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Aquabis(4-formylbenzoato)-$\kappa^2O,O';\kappa O$-(1,10-phenanthroline-κ^2N,N')-cadmium(II)

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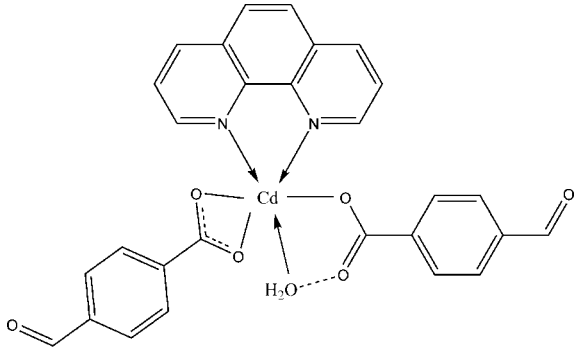
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.025; wR factor = 0.063; data-to-parameter ratio = 13.8.

The Cd^{II} atom in the title complex, $[Cd(C_8H_5O_3)_2(C_{12}H_8N_2)(H_2O)]$, is coordinated by three O atoms of two formylbenzoate ligands, two N atoms of a 1,10-phenanthroline ligand and one water molecule, giving rise to a trigonal–prismatic coordination geometry. Adjacent complex molecules are linked into a two-dimensional layer structure *via* hydrogen-bonding interactions.

Related literature

For the zinc phenanthroline adduct, see Deng, Gao, Huo *et al.* (2006), and for the cadmium phenanthroline complex, see Deng, Gao & Ng (2006).



Experimental

Crystal data

$[Cd(C_8H_5O_3)_2(C_{12}H_8N_2)(H_2O)]$
M_r = 608.86
Monoclinic, $P2_1$
a = 6.357 (1) Å
b = 19.668 (4) Å
c = 9.766 (2) Å
β = 90.11 (3)°
V = 1221.0 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.95 mm^{-1}
T = 295 (2) K
0.34 × 0.21 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.739, T_{max} = 0.848
11897 measured reflections
4825 independent reflections
4537 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.063
S = 1.05
4825 reflections
349 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), from 1957 Friedel pairs
Flack parameter: 0.01 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O2^{i}	0.86 (5)	1.89 (5)	2.735 (4)	168 (5)
O1W—H1W2···O5	0.86 (5)	1.88 (3)	2.590 (4)	140 (5)

Symmetry code: (i) $x+1, y, z$.

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: IM2036).

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supplementary materials

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Aquabis(4-formylbenzoato)-κ^2O,O';κO-(1,10-phenanthroline-κ^2N,N')cadmium(II)

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

Comment

An earlier report (Deng *et al.*, 2006*a*) detailed the synthesis and crystal structure of a zinc complex with 1,10-phenanthroline and 4-formylbenzoato ligands. Replacing zinc by cadmium in a similar reaction leads to the formation of the title complex, (I) (Fig. 1). The Cd(II) atom displays a trigonal prismatic geometry, which is different from the zinc complex and another cadmium phenanthroline adduct, (II) (Deng *et al.*, 2006*b*). The two basal planes of the trigonal prism are built up by O1, O1, N2 and O2, O4, N1, respectively. The Cd—O and Cd—N bond lengths are similar to complex (II). Interestingly, one of the 4-formylbenzoato ligands shows a coordination to cadmium only *via* one of the oxygen atoms whereas the other oxygen atom is engaged in a strong intramolecular hydrogen bond toward the aqua ligand. Adjacent complex molecules are linked into a two-dimensional layer structure *via* hydrogen-bonding interactions (Table 1, Fig. 2).

Experimental

Cadmium(II) diacetate trihydrate (0.14 g, 0.5 mmol) was added to an H_2O/EtOH solution (1:1 *v*/*v*) of 4-formylbenzoic acid (0.15 g, 1 mmol) and 1,10-phenanthroline (0.099 g 0.5 mmol). Sodium hydroxide (0.1 *M*) was added dropwise until the solution registered a pH of 5. Pale yellow single crystals separated from the filtered solution after several days. Elemental analysis: calcd. for $C_{28}H_{20}N_2O_7Cd$: C 55.23, H 3.31, N 4.60. Found: C 55.25, H 3.24, N 4.62.

