Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[diaqua(2,2′-bipyridine-κ^2N,N')cadmium(II)]-μ-phthalato-$\kappa^2O:O'$]

Xiao-Yan Wang,[a,b] Chen-Chen Dong,[a] Xiao-Tao Deng,[a,c] Cheng-Gang Wang[a]* and Bo Hu[a]

[a]Department of Chemistry, Central China Normal University, Wuhan, Hubei 430079, People's Republic of China, [b]Biology Department, West Anhui University, Liu an, Anhui 237000, People's Republic of China, and [c]Guang Zhou No. 6 Middle School, Guangzhou, Guangdong 510300, People's Republic of China
Correspondence e-mail: wangcg23@yahoo.com.cn

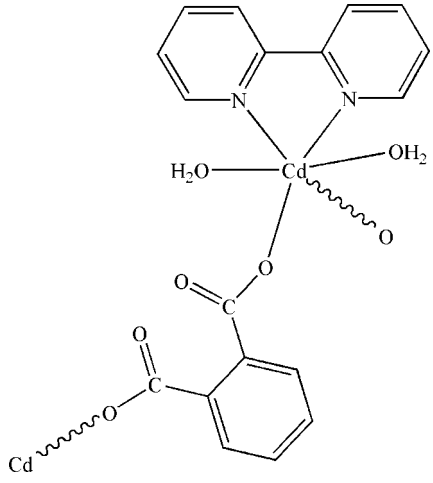
Received 14 June 2007; accepted 1 July 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.034; wR factor = 0.105; data-to-parameter ratio = 12.6.

In the title compound, $[Cd(C_8H_4O_4)(C_{10}H_8N_2)(H_2O)_2]_n$, the Cd atom has a distorted trigonal–prismatic coordination geometry, bonded to two N atoms from the 2,2′-bipyridine ligand, two water O atoms and two O atoms from two different phthalate ligands, thereby producing a linear coordination polymer. The crystal structure is stabilized by π–π interactions [centroid-to-centroid distance = 3.766 (3) Å] and hydrogen bonds.

Related literature

For related literature, see: Sun *et al.* (2005); Suresh *et al.* (2001); Wang *et al.* (2005).



Experimental

Crystal data

$[Cd(C_8H_4O_4)(C_{10}H_8N_2)(H_2O)_2]$
M_r = 468.73
Triclinic, $P\overline{1}$
a = 7.1268 (5) Å
b = 10.0900 (8) Å
c = 12.2110 (9) Å
α = 92.676 (1)°
β = 100.809 (1)°
γ = 90.382 (1)°
V = 861.5 (1) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.31 mm^{-1}
T = 293 (2) K
0.40 × 0.32 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.623, T_{max} = 0.972
(expected range = 0.481–0.750)
5178 measured reflections
3237 independent reflections
2993 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.106
S = 1.17
3237 reflections
256 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −1.11 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O4^{i}	0.82 (2)	1.92 (2)	2.709 (4)	161 (5)
O2W—H2WA···O4	0.81 (2)	2.08 (2)	2.884 (4)	172 (6)
O2W—H2WB···O2^{ii}	0.82 (2)	1.97 (2)	2.738 (4)	156 (5)
O1W—H1WB···O2^{ii}	0.82 (2)	2.08 (2)	2.877 (5)	164 (5)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the Hubei Key Laboratory of Novel Chemical Reactors and Green Chemical Technology (grant No. RCT2004011).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2023).

