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2,2′-[*m*-Phenylenebis(methyleneimino)]-dipyridinium dichloridobis(4-formylbenzoato-κ^2O,O')cadmate(II) dihydrate

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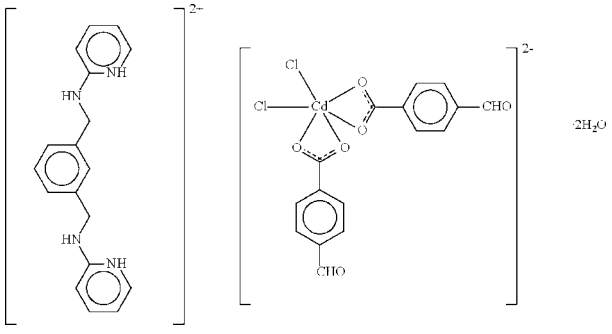
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.041; wR factor = 0.098; data-to-parameter ratio = 16.7.

The Cd^{II} atom in the title salt, $(C_{18}H_{20}N_4)[CdCl_2(C_8H_5O_3)_2]\cdot 2H_2O$, lies on a twofold rotation axis. It is chelated by the carboxylate group and exists in an octahedral geometry, with the Cl atoms *cis* to each other. The dication also lies on a twofold rotation axis. The cation and anion interact through one of the uncoordinated water molecules, forming a hydrogen-bonded chain structure that runs along the *a* axis.

Related literature

For the cadmium complexes with imidazole, benzimidazole and phenanthroline donor-ligands, see Deng *et al.* (2006*a*,*b*, 2007).



Experimental

Crystal data

$(C_{18}H_{20}N_4)[CdCl_2(C_8H_5O_3)_2]\cdot 2H_2O$
M_r = 809.95
Monoclinic, $P2/n$
a = 7.7856 (16) Å
b = 11.956 (2) Å
c = 18.509 (4) Å
β = 94.84 (3)°
V = 1716.8 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 295 (2) K
0.36 × 0.29 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.750, T_{max} = 0.862
16167 measured reflections
3918 independent reflections
2592 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.098
S = 1.10
3918 reflections
235 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −1.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···Cl1	0.86 (5)	2.37 (5)	3.209 (4)	167 (6)
O1W—H1W2···O1^{i}	0.86 (5)	2.21 (4)	3.035 (5)	167 (5)
N1—H1N···O1W	0.86 (4)	1.90 (4)	2.741 (6)	164 (5)
N2—H2N···O1W	0.86 (3)	2.49 (3)	3.164 (6)	136 (4)
N2—H2N···O1^{ii}	0.86 (3)	2.57 (4)	3.188 (5)	129 (4)

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

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: NG2347).

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  doi:10.1107/S1600536807052439

supplementary materials

Acta Cryst. (2007). E**63**, m2834 [**doi:10.1107/S1600536807052439**]

2,2'-[*m*-Phenylenebis(methyleneimino)]dipyridinium dichloridobis(4-formylbenzoato-κ^2O,O')cadmate(II) dihydrate

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

Comment

Cadmium bis(4-formylbenzoate) forms a hydrated 1:2 adduct with imidazole (Deng *et al.*, 2006*a*), two 1:1 aqua adducts with the larger benzimidazole ligand (Deng *et al.*, 2006*b*) as well as an adduct with 1,10-phenanthroline (Deng *et al.*, 2007). Replacing the these *N*-heterocycles by *N*,*N*'-(1,3-phenylenebis(methylene))dipyridin-2-amine furnishes the title compound as a salt whose anion has two 4-formylbenzoate ligands binding to the dichlorocadmium group; the *N*-heterocycle itself is displaced from the coordination sphere as it exists as a protonated cation (Fig.1). Hydrogen bonds link the cation, anion and lattice water into a chain structure along the *a* axis (Fig. 2).