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

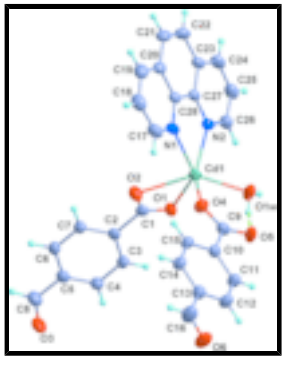


Fig. 1. Molecular structure of the title compound with 30% probability ellipsoid for the non-H atoms. Dashed lines indicate O—H···O hydrogen bonds.

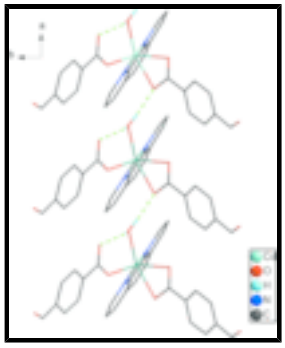


Fig. 2. Two-dimensional-layer structure of the title complex along the *ab* plane formed by hydrogen-bonding, with the O—H···O hydrogen bonds denoted by dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Aquabis(4-formylbenzoato)-κ^2*O*,*O*';κ*O*- (1,10-phenanthroline-κ^2*N*,*N*')cadmium(II)

Crystal data

$[Cd(C_8H_5O_3)_2(C_{12}H_8N_2)(H_2O)]$	F_{000} = 612
M_r = 608.86	D_x = 1.656 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 11052 reflections
a = 6.357 (1) Å	θ = 3.2–27.4º
b = 19.668 (4) Å	μ = 0.95 mm^{-1}
c = 9.766 (2) Å	T = 295 (2) K
β = 90.11 (3)º	Prism, pale yellow
V = 1221.0 (4) Å^3	0.34 × 0.21 × 0.18 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID diffractometer	4825 independent reflections
Radiation source: fine-focus sealed tube	4537 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 27.4º
T = 295(2) K	θ_{min} = 3.2º
ω scans	h = −8→8
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −25→21
T_{min} = 0.739, T_{max} = 0.848	l = −12→12
11897 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.025	$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 0.1062P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.063$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.56$ e Å^{-3}
4825 reflections	$\Delta\rho_{min} = -0.25$ e Å^{-3}
349 parameters	Extinction correction: none
4 restraints	Absolute structure: Flack (1983), from 1957 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.01 (2)
Secondary atom site location: difference Fourier map	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.77987 (3)	0.712516 (17)	0.315510 (15)	0.04216 (7)
O1W	1.1049 (4)	0.73572 (17)	0.3948 (3)	0.0812 (10)
H1W1	1.211 (7)	0.709 (3)	0.401 (5)	0.122*
H1W2	1.074 (8)	0.749 (3)	0.476 (2)	0.122*
O1	0.7527 (4)	0.61002 (14)	0.4439 (3)	0.0509 (6)
O2	0.4560 (4)	0.65579 (13)	0.3778 (3)	0.0565 (6)
O3	0.1403 (6)	0.3939 (2)	0.8716 (4)	0.1075 (12)
O4	0.6851 (4)	0.79973 (15)	0.4452 (3)	0.0553 (7)
O5	0.9706 (4)	0.82545 (17)	0.5680 (3)	0.0810 (10)
O6	0.3252 (5)	1.0274 (2)	0.9929 (3)	0.0981 (12)
N1	0.5860 (4)	0.75318 (13)	0.1303 (2)	0.0437 (6)
N2	0.9394 (4)	0.67398 (13)	0.1142 (2)	0.0424 (5)
C1	0.5570 (5)	0.61234 (16)	0.4443 (3)	0.0413 (6)
C2	0.4344 (5)	0.56143 (16)	0.5297 (3)	0.0404 (6)
C3	0.5283 (6)	0.53018 (18)	0.6406 (3)	0.0462 (7)
H3	0.6674	0.5400	0.6627	0.055*
C4	0.4147 (6)	0.48377 (18)	0.7196 (4)	0.0486 (8)
H4	0.4774	0.4634	0.7953	0.058*
C5	0.2109 (5)	0.46823 (19)	0.6856 (3)	0.0478 (7)
C6	0.1167 (5)	0.49958 (18)	0.5737 (3)	0.0491 (7)
H6	−0.0210	0.4887	0.5501	0.059*
C7	0.2267 (5)	0.54710 (16)	0.4970 (3)	0.0444 (6)
H7	0.1616	0.5692	0.4242	0.053*
C8	0.0849 (7)	0.4194 (2)	0.7671 (4)	0.0691 (10)
H8	−0.0476	0.4078	0.7340	0.083*
C9	0.7805 (5)	0.83037 (17)	0.5412 (3)	0.0505 (7)
C10	0.6485 (6)	0.87646 (16)	0.6317 (3)	0.0453 (7)
C11	0.7320 (5)	0.90185 (18)	0.7532 (3)	0.0499 (7)
H11	0.8690	0.8909	0.7784	0.060*
C12	0.6124 (5)	0.94315 (18)	0.8366 (3)	0.0528 (8)
H12	0.6685	0.9598	0.9180	0.063*
C13	0.4075 (5)	0.95998 (17)	0.7986 (4)	0.0495 (7)
C14	0.3249 (6)	0.93475 (19)	0.6781 (4)	0.0500 (8)
H14	0.1885	0.9461	0.6524	0.060*

