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Aqua(2,2′-bipyridine-κ^2N,N')bis(4-formylbenzoato-κ^2O,O')cadmium(II) monohydrate

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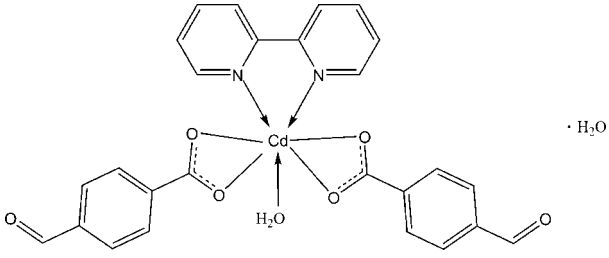
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.028; wR factor = 0.066; data-to-parameter ratio = 16.3.

In the mononuclear title compound, $[Cd(C_8H_5O_3)_2(C_{10}H_8N_2)(H_2O)]\cdot H_2O$, the Cd atom is O,O'-chelated by two 4-formylbenzoate monoanions and N,N'-chelated by 2,2′-bipyridine. It is also coordinated by a water molecule in a monocapped trigonal-prismatic geometry. The coordinated and solvent water molecules and O atoms of the monoanions engage in hydrogen bonding, resulting in a chain running along the b axis of the monoclinic unit cell.

Related literature

For the related cadmium phenanthroline adduct, see Deng *et al.* (2007).



Experimental

Crystal data

$[Cd(C_8H_5O_3)_2(C_{10}H_8N_2)(H_2O)]\cdot H_2O$
M_r = 602.86
Monoclinic, $P2_1/c$
a = 23.878 (5) Å
b = 6.3586 (13) Å
c = 17.048 (3) Å
β = 106.10 (3)°
V = 2486.8 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 295 (2) K
0.28 × 0.21 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.780, T_{max} = 0.865
22518 measured reflections
5636 independent reflections
4810 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.066
S = 1.08
5636 reflections
346 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O2W	0.85 (3)	1.85 (3)	2.685 (3)	167 (3)
O1W—H1W2···O5^{i}	0.85 (4)	1.93 (4)	2.740 (3)	159 (3)
O2W—H2W1···O3^{ii}	0.85 (4)	2.02 (4)	2.854 (3)	171 (4)
O2W—H2W2···O2^{i}	0.85 (3)	1.92 (3)	2.766 (3)	177 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); 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: NG2340).

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supplementary materials

Acta Cryst. (2007). E**63**, m2799 [**doi:10.1107/S160053680705115X**]

Aqua(2,2'-bipyridine-κ^2N,N')bis(4-formylbenzoato-κ^2O,O')cadmium(II) monohydrate

Z.-P. Deng, S. Gao, L.-H. Huo and H. Zhao

Comment

An earlier report (Deng *et al.*, 2007) detailed the crystal structure of cadmium phenanthroline adduct of 4-FBAH; the Cd^{II} atom is six-coordinated and the 4-FBA^- ligands act in both monodendate and chelating modes. Replacing the N-heterocycle by 2,2'-bipy furnishes the title compound as a monohydrated complex (Fig. 1) whose metal centre is seven-coordinate. It displays a mono-capped triangonal prismatic geometry (Fig. 2). The 4-FBA^- ligand is chelating. Hydrogen-bonding interactions between the water molecules and O atoms of 4-FBA^- ligands link the mononuclear complex into a chain structure along the *b* axis (Fig.3).

Experimental

Cadmium(II) diacetate dihydrate (2.66 g, 10 mmol) was added to an H_2O/EtOH solution (1:1 *v*/*v*) of 4-formylbenzoic acid (3.00 g, 20 mmol) and 2,2'-bipydine (1.56 g, 10 mmol). Sodium hydroxide (0.1 *M*) was added dropwise until the solution registered a pH of 5. Colorless single crystals separated from the filtered solution after several days. CH&N analysis. Calc. for $C_{26}H_{22}N_2O_8Cd$: C 51.80, H 3.68, N 4.65. Found: C 51.85, H 3.64, N 4.61.

Refinement

Carbon-bound H atoms were placed in calculated positions, with C—H = 0.93 and $U_{iso}(H) = 1.2U_{eq}(C)$, and were included in the refinement in the riding model approximation. The H atoms of water molecules were located in difference Fourier maps and refined with the O—H and H···H distance restraints to 0.85 (1) and 1.39 (1) Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

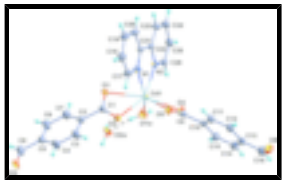


Fig. 1. Molecular structure of the title compound with 30% probability ellipsoid for the non-H atoms. Dashed lines indicate O—H···O hydrogen bonds.