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 *N*,*N*'-(1,3-phenylenebis(methylene))dipyridin-2-amine (2.92 g 10 mmol). Sodium hydroxide (0.1 *M*) was added dropwise until the pH value being 6. Colorless single crystals separated from the filtered solution after several days. CH&N analysis. Calc. for $C_{34}H_{34}N_4O_8Cl_2Cd$: C 50.42, H 4.23, N 6.92. Found: C 50.45, H 4.24, N 6.91.

Refinement

Carbon- and nitrogen bound H atoms were placed in calculated positions, with C—H = 0.93, N—H = 0.86 and U_{iso}(H) = 1.2U_{eq} (C,*N*), 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

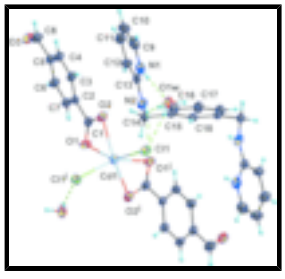


Fig. 1. **Figure 1**. Molecular structure of the title compound with 30% probability ellipsoid for the non-H atoms. Dashed lines indicate O—H···O hydrogen bonds.

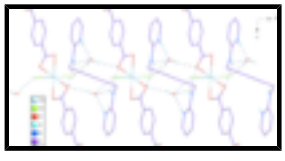


Fig. 2. **Figure 2**. Chain structure of the title complex along the *a* axis formed by hydrogen-bonding interactions, with the N—H···O O—H···O O—H···Cl hydrogen bonds denoted by dashed lines. H atoms not involved in hydrogen bonding have been omitted.

2,2'-[*m*-Phenylenebis(methyleneimino)]dipyridinium dichloridobis(4-formylbenzoato-κ^2O,O')cadmate(II) dihydrate