C15	0.4445 (6)	0.89241 (18)	0.5951 (4)	0.0480 (8)
H15	0.3871	0.8748	0.5149	0.058*
C16	0.2764 (7)	1.0020 (2)	0.8867 (5)	0.0696 (11)
H16	0.1397	1.0100	0.8568	0.083*
C17	0.4134 (6)	0.79067 (18)	0.1388 (4)	0.0572 (8)
H17	0.3730	0.8071	0.2241	0.069*
C18	0.2888 (6)	0.8067 (2)	0.0242 (5)	0.0632 (10)
H18	0.1673	0.8325	0.0338	0.076*
C19	0.3491 (6)	0.78362 (18)	−0.1008 (4)	0.0582 (8)
H19	0.2690	0.7940	−0.1778	0.070*
C20	0.5308 (5)	0.74446 (15)	−0.1141 (3)	0.0467 (7)
C21	0.6059 (6)	0.7193 (3)	−0.2424 (3)	0.0562 (8)
H21	0.5297	0.7282	−0.3218	0.067*
C22	0.7857 (6)	0.68279 (18)	−0.2503 (3)	0.0565 (8)
H22	0.8318	0.6680	−0.3355	0.068*
C23	0.9054 (5)	0.66654 (16)	−0.1326 (3)	0.0455 (7)
C24	1.0926 (6)	0.62859 (17)	−0.1353 (3)	0.0549 (8)
H24	1.1460	0.6134	−0.2185	0.066*
C25	1.1962 (6)	0.61390 (19)	−0.0170 (4)	0.0575 (9)
H25	1.3195	0.5885	−0.0186	0.069*
C26	1.1154 (5)	0.63739 (18)	0.1059 (3)	0.0510 (7)
H26	1.1872	0.6271	0.1863	0.061*
C27	0.8340 (5)	0.68927 (14)	−0.0025 (3)	0.0389 (6)
C28	0.6459 (5)	0.72926 (13)	0.0058 (3)	0.0399 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04758 (10)	0.04581 (11)	0.03311 (9)	−0.00347 (12)	0.00606 (6)	−0.00381 (13)
O1W	0.0490 (14)	0.102 (2)	0.0932 (19)	0.0088 (13)	−0.0024 (13)	−0.0504 (17)
O1	0.0371 (12)	0.0630 (16)	0.0527 (14)	−0.0030 (11)	0.0002 (10)	0.0125 (12)
O2	0.0487 (13)	0.0534 (14)	0.0675 (14)	0.0010 (10)	0.0033 (11)	0.0188 (12)
O3	0.102 (3)	0.120 (3)	0.100 (3)	−0.027 (2)	0.006 (2)	0.045 (2)
O4	0.0585 (17)	0.0584 (16)	0.0489 (13)	0.0005 (13)	−0.0046 (12)	−0.0139 (11)
O5	0.0510 (15)	0.095 (2)	0.097 (2)	−0.0037 (14)	0.0073 (14)	−0.0544 (19)
O6	0.087 (2)	0.116 (3)	0.091 (2)	0.032 (2)	−0.0099 (17)	−0.058 (2)
N1	0.0517 (14)	0.0401 (13)	0.0393 (12)	0.0007 (11)	0.0097 (10)	0.0020 (10)
N2	0.0485 (14)	0.0406 (13)	0.0381 (12)	−0.0036 (11)	0.0051 (10)	−0.0012 (10)
C1	0.0498 (17)	0.0401 (15)	0.0339 (13)	−0.0004 (13)	0.0027 (12)	−0.0038 (12)
C2	0.0404 (15)	0.0406 (16)	0.0401 (14)	0.0019 (12)	0.0044 (12)	−0.0039 (12)
C3	0.0381 (18)	0.0547 (19)	0.0460 (17)	−0.0008 (14)	−0.0046 (14)	0.0011 (15)
C4	0.0498 (19)	0.052 (2)	0.0441 (17)	0.0009 (15)	−0.0026 (14)	0.0085 (15)
C5	0.0509 (19)	0.0442 (18)	0.0482 (17)	−0.0007 (14)	0.0061 (14)	−0.0020 (13)
C6	0.0419 (16)	0.0565 (19)	0.0489 (16)	−0.0082 (13)	−0.0008 (13)	−0.0018 (14)
C7	0.0418 (15)	0.0490 (16)	0.0424 (14)	−0.0003 (13)	−0.0020 (11)	0.0007 (13)
C8	0.071 (3)	0.071 (3)	0.066 (2)	−0.014 (2)	0.0047 (19)	0.016 (2)
C9	0.058 (2)	0.0454 (18)	0.0481 (17)	−0.0082 (14)	0.0107 (14)	−0.0070 (14)
C10	0.0492 (18)	0.0404 (16)	0.0464 (15)	−0.0092 (13)	0.0018 (14)	−0.0046 (13)