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 doi:10.1107/S1600536807032035

supplementary materials

Acta Cryst. (2007). E**63**, m2079 [**doi:10.1107/S1600536807032035**]

catena-Poly[[diaqua(2,2'-bipyridine-κ^2N,N')cadmium(II)]-μ-phthalato-$\kappa^2O:O'$]

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Comment

The phthalate ligand was successfully used to design and synthesize a wide variety of metal complexes, those containing Cd(II) complexes are less considered (Sun *et al.*, 2005). Several structures of Cd(II) complexes with phth have been reported, for example, $[Cd(phth)_2(4,4'\text{-bpy})]_n$ (4,4'-bpy = 4,4'-bipyridine; Wang *et al.*, 2005), $[Cd(4,4'\text{-bpy})(phth)(H_2O)]_n \times 2H_2O$ (Suresh *et al.*, 2001). These structures were found to be two-dimensional or three-dimensional coordination polymers with the phth and 4,4'-bpy ligands serving as bridging units. In contrast $[Cd_2(phen)_4(phth)_2]$

$\times 4H_2O$ (phen = 1,10-phenanthroline; Sun *et al.*, 2005) is a binuclear complex. There have been no reports of one-dimensional Cd-bipy complexes in which phth ligands act as bridging ligands. The molecular structure of title compound is shown in Fig.1. The Cd^{II} cation is in a distorted trigonal prismatic CdN_2O_4 geometry coordinated by two N atomes of the bipy ligand and four O atoms of two bridging phth ligands and two coordinated water molecules. π-π stacking is observed between neighbouring parallel pyridine rings along 001 direction as shown in Fig.2. The distance between centroids is 3.766 (3) Å for N1 and $N2^i$-containing rings [symmetry code: (i) –*X*, –Y, 1-*Z*]. These interactions together with hydrogen bonds stabilize the crystal structure.

Experimental

A mixture of $Cd(CH_3COO)_2 \times 2(H_2O)$ (1 mmol, 0.266 g), phthalic acid (1 mmol, 0.168 g), bipy (2 mmol, 0.312 g) and H_2O (10 ml) was heated in a 23 ml stainless steel reactor with a teflon liner at 453 K for 72 h. Colorless block-shaped crystals of the title complex were obtained.

Refinement

H atoms bonded to O atoms were located in difference maps and then included in the refinement with restraints for bond-length of O–H = 0.82 (2) Å and $U_{iso}(H) = 1.5U_{eq}(O)$. H atoms bonded to C atoms were placed in calculated positions and included in the riding- model approximation, with C–H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}$ (C of aromatic).

Figures

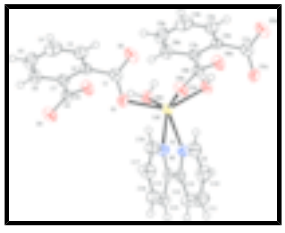


Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. The H atoms have been omitted for clarity [symmety code:(*b*) *x* + 1, *y*, *z*].

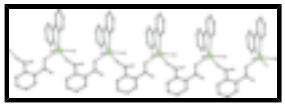


Fig. 2. The molecular structure of compound (I), showing the formation of π-π stacking. Packing diagram of one-dimensional chains structure along 001 direction.

catena-Poly[[diaqua(2,2'-bipyridine-κ^2*N*,*N*')cadmium(II)]- μ-phthalato-κ^2*O*:*O*']

Crystal data

$[Cd(C_8H_4O_4)(C_{10}H_8N_2)(H_2O)_2]$	$Z = 2$
$M_r = 468.73$	$F_{000} = 468$
Triclinic, $P\overline{1}$	$D_x = 1.807$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.1268$ (5) Å	Cell parameters from 4016 reflections
$b = 10.0900$ (8) Å	$\theta = 2.6$–28.3º
$c = 12.2110$ (9) Å	$\mu = 1.31$ mm^{-1}
$\alpha = 92.676$ (1)º	$T = 293$ (2) K
$\beta = 100.809$ (1)º	Block, colorless
$\gamma = 90.382$ (1)º	0.40 × 0.32 × 0.22 mm
$V = 861.5$ (1) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3237 independent reflections
Radiation source: fine-focus sealed tube	2993 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.053$
$T = 293$(2) K	$\theta_{max} = 25.8$º
φ and ω scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -7 \rightarrow 8$
$T_{min} = 0.623$, $T_{max} = 0.972$	$k = -12 \rightarrow 9$
5178 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.106$	$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.8703P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.17$	$(\Delta/\sigma)_{max} < 0.001$
3237 reflections	$\Delta\rho_{max} = 0.77$ e Å^{-3}
256 parameters	$\Delta\rho_{min} = -1.11$ e Å^{-3}
6 restraints	Extinction correction: none