Crystal data

$(C_{18}H_{20}N_4)[CdCl_2(C_8H_5O_3)_2]\cdot 2H_2O$	F_{000} = 824
M_r = 809.95	D_x = 1.567 Mg m^{-3}
Monoclinic, *P*2/*n*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yac	Cell parameters from 10612 reflections
a = 7.7856 (16) Å	θ = 3.1–27.5º
b = 11.956 (2) Å	μ = 0.85 mm^{-1}
c = 18.509 (4) Å	*T* = 295 (2) K
β = 94.84 (3)º	Prism, colorless
V = 1716.8 (6) Å^3	0.36 × 0.29 × 0.18 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID diffractometer	3918 independent reflections
Radiation source: fine-focus sealed tube	2592 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.057
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 27.5º
T = 295(2) K	θ_{min} = 3.1º
ω scans	*h* = −10→9
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*k* = −15→15
T_{min} = 0.750, T_{max} = 0.862	*l* = −23→23
16167 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
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.098	$w = 1/[\sigma^2(F_o^2) + 4.8999P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max} < 0.001$
3918 reflections	$\Delta\rho_{max}$ = 1.18 e Å^{-3}
235 parameters	$\Delta\rho_{min}$ = −1.51 e Å^{-3}
5 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	0.7500	0.53198 (4)	0.2500	0.03870 (14)
Cl1	0.49551 (16)	0.65424 (11)	0.25523 (7)	0.0566 (3)
O1W	0.3005 (5)	0.4707 (4)	0.3449 (2)	0.0804 (12)
H1W1	0.337 (7)	0.526 (4)	0.321 (3)	0.121*
H1W2	0.201 (4)	0.452 (5)	0.327 (3)	0.121*
O1	0.9408 (4)	0.3811 (3)	0.30373 (16)	0.0529 (8)
O2	0.7587 (4)	0.4687 (3)	0.36951 (16)	0.0486 (8)
O3	1.1884 (5)	0.0472 (3)	0.6110 (2)	0.0783 (12)
N1	0.4510 (5)	0.3320 (3)	0.4498 (3)	0.0532 (10)
H1N	0.409 (6)	0.386 (3)	0.423 (2)	0.064*
N2	0.5264 (5)	0.2507 (3)	0.3447 (2)	0.0486 (10)
H2N	0.495 (6)	0.312 (2)	0.323 (2)	0.058*
C1	0.8746 (6)	0.3968 (4)	0.3627 (2)	0.0403 (10)
C2	0.9362 (5)	0.3271 (3)	0.4277 (2)	0.0357 (9)
C3	0.9058 (6)	0.3627 (4)	0.4967 (2)	0.0431 (11)
H3	0.8470	0.4293	0.5030	0.052*
C4	0.9632 (6)	0.2992 (4)	0.5562 (2)	0.0457 (11)
H4	0.9448	0.3241	0.6026	0.055*
C5	1.0478 (5)	0.1988 (4)	0.5477 (2)	0.0427 (11)
C6	1.0754 (6)	0.1623 (4)	0.4780 (2)	0.0466 (11)
H6	1.1304	0.0944	0.4715	0.056*
C7	1.0212 (6)	0.2268 (4)	0.4191 (2)	0.0447 (11)
H7	1.0419	0.2028	0.3728	0.054*
C8	1.1105 (7)	0.1334 (4)	0.6124 (3)	0.0597 (14)
H8	1.0878	0.1613	0.6575	0.072*
C9	0.4429 (7)	0.3363 (5)	0.5225 (3)	0.0658 (15)
H9	0.3978	0.3994	0.5434	0.079*
C10	0.4993 (7)	0.2502 (5)	0.5646 (3)	0.0691 (16)