C11	0.0489 (17)	0.0514 (18)	0.0494 (17)	0.0017 (14)	−0.0025 (13)	−0.0106 (15)
C12	0.0541 (19)	0.0557 (19)	0.0484 (17)	0.0035 (15)	−0.0063 (14)	−0.0149 (15)
C13	0.0521 (18)	0.0422 (16)	0.0542 (18)	0.0016 (14)	0.0006 (14)	−0.0065 (15)
C14	0.045 (2)	0.053 (2)	0.0516 (19)	0.0052 (15)	−0.0092 (15)	−0.0007 (15)
C15	0.051 (2)	0.0509 (19)	0.0417 (17)	−0.0057 (15)	−0.0059 (14)	−0.0044 (15)
C16	0.060 (2)	0.071 (3)	0.078 (3)	0.0143 (19)	−0.0025 (19)	−0.026 (2)
C17	0.065 (2)	0.0492 (18)	0.0573 (19)	0.0038 (16)	0.0151 (16)	0.0040 (16)
C18	0.055 (2)	0.051 (2)	0.083 (3)	0.0109 (18)	0.0106 (19)	0.0154 (19)
C19	0.063 (2)	0.0502 (19)	0.062 (2)	−0.0018 (16)	−0.0046 (16)	0.0161 (16)
C20	0.0604 (19)	0.0378 (15)	0.0417 (14)	−0.0101 (14)	−0.0002 (13)	0.0074 (12)
C21	0.081 (2)	0.051 (2)	0.0364 (11)	−0.010 (2)	−0.0048 (12)	0.0092 (18)
C22	0.082 (2)	0.0528 (18)	0.0348 (14)	−0.0080 (17)	0.0051 (14)	−0.0051 (13)
C23	0.0585 (18)	0.0381 (15)	0.0399 (14)	−0.0081 (13)	0.0110 (13)	−0.0037 (12)
C24	0.067 (2)	0.0455 (18)	0.0519 (17)	−0.0034 (15)	0.0189 (15)	−0.0102 (15)
C25	0.057 (2)	0.0475 (19)	0.068 (2)	0.0011 (17)	0.0150 (18)	−0.0067 (17)
C26	0.0498 (18)	0.0514 (18)	0.0519 (17)	0.0006 (14)	0.0034 (13)	−0.0008 (15)
C27	0.0488 (16)	0.0327 (13)	0.0351 (12)	−0.0090 (10)	0.0049 (11)	−0.0009 (10)
C28	0.0488 (15)	0.0327 (17)	0.0382 (12)	−0.0085 (10)	0.0053 (10)	0.0022 (10)

Geometric parameters (Å, °)