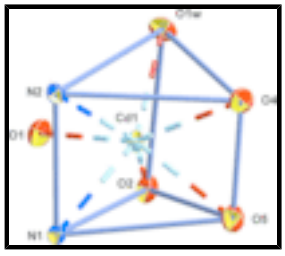


Fig. 2. The coordination polyhedron of the Cd atom in (I).

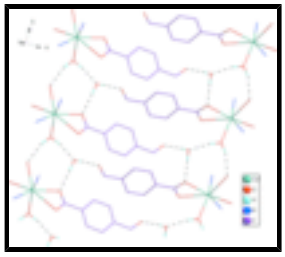


Fig. 3. Chain structure of the title complex along the *b* axis formed by hydrogen-bonding interactions, with the O—H···O hydrogen bonds denoted by dashed lines. H atoms not involved in hydrogen bonding and carbon atoms of 2,2-bipy ligand have been omitted.

Aqua(2,2'-bipyridine-κ^2*N*,*N*')bis(4-formylbenzoato-κ^2*O*,*O*')cadmium(II) monohydrate

Crystal data

$[Cd(C_8H_5O_3)_2(C_{10}H_8N_2)(H_2O)]\cdot H_2O$	F_{000} = 1216
M_r = 602.86	D_x = 1.610 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 18668 reflections
a = 23.878 (5) Å	θ = 3.1–27.4º
b = 6.3586 (13) Å	μ = 0.93 mm^{-1}
c = 17.048 (3) Å	T = 295 (2) K
β = 106.10 (3)º	Prism, colourless
V = 2486.8 (9) Å^3	0.28 × 0.21 × 0.16 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	5636 independent reflections
Radiation source: fine-focus sealed tube	4810 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 27.5º
T = 295(2) K	θ_{min} = 3.1º
ω scans	h = −30→30
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −8→8
T_{min} = 0.780, T_{max} = 0.865	l = −22→20
22518 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.028	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.066	$w = 1/[\sigma^2(F_o^2) + (0.0255P)^2 + 1.4537P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.08	$(\Delta/\sigma)_{max}$ = 0.002
5636 reflections	$\Delta\rho_{max}$ = 0.56 e Å^{-3}
346 parameters	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.761606 (7)	0.55282 (2)	0.604765 (9)	0.03165 (6)
O1W	0.76278 (8)	0.2404 (3)	0.67240 (12)	0.0517 (5)
H1W1	0.7304 (7)	0.194 (4)	0.676 (2)	0.078*
H1W2	0.7864 (9)	0.140 (3)	0.674 (2)	0.078*
O2W	0.67003 (10)	0.0390 (3)	0.69629 (17)	0.0674 (6)
H2W1	0.6537 (17)	0.045 (5)	0.7343 (18)	0.101*
H2W2	0.6727 (17)	−0.088 (2)	0.682 (2)	0.101*
O1	0.65529 (8)	0.4099 (3)	0.54083 (12)	0.0519 (5)
O2	0.67947 (7)	0.6319 (3)	0.64420 (11)	0.0473 (4)
O3	0.39562 (10)	0.5381 (4)	0.68703 (16)	0.0770 (7)
O4	0.85797 (9)	0.5509 (3)	0.69981 (13)	0.0623 (6)
O5	0.81462 (7)	0.8555 (3)	0.67383 (12)	0.0557 (5)
O6	1.06983 (12)	1.3180 (4)	0.92916 (16)	0.0933 (8)
N1	0.73508 (8)	0.7714 (3)	0.48969 (11)	0.0349 (4)
N2	0.79677 (8)	0.4103 (3)	0.50210 (11)	0.0330 (4)
C1	0.64311 (10)	0.5109 (4)	0.59560 (15)	0.0406 (5)
C2	0.58314 (10)	0.4899 (4)	0.60830 (15)	0.0419 (5)
C3	0.56186 (12)	0.6386 (6)	0.6514 (2)	0.0678 (9)
H3	0.5846	0.7547	0.6728	0.081*
C4	0.50721 (13)	0.6178 (6)	0.6633 (2)	0.0691 (9)
H4	0.4935	0.7196	0.6925	0.083*
C5	0.47330 (11)	0.4472 (5)	0.63218 (17)	0.0489 (6)
C6	0.49400 (12)	0.2990 (5)	0.5880 (2)	0.0605 (8)
H6	0.4710	0.1836	0.5662	0.073*
C7	0.54863 (11)	0.3205 (5)	0.57593 (18)	0.0541 (7)
H7	0.5621	0.2201	0.5458	0.065*
C8	0.41517 (12)	0.4242 (5)	0.6460 (2)	0.0630 (8)
H8	0.3922	0.3121	0.6207	0.076*
C9	0.85734 (10)	0.7444 (4)	0.70981 (14)	0.0405 (5)
C10	0.90945 (9)	0.8480 (4)	0.76737 (14)	0.0361 (5)
C11	0.92337 (11)	1.0556 (4)	0.75503 (16)	0.0423 (5)
H11	0.9002	1.1316	0.7114	0.051*
C12	0.97161 (11)	1.1490 (4)	0.80751 (16)	0.0465 (6)
H12	0.9812	1.2870	0.7986	0.056*
C13	1.00575 (10)	1.0371 (4)	0.87349 (17)	0.0457 (6)
C14	0.99173 (11)	0.8306 (4)	0.88568 (17)	0.0513 (6)
H14	1.0145	0.7553	0.9298	0.062*
C15	0.94405 (11)	0.7359 (4)	0.83257 (16)	0.0454 (6)