H10	0.4947	0.2528	0.6146	0.083*
C11	0.5647 (7)	0.1570 (5)	0.5314 (3)	0.0615 (14)
H11	0.6045	0.0967	0.5598	0.074*
C12	0.5720 (6)	0.1522 (4)	0.4585 (2)	0.0466 (11)
H12	0.6138	0.0885	0.4371	0.056*
C13	0.5161 (5)	0.2434 (4)	0.4161 (2)	0.0421 (11)
C14	0.5600 (5)	0.1570 (4)	0.2978 (2)	0.0440 (11)
H14A	0.6432	0.1074	0.3233	0.053*
H14B	0.6106	0.1849	0.2552	0.053*
C15	0.3994 (5)	0.0913 (4)	0.2741 (2)	0.0342 (9)
C16	0.3974 (6)	−0.0243 (4)	0.2739 (2)	0.0499 (11)
H16	0.4962	−0.0637	0.2899	0.060*
C17	0.2500	−0.0812 (6)	0.2500	0.064 (2)
H17	0.2500	−0.1590	0.2500	0.076*
C18	0.2500	0.1479 (5)	0.2500	0.0358 (13)
H18	0.2500	0.2257	0.2500	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0447 (3)	0.0372 (3)	0.0335 (2)	0.000	−0.00057 (18)	0.000
Cl1	0.0639 (8)	0.0584 (8)	0.0477 (7)	0.0228 (6)	0.0067 (6)	0.0049 (6)
O1W	0.061 (2)	0.087 (3)	0.091 (3)	0.001 (2)	−0.007 (2)	0.033 (3)
O1	0.066 (2)	0.058 (2)	0.0358 (18)	0.0016 (17)	0.0064 (15)	0.0077 (16)
O2	0.0547 (19)	0.0426 (18)	0.0472 (18)	0.0057 (16)	−0.0026 (14)	0.0094 (16)
O3	0.100 (3)	0.062 (3)	0.070 (3)	0.033 (2)	−0.007 (2)	0.013 (2)
N1	0.048 (2)	0.043 (3)	0.067 (3)	−0.0032 (19)	−0.001 (2)	−0.004 (2)
N2	0.053 (2)	0.040 (2)	0.050 (2)	−0.0052 (19)	−0.0097 (19)	0.0072 (19)
C1	0.043 (3)	0.034 (2)	0.042 (3)	−0.007 (2)	−0.004 (2)	0.001 (2)
C2	0.034 (2)	0.036 (2)	0.036 (2)	−0.0032 (18)	−0.0009 (17)	0.0023 (19)
C3	0.048 (3)	0.038 (2)	0.042 (3)	0.005 (2)	−0.002 (2)	−0.001 (2)
C4	0.054 (3)	0.047 (3)	0.036 (2)	0.005 (2)	0.000 (2)	−0.004 (2)
C5	0.043 (3)	0.041 (3)	0.042 (3)	0.002 (2)	−0.003 (2)	0.006 (2)
C6	0.053 (3)	0.043 (3)	0.044 (3)	0.011 (2)	0.002 (2)	0.000 (2)
C7	0.048 (3)	0.049 (3)	0.036 (2)	0.006 (2)	0.003 (2)	−0.003 (2)
C8	0.074 (4)	0.057 (3)	0.047 (3)	0.010 (3)	0.000 (3)	0.009 (3)
C9	0.057 (3)	0.058 (4)	0.084 (4)	−0.011 (3)	0.016 (3)	−0.023 (3)
C10	0.076 (4)	0.085 (5)	0.049 (3)	−0.021 (3)	0.016 (3)	−0.016 (3)
C11	0.072 (4)	0.062 (4)	0.050 (3)	−0.007 (3)	0.004 (3)	0.006 (3)
C12	0.056 (3)	0.043 (3)	0.042 (3)	−0.002 (2)	0.008 (2)	0.002 (2)
C13	0.037 (2)	0.043 (3)	0.045 (3)	−0.011 (2)	−0.002 (2)	−0.004 (2)
C14	0.037 (2)	0.057 (3)	0.038 (2)	−0.002 (2)	0.0004 (19)	0.008 (2)
C15	0.036 (2)	0.041 (2)	0.027 (2)	0.0027 (19)	0.0061 (16)	0.0030 (19)
C16	0.053 (3)	0.043 (3)	0.053 (3)	0.009 (2)	−0.001 (2)	0.003 (2)
C17	0.072 (5)	0.035 (4)	0.081 (6)	0.000	−0.009 (4)	0.000
C18	0.042 (3)	0.033 (3)	0.032 (3)	0.000	0.004 (3)	0.000