Cd1—O1	2.381 (3)	C10—C15	1.381 (5)
Cd1—O2	2.420 (2)	C10—C11	1.392 (5)
Cd1—O1W	2.252 (3)	C11—C12	1.379 (5)
Cd1—O4	2.216 (3)	C11—H11	0.9300
Cd1—N1	2.328 (3)	C12—C13	1.394 (5)
Cd1—N2	2.340 (2)	C12—H12	0.9300
Cd1—C1	2.735 (3)	C13—C14	1.380 (5)
O1W—H1W1	0.86 (5)	C13—C16	1.457 (5)
O1W—H1W2	0.86 (3)	C14—C15	1.390 (5)
O1—C1	1.245 (4)	C14—H14	0.9300
O2—C1	1.250 (4)	C15—H15	0.9300
O3—C8	1.190 (5)	C16—H16	0.9300
O4—C9	1.268 (4)	C17—C18	1.406 (6)
O5—C9	1.239 (4)	C17—H17	0.9300
O6—C16	1.191 (5)	C18—C19	1.358 (6)
N1—C17	1.324 (4)	C18—H18	0.9300
N1—C28	1.359 (3)	C19—C20	1.395 (5)
N2—C26	1.333 (4)	C19—H19	0.9300
N2—C27	1.355 (4)	C20—C28	1.412 (4)
C1—C2	1.519 (4)	C20—C21	1.430 (4)
C2—C3	1.380 (4)	C21—C22	1.352 (6)
C2—C7	1.387 (4)	C21—H21	0.9300
C3—C4	1.397 (5)	C22—C23	1.414 (5)
C3—H3	0.9300	C22—H22	0.9300
C4—C5	1.371 (5)	C23—C24	1.405 (5)
C4—H4	0.9300	C23—C27	1.422 (4)
C5—C6	1.389 (5)	C24—C25	1.360 (6)
C5—C8	1.483 (5)	C24—H24	0.9300

C6—C7	1.388 (5)	C25—C26	1.386 (5)
C6—H6	0.9300	C25—H25	0.9300
C7—H7	0.9300	C26—H26	0.9300
C8—H8	0.9300	C27—C28	1.434 (4)
C9—C10	1.520 (5)		
O4—Cd1—O1W	84.07 (10)	O5—C9—O4	125.7 (3)
O4—Cd1—N1	91.94 (10)	O5—C9—C10	117.6 (3)
O1W—Cd1—N1	132.97 (11)	O4—C9—C10	116.7 (3)
O4—Cd1—N2	148.15 (10)	C15—C10—C11	119.7 (3)
O1W—Cd1—N2	87.48 (9)	C15—C10—C9	120.3 (3)
N1—Cd1—N2	71.84 (9)	C11—C10—C9	120.0 (3)
O4—Cd1—O1	109.54 (9)	C12—C11—C10	120.3 (3)
O1W—Cd1—O1	93.32 (11)	C12—C11—H11	119.8
N1—Cd1—O1	131.38 (9)	C10—C11—H11	119.8
N2—Cd1—O1	101.55 (9)	C11—C12—C13	119.9 (3)
O4—Cd1—O2	88.91 (10)	C11—C12—H12	120.0
O1W—Cd1—O2	141.94 (10)	C13—C12—H12	120.0
N1—Cd1—O2	84.49 (9)	C14—C13—C12	119.7 (3)
N2—Cd1—O2	115.59 (9)	C14—C13—C16	119.4 (3)
O1—Cd1—O2	54.18 (8)	C12—C13—C16	120.9 (3)
O4—Cd1—C1	98.82 (10)	C13—C14—C15	120.4 (3)
O1W—Cd1—C1	117.62 (12)	C13—C14—H14	119.8
N1—Cd1—C1	109.32 (9)	C15—C14—H14	119.8
N2—Cd1—C1	112.26 (9)	C10—C15—C14	120.0 (3)
O1—Cd1—C1	27.05 (9)	C10—C15—H15	120.0
O2—Cd1—C1	27.21 (9)	C14—C15—H15	120.0
Cd1—O1W—H1W1	128 (4)	O6—C16—C13	127.2 (4)
Cd1—O1W—H1W2	100 (4)	O6—C16—H16	116.4
H1W1—O1W—H1W2	108 (5)	C13—C16—H16	116.4
C1—O1—Cd1	92.5 (2)	N1—C17—C18	122.7 (3)
C1—O2—Cd1	90.5 (2)	N1—C17—H17	118.6
C9—O4—Cd1	131.3 (3)	C18—C17—H17	118.6
C17—N1—C28	118.8 (3)	C19—C18—C17	118.8 (4)
C17—N1—Cd1	125.5 (2)	C19—C18—H18	120.6
C28—N1—Cd1	115.28 (19)	C17—C18—H18	120.6
C26—N2—C27	118.8 (3)	C18—C19—C20	120.2 (3)
C26—N2—Cd1	126.2 (2)	C18—C19—H19	119.9
C27—N2—Cd1	114.89 (19)	C20—C19—H19	119.9
O1—C1—O2	122.4 (3)	C19—C20—C28	117.9 (3)
O1—C1—C2	119.4 (3)	C19—C20—C21	123.4 (3)
O2—C1—C2	118.2 (3)	C28—C20—C21	118.7 (3)
O1—C1—Cd1	60.42 (18)	C22—C21—C20	121.2 (3)
O2—C1—Cd1	62.26 (17)	C22—C21—H21	119.4
C2—C1—Cd1	173.8 (2)	C20—C21—H21	119.4
C3—C2—C7	120.0 (3)	C21—C22—C23	121.8 (3)
C3—C2—C1	120.2 (3)	C21—C22—H22	119.1
C7—C2—C1	119.8 (3)	C23—C22—H22	119.1
C2—C3—C4	120.1 (3)	C24—C23—C22	124.0 (3)
C2—C3—H3	120.0	C24—C23—C27	117.1 (3)