H15	0.9352	0.5966	0.8406	0.054*
C16	1.05622 (13)	1.1379 (6)	0.9315 (2)	0.0645 (8)
H16	1.0792	1.0548	0.9730	0.077*
C17	0.70356 (11)	0.9470 (4)	0.48623 (16)	0.0429 (5)
H17	0.6942	0.9908	0.5331	0.051*
C18	0.68434 (12)	1.0655 (4)	0.41651 (17)	0.0494 (6)
H18	0.6624	1.1865	0.4161	0.059*
C19	0.69833 (13)	1.0009 (4)	0.34751 (17)	0.0500 (6)
H19	0.6857	1.0774	0.2993	0.060*
C20	0.73139 (11)	0.8216 (4)	0.35019 (14)	0.0438 (6)
H20	0.7416	0.7768	0.3040	0.053*
C21	0.74927 (9)	0.7089 (3)	0.42260 (13)	0.0325 (4)
C22	0.78480 (9)	0.5124 (3)	0.43018 (13)	0.0311 (4)
C23	0.80441 (11)	0.4359 (4)	0.36645 (15)	0.0428 (6)
H23	0.7964	0.5092	0.3174	0.051*
C24	0.83584 (11)	0.2510 (4)	0.37576 (16)	0.0472 (6)
H24	0.8485	0.1972	0.3329	0.057*
C25	0.84809 (11)	0.1478 (4)	0.44941 (15)	0.0451 (6)
H25	0.8696	0.0237	0.4576	0.054*
C26	0.82783 (10)	0.2323 (4)	0.51076 (14)	0.0408 (5)
H26	0.8361	0.1624	0.5606	0.049*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03319 (9)	0.03734 (9)	0.02606 (8)	−0.00243 (7)	0.01094 (6)	−0.00048 (7)
O1W	0.0478 (10)	0.0509 (10)	0.0589 (11)	−0.0039 (8)	0.0190 (9)	0.0167 (10)
O2W	0.0700 (14)	0.0525 (11)	0.0972 (19)	−0.0107 (11)	0.0524 (13)	−0.0017 (12)
O1	0.0484 (10)	0.0616 (11)	0.0518 (11)	−0.0034 (9)	0.0242 (8)	−0.0124 (9)
O2	0.0363 (8)	0.0622 (11)	0.0465 (10)	−0.0096 (8)	0.0167 (7)	−0.0118 (9)
O3	0.0558 (13)	0.1004 (18)	0.0884 (18)	0.0093 (12)	0.0427 (12)	0.0183 (14)
O4	0.0636 (12)	0.0451 (11)	0.0648 (13)	−0.0172 (9)	−0.0045 (10)	−0.0019 (10)
O5	0.0371 (9)	0.0670 (12)	0.0555 (11)	0.0047 (9)	0.0004 (8)	−0.0118 (10)
O6	0.0939 (18)	0.0898 (18)	0.0856 (18)	−0.0442 (16)	0.0074 (14)	−0.0313 (15)
N1	0.0409 (10)	0.0330 (9)	0.0307 (9)	0.0005 (8)	0.0098 (8)	−0.0010 (8)
N2	0.0357 (9)	0.0369 (10)	0.0266 (9)	0.0004 (8)	0.0090 (7)	0.0026 (8)
C1	0.0372 (12)	0.0481 (13)	0.0396 (13)	0.0018 (10)	0.0160 (10)	0.0017 (11)
C2	0.0337 (11)	0.0537 (14)	0.0391 (13)	−0.0040 (11)	0.0115 (10)	−0.0035 (11)
C3	0.0487 (15)	0.082 (2)	0.082 (2)	−0.0246 (16)	0.0342 (15)	−0.0409 (19)
C4	0.0489 (16)	0.091 (2)	0.077 (2)	−0.0111 (16)	0.0333 (15)	−0.0319 (19)
C5	0.0356 (12)	0.0637 (17)	0.0491 (15)	−0.0037 (12)	0.0147 (11)	0.0068 (13)
C6	0.0457 (15)	0.0585 (17)	0.078 (2)	−0.0136 (13)	0.0180 (14)	−0.0069 (16)
C7	0.0466 (14)	0.0538 (16)	0.0648 (17)	−0.0038 (13)	0.0202 (13)	−0.0095 (14)
C8	0.0416 (14)	0.076 (2)	0.073 (2)	−0.0041 (14)	0.0192 (14)	0.0151 (17)
C9	0.0381 (12)	0.0498 (14)	0.0348 (12)	−0.0104 (11)	0.0121 (10)	−0.0062 (11)
C10	0.0325 (11)	0.0389 (12)	0.0377 (11)	−0.0019 (10)	0.0113 (9)	−0.0044 (11)
C11	0.0407 (12)	0.0415 (13)	0.0433 (13)	0.0003 (11)	0.0095 (10)	0.0011 (11)
C12	0.0462 (13)	0.0380 (12)	0.0572 (15)	−0.0073 (11)	0.0176 (12)	−0.0089 (12)