Geometric parameters (Å, °)

Cd1—O2^{i}	2.333 (3)	C5—C6	1.396 (6)
Cd1—O2	2.333 (3)	C5—C8	1.477 (6)
Cd1—Cl1^{i}	2.4707 (12)	C6—C7	1.372 (6)
Cd1—Cl1	2.4707 (12)	C6—H6	0.9300
Cd1—O1^{i}	2.490 (3)	C7—H7	0.9300
Cd1—O1	2.490 (3)	C8—H8	0.9300
Cd1—C1^{i}	2.750 (4)	C9—C10	1.342 (8)
Cd1—C1	2.750 (4)	C9—H9	0.9300
O1W—H1W1	0.86 (5)	C10—C11	1.390 (7)
O1W—H1W2	0.86 (5)	C10—H10	0.9300
O1—C1	1.260 (5)	C11—C12	1.357 (6)
O2—C1	1.260 (5)	C11—H11	0.9300
O3—C8	1.197 (6)	C12—C13	1.392 (6)
N1—C13	1.350 (6)	C12—H12	0.9300
N1—C9	1.353 (7)	C14—C15	1.510 (6)

N1—H1N	0.86 (4)	C14—H14A	0.9700
N2—C13	1.332 (6)	C14—H14B	0.9700
N2—C14	1.455 (6)	C15—C16	1.382 (6)
N2—H2N	0.86 (3)	C15—C18	1.386 (5)
C1—C2	1.508 (6)	C16—C17	1.375 (6)
C2—C7	1.385 (6)	C16—H16	0.9300
C2—C3	1.387 (6)	C17—C16^{ii}	1.375 (6)
C3—C4	1.381 (6)	C17—H17	0.9300
C3—H3	0.9300	C18—C15^{ii}	1.386 (5)
C4—C5	1.384 (6)	C18—H18	0.9300
C4—H4	0.9300		
O2^{i}—Cd1—O2	142.15 (16)	C3—C4—C5	120.8 (4)
O2^{i}—Cd1—Cl1^{i}	96.55 (8)	C3—C4—H4	119.6
O2—Cd1—Cl1^{i}	105.65 (8)	C5—C4—H4	119.6
O2^{i}—Cd1—Cl1	105.65 (8)	C4—C5—C6	119.2 (4)
O2—Cd1—Cl1	96.55 (8)	C4—C5—C8	119.6 (4)
Cl1^{i}—Cd1—Cl1	107.45 (7)	C6—C5—C8	121.1 (4)
O2^{i}—Cd1—O1^{i}	54.40 (10)	C7—C6—C5	119.8 (4)
O2—Cd1—O1^{i}	96.45 (11)	C7—C6—H6	120.1
Cl1^{i}—Cd1—O1^{i}	150.04 (8)	C5—C6—H6	120.1
Cl1—Cd1—O1^{i}	89.47 (8)	C6—C7—C2	120.9 (4)
O2^{i}—Cd1—O1	96.45 (11)	C6—C7—H7	119.5
O2—Cd1—O1	54.40 (10)	C2—C7—H7	119.5
Cl1^{i}—Cd1—O1	89.47 (8)	O3—C8—C5	124.9 (5)
Cl1—Cd1—O1	150.04 (8)	O3—C8—H8	117.6
O1^{i}—Cd1—O1	87.16 (15)	C5—C8—H8	117.6
O2^{i}—Cd1—C1^{i}	27.16 (12)	C10—C9—N1	120.5 (5)
O2—Cd1—C1^{i}	120.56 (13)	C10—C9—H9	119.7
Cl1^{i}—Cd1—C1^{i}	123.42 (10)	N1—C9—H9	119.7
Cl1—Cd1—C1^{i}	98.32 (9)	C9—C10—C11	118.2 (5)
O1^{i}—Cd1—C1^{i}	27.24 (11)	C9—C10—H10	120.9
O1—Cd1—C1^{i}	92.15 (11)	C11—C10—H10	120.9
O2^{i}—Cd1—C1	120.56 (13)	C12—C11—C10	121.4 (5)
O2—Cd1—C1	27.16 (11)	C12—C11—H11	119.3
Cl1^{i}—Cd1—C1	98.32 (9)	C10—C11—H11	119.3
Cl1—Cd1—C1	123.42 (10)	C11—C12—C13	119.4 (5)
O1^{i}—Cd1—C1	92.15 (11)	C11—C12—H12	120.3
O1—Cd1—C1	27.24 (11)	C13—C12—H12	120.3
C1^{i}—Cd1—C1	108.00 (18)	N2—C13—N1	117.6 (4)
H1W1—O1W—H1W2	110 (5)	N2—C13—C12	124.6 (4)
C1—O1—Cd1	87.9 (3)	N1—C13—C12	117.7 (4)
C1—O2—Cd1	95.2 (3)	N2—C14—C15	112.8 (3)
C13—N1—C9	122.8 (5)	N2—C14—H14A	109.0
C13—N1—H1N	117 (3)	C15—C14—H14A	109.0