C4—C3—H3	120.0	C22—C23—C27	118.9 (3)
C5—C4—C3	120.0 (3)	C25—C24—C23	120.4 (3)
C5—C4—H4	120.0	C25—C24—H24	119.8
C3—C4—H4	120.0	C23—C24—H24	119.8
C4—C5—C6	119.8 (3)	C24—C25—C26	119.0 (4)
C4—C5—C8	121.7 (3)	C24—C25—H25	120.5
C6—C5—C8	118.5 (3)	C26—C25—H25	120.5
C7—C6—C5	120.4 (3)	N2—C26—C25	123.0 (3)
C7—C6—H6	119.8	N2—C26—H26	118.5
C5—C6—H6	119.8	C25—C26—H26	118.5
C2—C7—C6	119.6 (3)	N2—C27—C23	121.6 (3)
C2—C7—H7	120.2	N2—C27—C28	119.0 (2)
C6—C7—H7	120.2	C23—C27—C28	119.4 (3)
O3—C8—C5	125.0 (4)	N1—C28—C20	121.6 (3)
O3—C8—H8	117.5	N1—C28—C27	118.4 (3)
C5—C8—H8	117.5	C20—C28—C27	120.0 (2)
O4—Cd1—O1—C1	70.3 (2)	C4—C5—C6—C7	−0.7 (5)
O1W—Cd1—O1—C1	155.2 (2)	C8—C5—C6—C7	178.1 (3)
N1—Cd1—O1—C1	−40.9 (2)	C3—C2—C7—C6	−2.1 (4)
N2—Cd1—O1—C1	−116.7 (2)	C1—C2—C7—C6	178.7 (3)
O2—Cd1—O1—C1	−3.40 (18)	C5—C6—C7—C2	2.3 (5)
O4—Cd1—O2—C1	−111.9 (2)	C4—C5—C8—O3	5.8 (7)
O1W—Cd1—O2—C1	−32.9 (3)	C6—C5—C8—O3	−173.0 (5)
N1—Cd1—O2—C1	156.09 (19)	Cd1—O4—C9—O5	14.3 (6)
N2—Cd1—O2—C1	89.3 (2)	Cd1—O4—C9—C10	−165.0 (2)
O1—Cd1—O2—C1	3.38 (18)	O5—C9—C10—C15	169.9 (3)
O1W—Cd1—O4—C9	−15.6 (3)	O4—C9—C10—C15	−10.7 (5)
N1—Cd1—O4—C9	−148.6 (3)	O5—C9—C10—C11	−11.1 (5)
N2—Cd1—O4—C9	−91.0 (4)	O4—C9—C10—C11	168.2 (3)
O1—Cd1—O4—C9	75.9 (3)	C15—C10—C11—C12	−0.4 (5)
O2—Cd1—O4—C9	127.0 (3)	C9—C10—C11—C12	−179.4 (3)
C1—Cd1—O4—C9	101.5 (3)	C10—C11—C12—C13	−0.4 (5)
O4—Cd1—N1—C17	−29.0 (3)	C11—C12—C13—C14	0.5 (5)
O1W—Cd1—N1—C17	−112.7 (3)	C11—C12—C13—C16	178.4 (4)
N2—Cd1—N1—C17	179.0 (3)	C12—C13—C14—C15	0.4 (5)
O1—Cd1—N1—C17	89.5 (3)	C16—C13—C14—C15	−177.6 (4)
O2—Cd1—N1—C17	59.8 (3)	C11—C10—C15—C14	1.3 (5)
C1—Cd1—N1—C17	71.1 (3)	C9—C10—C15—C14	−179.8 (3)
O4—Cd1—N1—C28	158.7 (2)	C13—C14—C15—C10	−1.3 (5)
O1W—Cd1—N1—C28	75.0 (2)	C14—C13—C16—O6	−179.9 (5)
N2—Cd1—N1—C28	6.61 (19)	C12—C13—C16—O6	2.2 (7)
O1—Cd1—N1—C28	−82.9 (2)	C28—N1—C17—C18	0.2 (5)
O2—Cd1—N1—C28	−112.6 (2)	Cd1—N1—C17—C18	−171.9 (3)
C1—Cd1—N1—C28	−101.3 (2)	N1—C17—C18—C19	−1.0 (6)
O4—Cd1—N2—C26	115.0 (3)	C17—C18—C19—C20	0.4 (6)
O1W—Cd1—N2—C26	40.4 (3)	C18—C19—C20—C28	0.8 (5)
N1—Cd1—N2—C26	177.5 (3)	C18—C19—C20—C21	−179.0 (4)
O1—Cd1—N2—C26	−52.4 (3)	C19—C20—C21—C22	178.5 (4)
O2—Cd1—N2—C26	−108.1 (3)	C28—C20—C21—C22	−1.3 (6)

