C6—N2	0.4 (3)
O3^{i}—Cd1—N2—C10	−96.8 (2)	C4—C5—C6—N2	179.4 (2)
O2—Cd1—N2—C6	−20.8 (3)	N1—C5—C6—C7	180.0 (2)
N3^{i}—Cd1—N2—C6	146.84 (16)	C4—C5—C6—C7	−1.0 (4)
O4^{ii}—Cd1—N2—C6	−99.25 (16)	Cd1—O2—C11—O1	−45.6 (3)
N1—Cd1—N2—C6	−4.04 (15)	Cd1—O2—C11—C12	135.58 (16)
O3^{i}—Cd1—N2—C6	79.84 (16)	C13—C12—C11—O1	−168.4 (2)
O2—Cd1—N1—C1	−5.54 (19)	C16—C12—C11—O1	12.5 (3)
N3^{i}—Cd1—N1—C1	93.2 (2)	C13—C12—C11—O2	10.5 (3)
O4^{ii}—Cd1—N1—C1	−88.15 (19)	C16—C12—C11—O2	−168.6 (2)
N2—Cd1—N1—C1	−179.4 (2)	C5—N1—C1—C2	0.6 (4)
O3^{i}—Cd1—N1—C1	93.90 (19)	Cd1—N1—C1—C2	−175.6 (2)
O2—Cd1—N1—C5	178.17 (15)	C3—C2—C1—N1	−1.1 (4)
N3^{i}—Cd1—N1—C5	−83.1 (2)	N2—C6—C7—C8	−0.3 (4)
O4^{ii}—Cd1—N1—C5	95.56 (15)	C5—C6—C7—C8	−179.8 (2)
N2—Cd1—N1—C5	4.33 (15)	C1—C2—C3—C4	0.4 (5)
O3^{i}—Cd1—N1—C5	−82.39 (15)	C5—C4—C3—C2	0.6 (4)
C14—N3—C15—C16	−3.9 (3)	C10—C9—C8—C7	0.6 (5)
Cd1^{iii}—N3—C15—C16	−179.49 (16)	C6—C7—C8—C9	−0.4 (5)
C14—N3—C15—C17	172.7 (2)	Cd1^{iii}—O3—C17—O4	179.41 (17)
Cd1^{iii}—N3—C15—C17	−2.9 (2)	Cd1^{iii}—O3—C17—C15	1.8 (3)
N2—C10—C9—C8	−0.1 (5)	N3—C15—C17—O3	0.6 (3)

C1—N1—C5—C4	0.4 (3)	C16—C15—C17—O3	177.2 (2)
Cd1—N1—C5—C4	176.85 (18)	N3—C15—C17—O4	−177.16 (19)
C1—N1—C5—C6	179.4 (2)	C16—C15—C17—O4	−0.5 (3)
Cd1—N1—C5—C6	−4.2 (2)	O3—C17—O4—Cd1^{ii}	−23.7 (3)
C3—C4—C5—N1	−1.0 (4)	C15—C17—O4—Cd1^{ii}	153.94 (14)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1W···O1	0.81	2.06	2.783 (4)	149
O5—H2W···O2^{iv}	1.06	2.38	3.308 (4)	145
O5—H2W···O1^{iv}	1.06	2.57	3.333 (4)	129

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

Fig. 1

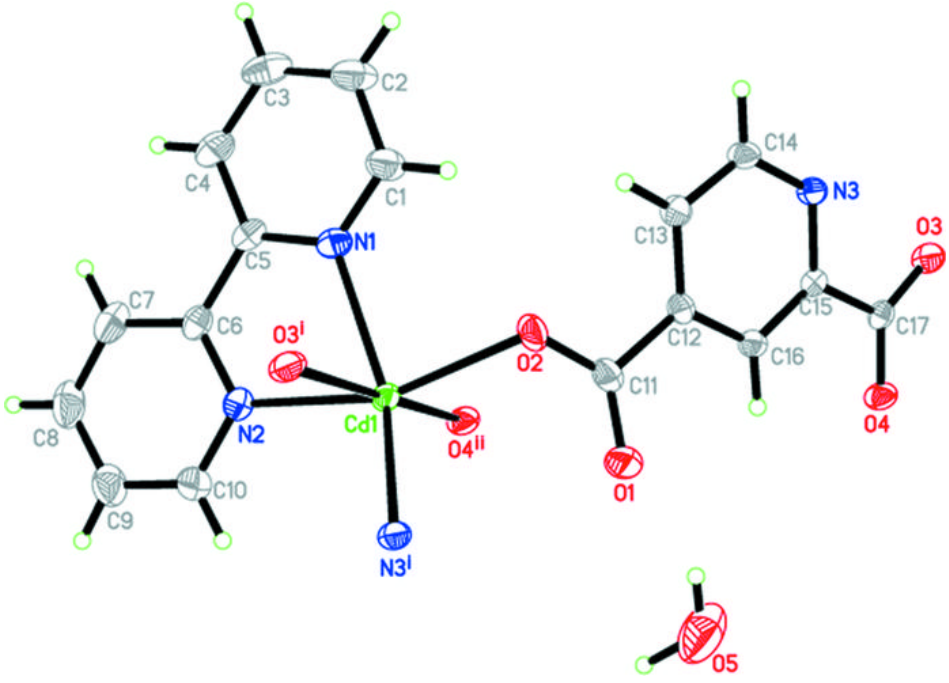
C3
C2
C4
C1
C5
N1
C7
C6
O3I
O2
C14
N3
C13
O3
C15
C17
C12
C16
C11
O4
C8
N2
Cd1
O4II
O1
C10
C9
N3I
O5

Fig. 2