C13	0.0345 (12)	0.0512 (14)	0.0504 (15)	−0.0048 (11)	0.0104 (10)	−0.0147 (12)
C14	0.0443 (13)	0.0539 (16)	0.0487 (14)	0.0042 (12)	0.0015 (11)	−0.0008 (13)
C15	0.0466 (13)	0.0376 (12)	0.0493 (14)	−0.0028 (11)	0.0089 (11)	−0.0003 (11)
C16	0.0487 (16)	0.075 (2)	0.0651 (19)	−0.0121 (16)	0.0086 (14)	−0.0249 (18)
C17	0.0511 (14)	0.0392 (12)	0.0390 (13)	0.0011 (11)	0.0134 (11)	−0.0082 (11)
C18	0.0565 (15)	0.0361 (13)	0.0511 (15)	0.0085 (11)	0.0075 (12)	0.0001 (12)
C19	0.0643 (17)	0.0387 (13)	0.0408 (14)	0.0054 (12)	0.0042 (12)	0.0088 (11)
C20	0.0602 (15)	0.0414 (13)	0.0293 (11)	0.0013 (12)	0.0114 (10)	0.0037 (10)
C21	0.0374 (11)	0.0316 (10)	0.0282 (10)	−0.0065 (9)	0.0086 (8)	−0.0023 (9)
C22	0.0339 (10)	0.0320 (10)	0.0283 (10)	−0.0039 (9)	0.0099 (8)	−0.0007 (9)
C23	0.0563 (15)	0.0446 (13)	0.0314 (11)	0.0053 (12)	0.0187 (10)	0.0058 (10)
C24	0.0546 (15)	0.0504 (14)	0.0415 (13)	0.0092 (12)	0.0215 (11)	−0.0028 (12)
C25	0.0454 (13)	0.0430 (13)	0.0484 (14)	0.0117 (11)	0.0151 (11)	0.0025 (12)
C26	0.0417 (12)	0.0451 (13)	0.0355 (12)	0.0065 (11)	0.0102 (10)	0.0093 (11)

Geometric parameters (Å, °)