Primary atom site location: structure-invariant direct methods

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}
Cd2	0.17038 (4)	0.02430 (3)	0.23625 (2)	0.02881 (13)
N1	0.1757 (5)	−0.1635 (4)	0.3463 (3)	0.0335 (8)
N2	0.2500 (5)	0.0849 (4)	0.4289 (3)	0.0358 (8)
O1	−0.0341 (4)	0.1911 (3)	0.2320 (3)	0.0367 (7)
O1W	0.3260 (5)	−0.1045 (3)	0.1228 (3)	0.0368 (7)
O2W	−0.1092 (5)	−0.0851 (3)	0.1248 (3)	0.0378 (7)
C1	−0.0826 (6)	0.2393 (4)	0.1376 (4)	0.0318 (9)
C2	−0.2245 (6)	0.3485 (4)	0.1321 (3)	0.0272 (8)
C3	−0.1681 (7)	0.4770 (4)	0.1130 (4)	0.0371 (10)
H3	−0.0472	0.4919	0.0973	0.045*
C4	−0.2906 (8)	0.5825 (5)	0.1172 (4)	0.0511 (13)
H4	−0.2524	0.6674	0.1032	0.061*
C5	−0.4691 (8)	0.5617 (5)	0.1420 (4)	0.0480 (12)
H5	−0.5498	0.6330	0.1462	0.058*
C6	−0.5291 (7)	0.4355 (5)	0.1608 (4)	0.0388 (10)
H6	−0.6495	0.4219	0.1777	0.047*
C7	−0.4064 (6)	0.3275 (4)	0.1542 (3)	0.0300 (8)
C8	−0.4824 (6)	0.1897 (4)	0.1651 (3)	0.0290 (8)
C9	0.1466 (7)	−0.2885 (5)	0.3006 (4)	0.0436 (11)
H9	0.1229	−0.3007	0.2232	0.052*
C10	0.1505 (8)	−0.3987 (5)	0.3640 (5)	0.0520 (13)
H10	0.1322	−0.4835	0.3301	0.062*
C11	0.1822 (9)	−0.3802 (5)	0.4781 (5)	0.0537 (13)
H11	0.1841	−0.4525	0.5229	0.064*
C12	0.2110 (8)	−0.2535 (5)	0.5255 (4)	0.0462 (11)
H12	0.2329	−0.2397	0.6027	0.055*
C13	0.2073 (6)	−0.1463 (4)	0.4578 (3)	0.0321 (9)
C14	0.2451 (6)	−0.0068 (4)	0.5035 (3)	0.0314 (9)
C15	0.2745 (7)	0.0255 (5)	0.6174 (4)	0.0392 (10)
H15	0.2672	−0.0394	0.6681	0.047*
C16	0.3146 (7)	0.1553 (5)	0.6536 (4)	0.0440 (11)