C9—N1—H1N	120 (4)	N2—C14—H14B	109.0
C13—N2—C14	124.8 (4)	C15—C14—H14B	109.0
C13—N2—H2N	119 (3)	H14A—C14—H14B	107.8
C14—N2—H2N	115 (3)	C16—C15—C18	118.6 (4)
O1—C1—O2	122.5 (4)	C16—C15—C14	122.0 (4)
O1—C1—C2	118.9 (4)	C18—C15—C14	119.4 (4)
O2—C1—C2	118.6 (4)	C17—C16—C15	120.3 (5)
O1—C1—Cd1	64.8 (2)	C17—C16—H16	119.8
O2—C1—Cd1	57.7 (2)	C15—C16—H16	119.8
C2—C1—Cd1	176.3 (3)	C16—C17—C16^{ii}	120.6 (7)
C7—C2—C3	119.4 (4)	C16—C17—H17	119.7
C7—C2—C1	120.7 (4)	C16^{ii}—C17—H17	119.7
C3—C2—C1	119.9 (4)	C15^{ii}—C18—C15	121.6 (6)
C4—C3—C2	119.8 (4)	C15^{ii}—C18—H18	119.2
C4—C3—H3	120.1	C15—C18—H18	119.2
C2—C3—H3	120.1		
O2^{i}—Cd1—O1—C1	−154.0 (2)	O2—C1—C2—C3	−19.0 (6)
O2—Cd1—O1—C1	−0.3 (2)	C7—C2—C3—C4	1.2 (6)
Cl1^{i}—Cd1—O1—C1	109.5 (2)	C1—C2—C3—C4	−179.6 (4)
Cl1—Cd1—O1—C1	−16.3 (3)	C2—C3—C4—C5	−1.4 (7)
O1^{i}—Cd1—O1—C1	−100.3 (3)	C3—C4—C5—C6	0.3 (7)
C1^{i}—Cd1—O1—C1	−127.1 (2)	C3—C4—C5—C8	178.9 (4)
O2^{i}—Cd1—O2—C1	46.1 (2)	C4—C5—C6—C7	1.0 (7)
Cl1^{i}—Cd1—O2—C1	−77.5 (3)	C8—C5—C6—C7	−177.6 (4)
Cl1—Cd1—O2—C1	172.3 (2)	C5—C6—C7—C2	−1.2 (7)
O1^{i}—Cd1—O2—C1	82.1 (3)	C3—C2—C7—C6	0.1 (7)
O1—Cd1—O2—C1	0.3 (2)	C1—C2—C7—C6	−179.1 (4)
C1^{i}—Cd1—O2—C1	68.6 (3)	C4—C5—C8—O3	−178.1 (5)
Cd1—O1—C1—O2	0.5 (4)	C6—C5—C8—O3	0.5 (8)
Cd1—O1—C1—C2	−179.5 (3)	C13—N1—C9—C10	−0.6 (8)
Cd1—O2—C1—O1	−0.5 (4)	N1—C9—C10—C11	−0.4 (8)
Cd1—O2—C1—C2	179.4 (3)	C9—C10—C11—C12	−0.1 (8)
O2^{i}—Cd1—C1—O1	30.4 (3)	C10—C11—C12—C13	1.4 (8)
O2—Cd1—C1—O1	179.5 (4)	C14—N2—C13—N1	−167.1 (4)
Cl1^{i}—Cd1—C1—O1	−72.3 (2)	C14—N2—C13—C12	14.7 (7)
Cl1—Cd1—C1—O1	170.4 (2)	C9—N1—C13—N2	−176.4 (4)
O1^{i}—Cd1—C1—O1	79.6 (3)	C9—N1—C13—C12	1.9 (7)
C1^{i}—Cd1—C1—O1	57.0 (2)	C11—C12—C13—N2	175.9 (4)
O2^{i}—Cd1—C1—O2	−149.1 (2)	C11—C12—C13—N1	−2.3 (7)
Cl1^{i}—Cd1—C1—O2	108.2 (2)	C13—N2—C14—C15	83.6 (5)
Cl1—Cd1—C1—O2	−9.2 (3)	N2—C14—C15—C16	−136.2 (4)
O1^{i}—Cd1—C1—O2	−100.0 (2)	N2—C14—C15—C18	45.5 (5)
O1—Cd1—C1—O2	−179.5 (4)	C18—C15—C16—C17	0.2 (6)
C1^{i}—Cd1—C1—O2	−122.5 (3)	C14—C15—C16—C17	−178.2 (3)