Cd1—O1W	2.2930 (18)	C7—H7	0.9300
Cd1—O2	2.2983 (17)	C8—H8	0.9300
Cd1—N2	2.3248 (19)	C9—C10	1.506 (3)
Cd1—N1	2.3438 (19)	C10—C15	1.385 (3)
Cd1—O4	2.419 (2)	C10—C11	1.391 (3)
Cd1—O5	2.422 (2)	C11—C12	1.381 (3)
Cd1—O1	2.6312 (19)	C11—H11	0.9300
O1W—H1W1	0.85 (3)	C12—C13	1.388 (4)
O1W—H1W2	0.85 (4)	C12—H12	0.9300
O2W—H2W1	0.85 (4)	C13—C14	1.385 (4)
O2W—H2W2	0.85 (3)	C13—C16	1.476 (4)
O1—C1	1.233 (3)	C14—C15	1.381 (3)
O2—C1	1.278 (3)	C14—H14	0.9300
O3—C8	1.188 (4)	C15—H15	0.9300
O4—C9	1.242 (3)	C16—H16	0.9300
O5—C9	1.253 (3)	C17—C18	1.374 (4)
O6—C16	1.194 (4)	C17—H17	0.9300
N1—C17	1.339 (3)	C18—C19	1.372 (4)
N1—C21	1.340 (3)	C18—H18	0.9300
N2—C26	1.339 (3)	C19—C20	1.381 (4)
N2—C22	1.346 (3)	C19—H19	0.9300
C1—C2	1.512 (3)	C20—C21	1.388 (3)
C2—C7	1.375 (4)	C20—H20	0.9300
C2—C3	1.378 (4)	C21—C22	1.496 (3)
C3—C4	1.382 (4)	C22—C23	1.385 (3)
C3—H3	0.9300	C23—C24	1.380 (3)
C4—C5	1.369 (4)	C23—H23	0.9300
C4—H4	0.9300	C24—C25	1.375 (3)
C5—C6	1.380 (4)	C24—H24	0.9300
C5—C8	1.478 (4)	C25—C26	1.378 (3)
C6—C7	1.383 (4)	C25—H25	0.9300
C6—H6	0.9300	C26—H26	0.9300

O1W—Cd1—O2	86.27 (7)	O3—C8—H8	117.5
O1W—Cd1—N2	94.83 (7)	C5—C8—H8	117.5
O2—Cd1—N2	145.20 (6)	O4—C9—O5	122.0 (2)
O1W—Cd1—N1	153.83 (7)	O4—C9—C10	118.9 (2)
O2—Cd1—N1	93.47 (7)	O5—C9—C10	119.0 (2)
N2—Cd1—N1	70.81 (6)	C15—C10—C11	119.7 (2)
O1W—Cd1—O4	77.42 (7)	C15—C10—C9	119.9 (2)
O2—Cd1—O4	122.37 (7)	C11—C10—C9	120.4 (2)
N2—Cd1—O4	91.56 (8)	C12—C11—C10	120.1 (2)
N1—Cd1—O4	123.34 (7)	C12—C11—H11	120.0
O1W—Cd1—O5	120.81 (7)	C10—C11—H11	120.0
O2—Cd1—O5	93.28 (6)	C11—C12—C13	120.1 (2)
N2—Cd1—O5	115.25 (7)	C11—C12—H12	120.0
N1—Cd1—O5	85.35 (7)	C13—C12—H12	120.0
O4—Cd1—O5	53.60 (6)	C14—C13—C12	119.7 (2)
O1W—Cd1—O1	77.58 (7)	C14—C13—C16	119.8 (3)
O2—Cd1—O1	52.65 (6)	C12—C13—C16	120.4 (3)
N2—Cd1—O1	93.55 (6)	C15—C14—C13	120.3 (2)
N1—Cd1—O1	81.51 (7)	C15—C14—H14	119.9
O4—Cd1—O1	154.81 (6)	C13—C14—H14	119.9
O5—Cd1—O1	142.17 (6)	C14—C15—C10	120.1 (2)
Cd1—O1W—H1W1	117 (2)	C14—C15—H15	119.9
Cd1—O1W—H1W2	126 (2)	C10—C15—H15	119.9
H1W1—O1W—H1W2	110.2 (16)	O6—C16—C13	125.0 (3)
H2W1—O2W—H2W2	110.6 (17)	O6—C16—H16	117.5
C1—O1—Cd1	84.80 (15)	C13—C16—H16	117.5
C1—O2—Cd1	99.20 (15)	N1—C17—C18	123.0 (2)
C9—O4—Cd1	92.39 (16)	N1—C17—H17	118.5
C9—O5—Cd1	91.97 (16)	C18—C17—H17	118.5
C17—N1—C21	118.8 (2)	C19—C18—C17	118.4 (2)
C17—N1—Cd1	123.34 (16)	C19—C18—H18	120.8
C21—N1—Cd1	117.69 (14)	C17—C18—H18	120.8
C26—N2—C22	118.64 (19)	C18—C19—C20	119.5 (2)
C26—N2—Cd1	123.46 (15)	C18—C19—H19	120.3
C22—N2—Cd1	117.90 (14)	C20—C19—H19	120.3
O1—C1—O2	123.0 (2)	C19—C20—C21	119.2 (2)
O1—C1—C2	119.6 (2)	C19—C20—H20	120.4
O2—C1—C2	117.4 (2)	C21—C20—H20	120.4
C7—C2—C3	118.9 (2)	N1—C21—C20	121.2 (2)
C7—C2—C1	119.8 (2)	N1—C21—C22	116.48 (19)
C3—C2—C1	121.3 (2)	C20—C21—C22	122.4 (2)
C2—C3—C4	121.1 (3)	N2—C22—C23	120.8 (2)
C2—C3—H3	119.5	N2—C22—C21	116.98 (19)
C4—C3—H3	119.5	C23—C22—C21	122.2 (2)
C5—C4—C3	120.0 (3)	C24—C23—C22	120.0 (2)
C5—C4—H4	120.0	C24—C23—H23	120.0
C3—C4—H4	120.0	C22—C23—H23	120.0
C4—C5—C6	119.3 (3)	C25—C24—C23	118.9 (2)
C4—C5—C8	119.8 (3)	C25—C24—H24	120.6