H16	0.3362	0.1790	0.7295	0.053*
C17	0.3227 (7)	0.2497 (5)	0.5776 (4)	0.0436 (11)
H17	0.3508	0.3380	0.6007	0.052*
C18	0.2879 (7)	0.2104 (5)	0.4658 (4)	0.0423 (11)
H18	0.2911	0.2744	0.4138	0.051*
O2	−0.0222 (5)	0.2038 (4)	0.0518 (3)	0.0463 (8)
O3	−0.6024 (5)	0.1793 (3)	0.2278 (3)	0.0413 (7)
O4	−0.4241 (4)	0.0953 (3)	0.1102 (3)	0.0391 (7)
H1WA	0.399 (7)	−0.051 (5)	0.104 (4)	0.059*
H2WA	−0.191 (6)	−0.029 (4)	0.118 (4)	0.059*
H2WB	−0.097 (8)	−0.110 (5)	0.062 (2)	0.059*
H1WB	0.257 (7)	−0.134 (5)	0.065 (3)	0.059*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd2	0.02976 (19)	0.03001 (19)	0.02768 (19)	0.00116 (12)	0.00831 (12)	0.00022 (12)
N1	0.0322 (18)	0.036 (2)	0.0335 (19)	0.0057 (15)	0.0087 (15)	−0.0001 (15)
N2	0.042 (2)	0.036 (2)	0.0293 (18)	−0.0033 (16)	0.0057 (15)	0.0006 (15)
O1	0.0343 (16)	0.0360 (17)	0.0393 (17)	0.0116 (13)	0.0054 (13)	0.0012 (13)
O1W	0.0405 (18)	0.0376 (17)	0.0347 (16)	0.0052 (14)	0.0138 (14)	−0.0025 (13)
O2W	0.0354 (17)	0.0392 (18)	0.0403 (17)	0.0083 (13)	0.0114 (14)	−0.0014 (14)
C1	0.029 (2)	0.032 (2)	0.034 (2)	−0.0082 (17)	0.0063 (17)	−0.0033 (17)
C2	0.031 (2)	0.027 (2)	0.0227 (18)	−0.0014 (16)	0.0054 (15)	−0.0027 (15)
C3	0.039 (2)	0.034 (2)	0.037 (2)	−0.0018 (18)	0.0064 (19)	0.0031 (18)
C4	0.071 (4)	0.029 (2)	0.050 (3)	−0.009 (2)	0.004 (3)	0.005 (2)
C5	0.054 (3)	0.032 (2)	0.056 (3)	0.015 (2)	0.007 (2)	−0.002 (2)
C6	0.034 (2)	0.039 (2)	0.043 (3)	0.0064 (19)	0.0091 (19)	−0.0056 (19)
C7	0.032 (2)	0.030 (2)	0.028 (2)	0.0008 (17)	0.0066 (16)	−0.0004 (16)
C8	0.0262 (19)	0.030 (2)	0.030 (2)	−0.0011 (16)	0.0053 (16)	0.0014 (16)
C9	0.050 (3)	0.037 (3)	0.044 (3)	0.002 (2)	0.010 (2)	−0.002 (2)
C10	0.056 (3)	0.032 (3)	0.069 (4)	0.003 (2)	0.015 (3)	0.000 (2)
C11	0.071 (4)	0.036 (3)	0.055 (3)	−0.003 (2)	0.010 (3)	0.012 (2)
C12	0.055 (3)	0.044 (3)	0.040 (3)	0.000 (2)	0.006 (2)	0.011 (2)
C13	0.027 (2)	0.037 (2)	0.032 (2)	0.0065 (17)	0.0055 (16)	0.0013 (17)
C14	0.0217 (18)	0.038 (2)	0.035 (2)	0.0072 (16)	0.0071 (16)	0.0049 (18)
C15	0.044 (3)	0.044 (3)	0.030 (2)	0.010 (2)	0.0092 (19)	0.0020 (19)
C16	0.044 (3)	0.051 (3)	0.034 (2)	0.005 (2)	0.002 (2)	−0.005 (2)
C17	0.050 (3)	0.038 (3)	0.040 (3)	−0.007 (2)	0.004 (2)	−0.009 (2)
C18	0.050 (3)	0.037 (2)	0.041 (3)	−0.004 (2)	0.010 (2)	0.0032 (19)
O2	0.0446 (19)	0.052 (2)	0.0456 (19)	−0.0010 (16)	0.0219 (16)	−0.0116 (16)
O3	0.0431 (18)	0.0395 (18)	0.0457 (18)	−0.0065 (14)	0.0213 (15)	−0.0042 (14)
O4	0.0381 (17)	0.0321 (16)	0.0505 (19)	−0.0041 (13)	0.0194 (15)	−0.0047 (14)

Geometric parameters (Å, °)

Cd2—O1	2.229 (3)	C5—H5	0.9300
Cd2—O3^{i}	2.264 (3)	C6—C7	1.410 (6)