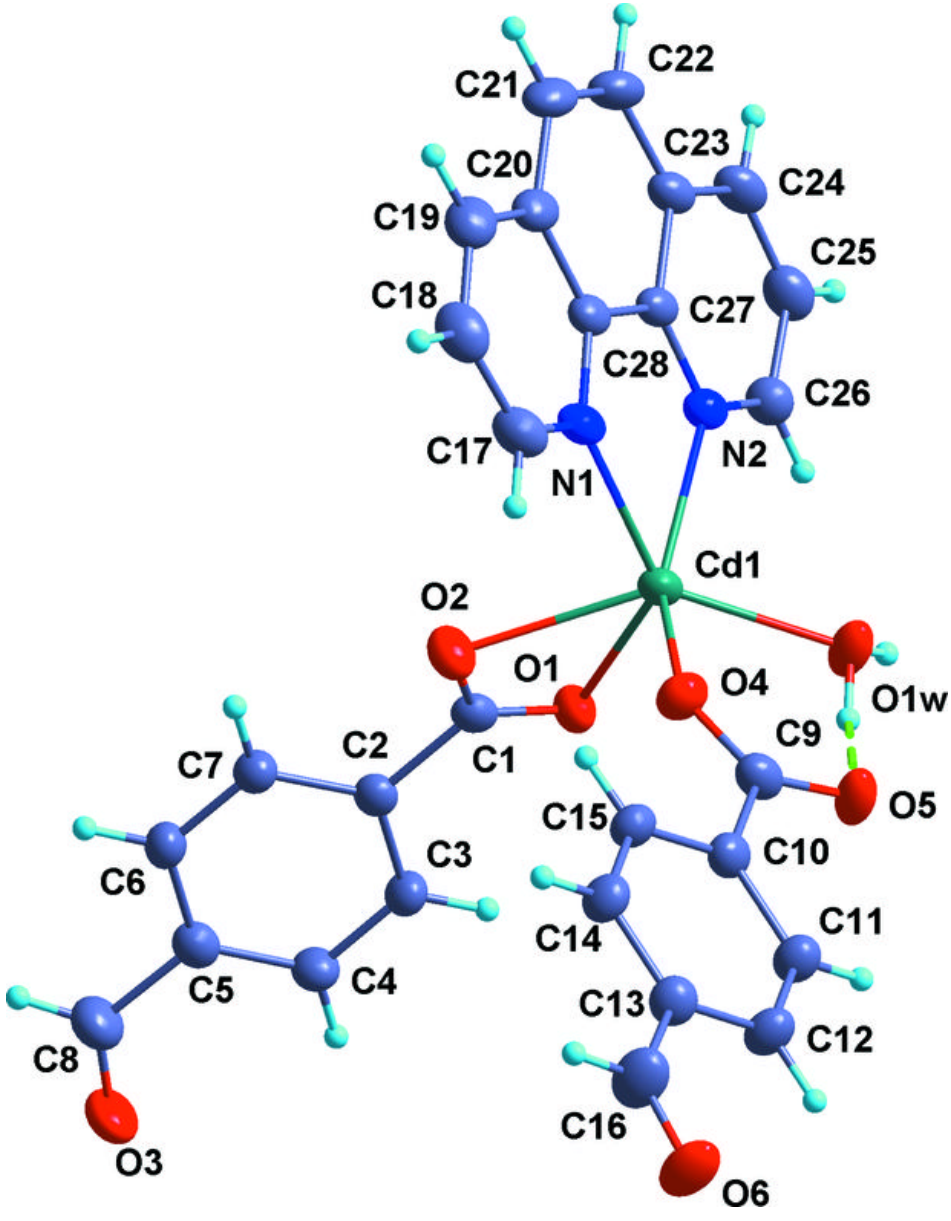
C1—Cd1—N2—C26	−78.5 (3)	C20—C21—C22—C23	1.3 (6)
O4—Cd1—N2—C27	−67.5 (3)	C21—C22—C23—C24	179.8 (4)
O1W—Cd1—N2—C27	−142.1 (2)	C21—C22—C23—C27	0.1 (5)
N1—Cd1—N2—C27	−4.96 (19)	C22—C23—C24—C25	−178.6 (3)
O1—Cd1—N2—C27	125.07 (19)	C27—C23—C24—C25	1.1 (5)
O2—Cd1—N2—C27	69.4 (2)	C23—C24—C25—C26	−0.5 (5)
C1—Cd1—N2—C27	99.0 (2)	C27—N2—C26—C25	−0.2 (5)
Cd1—O1—C1—O2	6.3 (3)	Cd1—N2—C26—C25	177.2 (3)
Cd1—O1—C1—C2	−172.9 (2)	C24—C25—C26—N2	0.0 (6)
Cd1—O2—C1—O1	−6.2 (3)	C26—N2—C27—C23	0.8 (4)
Cd1—O2—C1—C2	173.0 (2)	Cd1—N2—C27—C23	−176.9 (2)
O4—Cd1—C1—O1	−116.14 (19)	C26—N2—C27—C28	−179.3 (3)
O1W—Cd1—C1—O1	−28.2 (2)	Cd1—N2—C27—C28	3.0 (3)
N1—Cd1—C1—O1	148.7 (2)	C24—C23—C27—N2	−1.2 (4)
N2—Cd1—C1—O1	71.0 (2)	C22—C23—C27—N2	178.5 (3)
O2—Cd1—C1—O1	174.0 (3)	C24—C23—C27—C28	178.9 (3)
O4—Cd1—C1—O2	69.9 (2)	C22—C23—C27—C28	−1.4 (4)
O1W—Cd1—C1—O2	157.79 (18)	C17—N1—C28—C20	1.1 (4)
N1—Cd1—C1—O2	−25.3 (2)	Cd1—N1—C28—C20	174.1 (2)