C6—C5—C8	120.9 (3)	C23—C24—H24	120.6
C5—C6—C7	120.6 (3)	C24—C25—C26	118.5 (2)
C5—C6—H6	119.7	C24—C25—H25	120.8
C7—C6—H6	119.7	C26—C25—H25	120.8
C2—C7—C6	120.2 (3)	N2—C26—C25	123.1 (2)
C2—C7—H7	119.9	N2—C26—H26	118.4
C6—C7—H7	119.9	C25—C26—H26	118.4
O3—C8—C5	125.0 (3)		
O1W—Cd1—O1—C1	91.39 (16)	C1—C2—C3—C4	−179.5 (3)
O2—Cd1—O1—C1	−3.45 (15)	C2—C3—C4—C5	0.1 (6)
N2—Cd1—O1—C1	−174.44 (15)	C3—C4—C5—C6	−0.9 (5)
N1—Cd1—O1—C1	−104.45 (16)	C3—C4—C5—C8	179.2 (3)
O4—Cd1—O1—C1	84.2 (2)	C4—C5—C6—C7	0.7 (5)
O5—Cd1—O1—C1	−33.5 (2)	C8—C5—C6—C7	−179.4 (3)
O1W—Cd1—O2—C1	−73.86 (16)	C3—C2—C7—C6	−1.2 (4)
N2—Cd1—O2—C1	19.2 (2)	C1—C2—C7—C6	179.3 (3)
N1—Cd1—O2—C1	79.92 (16)	C5—C6—C7—C2	0.4 (5)
O4—Cd1—O2—C1	−146.42 (15)	C4—C5—C8—O3	−4.5 (5)
O5—Cd1—O2—C1	165.45 (16)	C6—C5—C8—O3	175.5 (3)
O1—Cd1—O2—C1	3.35 (14)	Cd1—O4—C9—O5	0.1 (3)
O1W—Cd1—O4—C9	−144.78 (18)	Cd1—O4—C9—C10	179.72 (19)
O2—Cd1—O4—C9	−67.51 (18)	Cd1—O5—C9—O4	−0.1 (3)
N2—Cd1—O4—C9	120.62 (17)	Cd1—O5—C9—C10	−179.72 (19)
N1—Cd1—O4—C9	52.7 (2)	O4—C9—C10—C15	−28.3 (4)
O5—Cd1—O4—C9	−0.05 (15)	O5—C9—C10—C15	151.4 (2)
O1—Cd1—O4—C9	−137.63 (16)	O4—C9—C10—C11	151.2 (3)
O1W—Cd1—O5—C9	41.05 (17)	O5—C9—C10—C11	−29.2 (3)
O2—Cd1—O5—C9	128.66 (15)	C15—C10—C11—C12	0.2 (4)
N2—Cd1—O5—C9	−71.88 (16)	C9—C10—C11—C12	−179.3 (2)
N1—Cd1—O5—C9	−138.11 (15)	C10—C11—C12—C13	−1.1 (4)
O4—Cd1—O5—C9	0.05 (15)	C11—C12—C13—C14	1.0 (4)
O1—Cd1—O5—C9	152.14 (14)	C11—C12—C13—C16	−177.9 (3)
O1W—Cd1—N1—C17	119.2 (2)	C12—C13—C14—C15	0.0 (4)
O2—Cd1—N1—C17	30.57 (18)	C16—C13—C14—C15	178.9 (3)
N2—Cd1—N1—C17	178.78 (19)	C13—C14—C15—C10	−0.9 (4)
O4—Cd1—N1—C17	−102.43 (19)	C11—C10—C15—C14	0.8 (4)
O5—Cd1—N1—C17	−62.44 (18)	C9—C10—C15—C14	−179.8 (2)
O1—Cd1—N1—C17	81.99 (18)	C14—C13—C16—O6	−175.4 (3)
O1W—Cd1—N1—C21	−56.5 (2)	C12—C13—C16—O6	3.6 (5)
O2—Cd1—N1—C21	−145.07 (16)	C21—N1—C17—C18	0.8 (4)
N2—Cd1—N1—C21	3.14 (15)	Cd1—N1—C17—C18	−174.77 (19)
O4—Cd1—N1—C21	81.93 (17)	N1—C17—C18—C19	−0.2 (4)
O5—Cd1—N1—C21	121.92 (16)	C17—C18—C19—C20	−0.5 (4)
O1—Cd1—N1—C21	−93.65 (16)	C18—C19—C20—C21	0.7 (4)
O1W—Cd1—N2—C26	−23.32 (18)	C17—N1—C21—C20	−0.6 (3)
O2—Cd1—N2—C26	−113.74 (19)	Cd1—N1—C21—C20	175.21 (17)
N1—Cd1—N2—C26	179.12 (19)	C17—N1—C21—C22	179.7 (2)
O4—Cd1—N2—C26	54.18 (18)	Cd1—N1—C21—C22	−4.5 (2)
O5—Cd1—N2—C26	104.13 (18)	C19—C20—C21—N1	−0.1 (4)