Cd2—O1W	2.295 (3)	C6—H6	0.9300
Cd2—N2	2.364 (4)	C7—C8	1.510 (6)
Cd2—N1	2.370 (4)	C8—O4	1.256 (5)
Cd2—O2W	2.419 (3)	C8—O3	1.257 (5)
N1—C13	1.341 (6)	C9—C10	1.382 (7)
N1—C9	1.353 (6)	C9—H9	0.9300
N2—C18	1.333 (6)	C10—C11	1.373 (8)
N2—C14	1.334 (5)	C10—H10	0.9300
O1—C1	1.262 (5)	C11—C12	1.376 (7)
O1W—H1WA	0.817 (19)	C11—H11	0.9300
O1W—H1WB	0.821 (19)	C12—C13	1.389 (6)
O2W—H2WA	0.807 (19)	C12—H12	0.9300
O2W—H2WB	0.821 (19)	C13—C14	1.494 (6)
C1—O2	1.243 (5)	C14—C15	1.390 (6)
C1—C2	1.496 (6)	C15—C16	1.373 (7)
C2—C7	1.389 (6)	C15—H15	0.9300
C2—C3	1.398 (6)	C16—C17	1.369 (7)
C3—C4	1.386 (7)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.380 (7)
C4—C5	1.379 (8)	C17—H17	0.9300
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.383 (7)	O3—Cd2^{ii}	2.264 (3)
O1—Cd2—O3^{i}	86.89 (12)	C6—C5—H5	119.7
O1—Cd2—O1W	141.77 (11)	C5—C6—C7	119.5 (4)
O3^{i}—Cd2—O1W	85.07 (11)	C5—C6—H6	120.2
O1—Cd2—N2	84.07 (12)	C7—C6—H6	120.2
O3^{i}—Cd2—N2	81.96 (12)	C2—C7—C6	120.1 (4)
O1W—Cd2—N2	131.33 (12)	C2—C7—C8	121.6 (4)
O1—Cd2—N1	125.60 (12)	C6—C7—C8	118.2 (4)
O3^{i}—Cd2—N1	131.22 (12)	O4—C8—O3	125.2 (4)
O1W—Cd2—N1	86.34 (12)	O4—C8—C7	118.2 (4)
N2—Cd2—N1	68.64 (12)	O3—C8—C7	116.6 (4)
O1—Cd2—O2W	81.03 (11)	N1—C9—C10	122.8 (5)
O3^{i}—Cd2—O2W	141.92 (12)	N1—C9—H9	118.6
O1W—Cd2—O2W	82.64 (11)	C10—C9—H9	118.6
N2—Cd2—O2W	131.78 (12)	C11—C10—C9	118.5 (5)
N1—Cd2—O2W	83.77 (12)	C11—C10—H10	120.8
C13—N1—C9	118.3 (4)	C9—C10—H10	120.8
C13—N1—Cd2	119.3 (3)	C10—C11—C12	119.2 (5)
C9—N1—Cd2	122.3 (3)	C10—C11—H11	120.4
C18—N2—C14	118.4 (4)	C12—C11—H11	120.4
C18—N2—Cd2	121.9 (3)	C11—C12—C13	119.9 (5)
C14—N2—Cd2	119.6 (3)	C11—C12—H12	120.0
C1—O1—Cd2	114.5 (3)	C13—C12—H12	120.0
Cd2—O1W—H1WA	102 (4)	N1—C13—C12	121.3 (4)
Cd2—O1W—H1WB	114 (4)	N1—C13—C14	115.9 (4)
H1WA—O1W—H1WB	107 (3)	C12—C13—C14	122.8 (4)