O1—C1—C2—C7	−19.8 (6)	C15—C16—C17—C16^{ii}	−0.1 (3)
O2—C1—C2—C7	160.3 (4)	C16—C15—C18—C15^{ii}	−0.1 (3)
O1—C1—C2—C3	161.0 (4)	C14—C15—C18—C15^{ii}	178.3 (4)

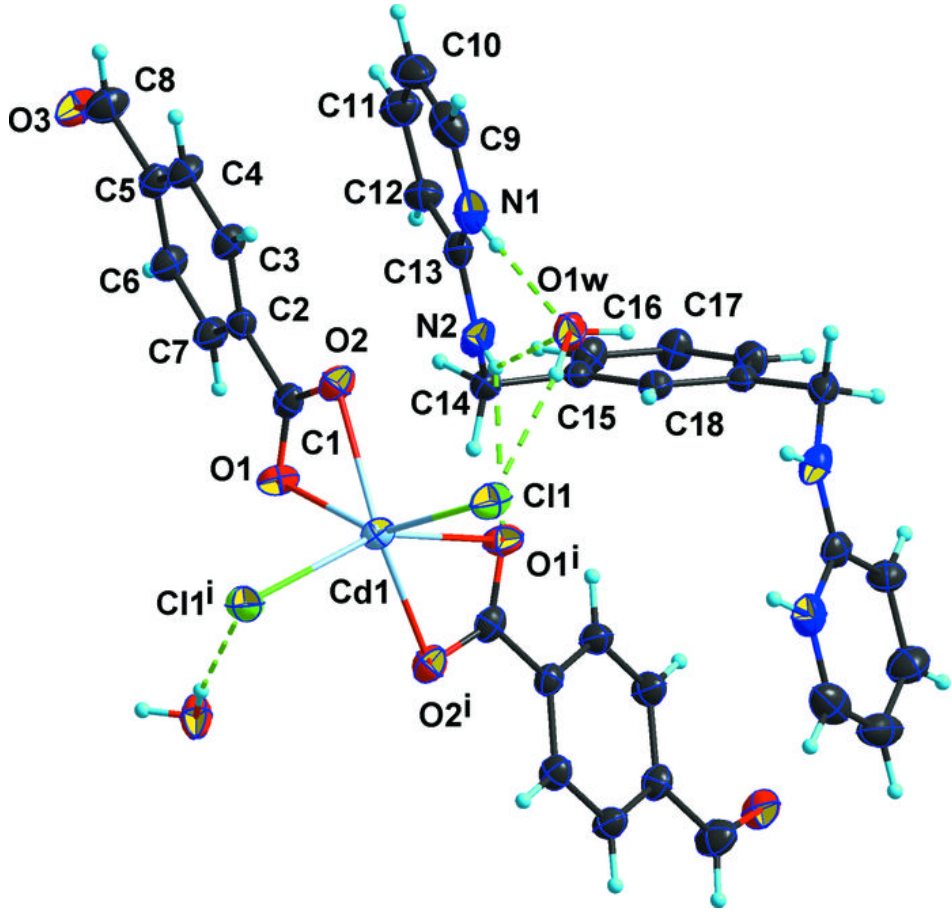
Symmetry codes: (i) −*x*+3/2, *y*, −*z*+1/2; (ii) −*x*+1/2, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···Cl1	0.86 (5)	2.37 (5)	3.209 (4)	167 (6)
O1W—H1W2···O1^{iii}	0.86 (5)	2.21 (4)	3.035 (5)	167 (5)
N1—H1N···O1W	0.86 (4)	1.90 (4)	2.741 (6)	164 (5)
N2—H2N···O1W	0.86 (3)	2.49 (3)	3.164 (6)	136 (4)
N2—H2N···O1^{i}	0.86 (3)	2.57 (4)	3.188 (5)	129 (4)

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

Fig. 1


C10
C8
O3
C11
C9
C5
C4
C12
N1
C6
C3
C13
O1w
C16
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C7
C2
N2
O2
C14
C15
C18
C1
O1
Cl1
O1i
Cl1i
Cd1
O2i

Fig. 2