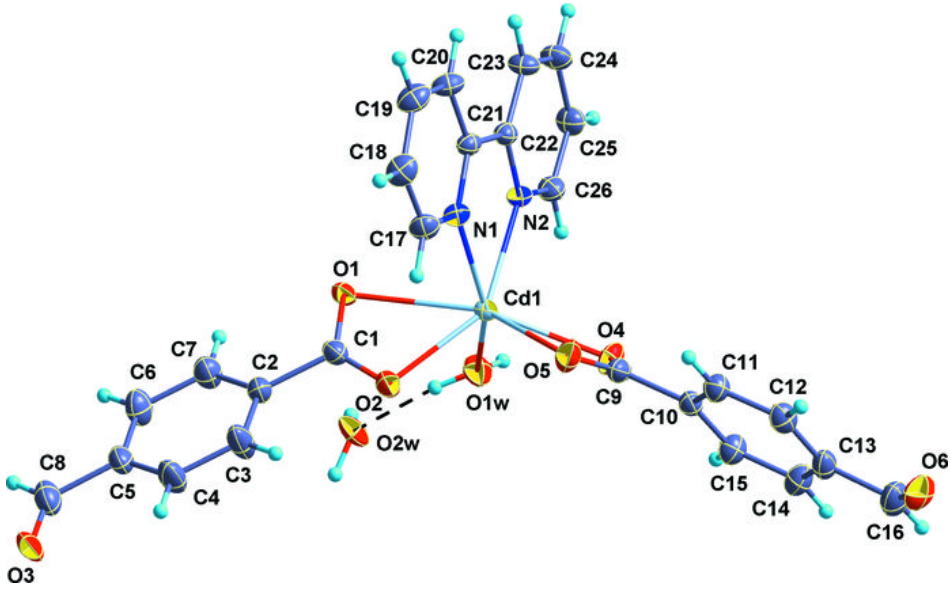
O1—Cd1—N2—C26	−101.14 (18)	C19—C20—C21—C22	179.6 (2)
O1W—Cd1—N2—C22	156.28 (15)	C26—N2—C22—C23	−0.3 (3)
O2—Cd1—N2—C22	65.9 (2)	Cd1—N2—C22—C23	−179.96 (17)
N1—Cd1—N2—C22	−1.28 (15)	C26—N2—C22—C21	179.14 (19)
O4—Cd1—N2—C22	−126.21 (16)	Cd1—N2—C22—C21	−0.5 (2)
O5—Cd1—N2—C22	−76.26 (16)	N1—C21—C22—N2	3.3 (3)
O1—Cd1—N2—C22	78.46 (16)	C20—C21—C22—N2	−176.4 (2)
Cd1—O1—C1—O2	5.9 (2)	N1—C21—C22—C23	−177.2 (2)
Cd1—O1—C1—C2	−172.8 (2)	C20—C21—C22—C23	3.1 (3)
Cd1—O2—C1—O1	−6.8 (3)	N2—C22—C23—C24	1.1 (4)
Cd1—O2—C1—C2	171.87 (19)	C21—C22—C23—C24	−178.4 (2)
O1—C1—C2—C7	18.1 (4)	C22—C23—C24—C25	−1.2 (4)
O2—C1—C2—C7	−160.6 (3)	C23—C24—C25—C26	0.7 (4)
O1—C1—C2—C3	−161.4 (3)	C22—N2—C26—C25	−0.2 (3)
O2—C1—C2—C3	19.9 (4)	Cd1—N2—C26—C25	179.41 (19)
C7—C2—C3—C4	1.0 (5)	C24—C25—C26—N2	0.0 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O2W	0.85 (3)	1.85 (3)	2.685 (3)	167 (3)
O1W—H1W2···O5^{i}	0.85 (4)	1.93 (4)	2.740 (3)	159 (3)
O2W—H2W1···O3^{ii}	0.85 (4)	2.02 (4)	2.854 (3)	171 (4)
O2W—H2W2···O2^{i}	0.85 (3)	1.92 (3)	2.766 (3)	177 (3)