Cd2—O2W—H2WA	105 (4)	N2—C14—C15	121.9 (4)
Cd2—O2W—H2WB	115 (4)	N2—C14—C13	116.2 (4)
H2WA—O2W—H2WB	107 (3)	C15—C14—C13	121.9 (4)
O2—C1—O1	125.5 (4)	C16—C15—C14	118.7 (4)
O2—C1—C2	119.2 (4)	C16—C15—H15	120.6
O1—C1—C2	115.3 (4)	C14—C15—H15	120.6
C7—C2—C3	119.0 (4)	C17—C16—C15	119.8 (4)
C7—C2—C1	121.5 (4)	C17—C16—H16	120.1
C3—C2—C1	119.2 (4)	C15—C16—H16	120.1
C4—C3—C2	120.7 (4)	C16—C17—C18	118.1 (4)
C4—C3—H3	119.7	C16—C17—H17	120.9
C2—C3—H3	119.7	C18—C17—H17	120.9
C5—C4—C3	120.0 (4)	N2—C18—C17	123.1 (4)
C5—C4—H4	120.0	N2—C18—H18	118.5
C3—C4—H4	120.0	C17—C18—H18	118.5
C4—C5—C6	120.6 (4)	C8—O3—Cd2^{ii}	132.5 (3)
C4—C5—H5	119.7		
O1—Cd2—N1—C13	−61.5 (3)	C1—C2—C7—C6	172.8 (4)
O3^{i}—Cd2—N1—C13	61.1 (4)	C3—C2—C7—C8	174.3 (4)
O1W—Cd2—N1—C13	141.3 (3)	C1—C2—C7—C8	−10.7 (6)
N2—Cd2—N1—C13	3.9 (3)	C5—C6—C7—C2	1.9 (7)
O2W—Cd2—N1—C13	−135.7 (3)	C5—C6—C7—C8	−174.7 (4)
O1—Cd2—N1—C9	118.0 (3)	C2—C7—C8—O4	−30.1 (6)
O3^{i}—Cd2—N1—C9	−119.4 (3)	C6—C7—C8—O4	146.4 (4)
O1W—Cd2—N1—C9	−39.2 (3)	C2—C7—C8—O3	150.9 (4)
N2—Cd2—N1—C9	−176.6 (4)	C6—C7—C8—O3	−32.5 (6)
O2W—Cd2—N1—C9	43.8 (3)	C13—N1—C9—C10	−0.9 (7)
O1—Cd2—N2—C18	−48.8 (4)	Cd2—N1—C9—C10	179.6 (4)
O3^{i}—Cd2—N2—C18	38.9 (4)	N1—C9—C10—C11	1.1 (8)
O1W—Cd2—N2—C18	115.0 (4)	C9—C10—C11—C12	−0.8 (9)
N1—Cd2—N2—C18	179.2 (4)	C10—C11—C12—C13	0.2 (8)
O2W—Cd2—N2—C18	−121.1 (4)	C9—N1—C13—C12	0.2 (6)
O1—Cd2—N2—C14	126.7 (3)	Cd2—N1—C13—C12	179.8 (3)
O3^{i}—Cd2—N2—C14	−145.6 (3)	C9—N1—C13—C14	178.0 (4)
O1W—Cd2—N2—C14	−69.5 (4)	Cd2—N1—C13—C14	−2.5 (5)
N1—Cd2—N2—C14	−5.3 (3)	C11—C12—C13—N1	0.1 (7)
O2W—Cd2—N2—C14	54.4 (4)	C11—C12—C13—C14	−177.5 (5)
O3^{i}—Cd2—O1—C1	74.7 (3)	C18—N2—C14—C15	1.3 (6)
O1W—Cd2—O1—C1	−3.3 (4)	Cd2—N2—C14—C15	−174.4 (3)
N2—Cd2—O1—C1	157.0 (3)	C18—N2—C14—C13	−178.4 (4)
N1—Cd2—O1—C1	−144.7 (3)	Cd2—N2—C14—C13	6.0 (5)
O2W—Cd2—O1—C1	−69.0 (3)	N1—C13—C14—N2	−2.3 (5)
Cd2—O1—C1—O2	−2.1 (5)	C12—C13—C14—N2	175.5 (4)
Cd2—O1—C1—C2	178.2 (2)	N1—C13—C14—C15	178.1 (4)
O2—C1—C2—C7	118.2 (4)	C12—C13—C14—C15	−4.2 (6)
O1—C1—C2—C7	−62.0 (5)	N2—C14—C15—C16	−1.7 (7)
O2—C1—C2—C3	−66.8 (5)	C13—C14—C15—C16	177.9 (4)