N2—Cd1—C1—O2	−103.0 (2)	C17—N1—C28—C27	179.4 (3)
O1—Cd1—C1—O2	−174.0 (3)	Cd1—N1—C28—C27	−7.7 (3)
O1—C1—C2—C3	23.3 (4)	C19—C20—C28—N1	−1.6 (4)
O2—C1—C2—C3	−155.9 (3)	C21—C20—C28—N1	178.2 (3)
O1—C1—C2—C7	−157.6 (3)	C19—C20—C28—C27	−179.9 (3)
O2—C1—C2—C7	23.2 (4)	C21—C20—C28—C27	0.0 (4)
C7—C2—C3—C4	0.4 (5)	N2—C27—C28—N1	3.2 (4)
C1—C2—C3—C4	179.5 (3)	C23—C27—C28—N1	−176.9 (3)
C2—C3—C4—C5	1.2 (5)	N2—C27—C28—C20	−178.5 (3)
C3—C4—C5—C6	−1.1 (5)	C23—C27—C28—C20	1.4 (4)
C3—C4—C5—C8	−179.8 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O2^{i}	0.86 (5)	1.89 (5)	2.735 (4)	168 (5)
O1W—H1W2···O5	0.86 (5)	1.88 (3)	2.590 (4)	140 (5)

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

Fig. 1


C22
C21
C23
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C28
C26
C17
N1
N2
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O1
O4
O1w
C9
C2
C1
C7
C15
O5
C3
C10
C6
C14
C11
C5
C4
C13
C12
C8
C16
O3
O6

Fig. 2