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

Fig. 1


C20
C23
C24
C19
C21
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C26
N2
C17
N1
O1
Cd1
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C2
C6
O4
O5
C11
C12
C9
C10
O2
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O2w
C8
C5
C3
C4
C13
O6
C15
C14
C16
O3

Fig. 2

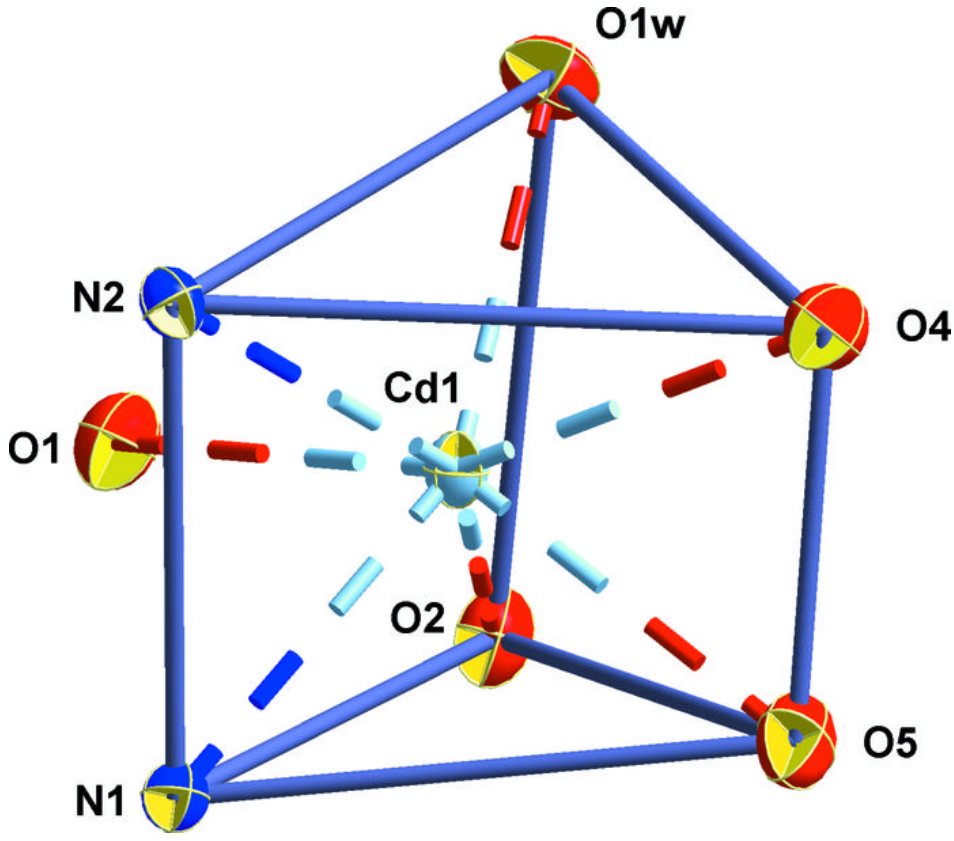

Fig. 3