O1—C1—C2—C3	112.9 (4)	C14—C15—C16—C17	0.7 (7)
C7—C2—C3—C4	0.8 (6)	C15—C16—C17—C18	0.6 (8)
C1—C2—C3—C4	−174.3 (4)	C14—N2—C18—C17	0.1 (7)
C2—C3—C4—C5	1.0 (7)	Cd2—N2—C18—C17	175.7 (4)
C3—C4—C5—C6	−1.3 (8)	C16—C17—C18—N2	−1.1 (8)
C4—C5—C6—C7	−0.1 (8)	O4—C8—O3—Cd2^{ii}	−21.6 (7)
C3—C2—C7—C6	−2.2 (6)	C7—C8—O3—Cd2^{ii}	157.3 (3)

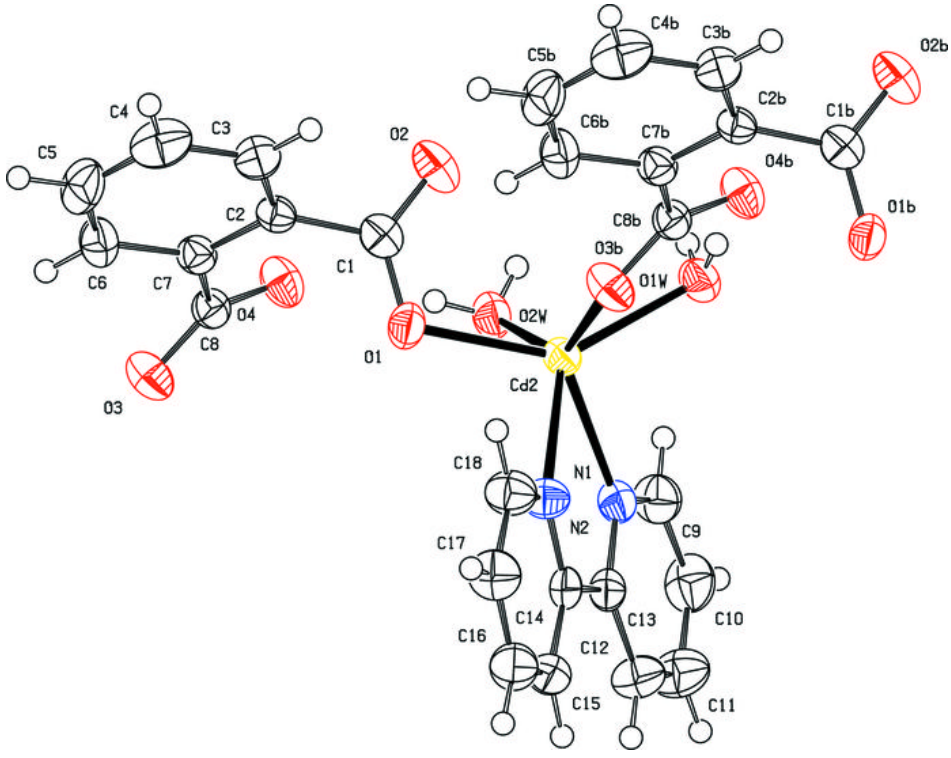
Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*−1, *y*, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O4^{i}	0.82 (2)	1.92 (2)	2.709 (4)	161 (5)
O2W—H2WA···O4	0.81 (2)	2.08 (2)	2.884 (4)	172 (6)
O2W—H2WB···O2^{iii}	0.82 (2)	1.97 (2)	2.738 (4)	156 (5)
O1W—H1WB···O2^{iii}	0.82 (2)	2.08 (2)	2.877 (5)	164 (5)

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

Fig. 1


C4b
C3b
C5b
O2b
C2b
C1b
C6b
C7b
C4
C3
O2
C5
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C8b
C2
O3b
O1W
C1
C6
C7
O4
O2W
C8
O1
Cd2
O3
C18
N1
N2
C9
C17
C14
C13
C10
C16
C12
C15
C11

Fig. 2