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(Acetato-κ^2O,O')bis(1,10-phenanthroline-κ^2N,N')cadmium(II) perchlorate dihydrate

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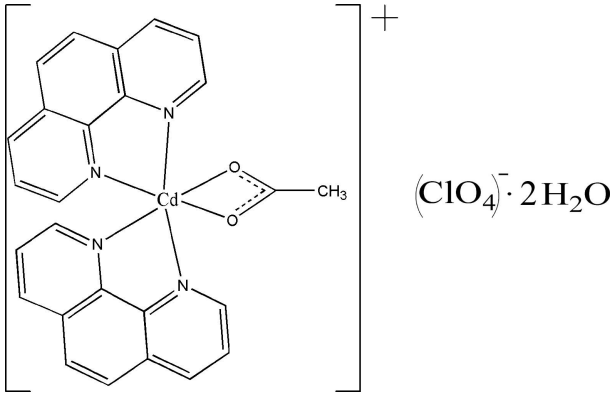
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.059; wR factor = 0.155; data-to-parameter ratio = 15.3.

In the title compound, $[Cd(C_2H_4O_2)(C_{12}H_8N_2)_2]ClO_4\cdot H_2O$, the Cu^{II} ion is in a distorted octahedral coordination geometry with normal Cd—O and Cd—N bond lengths. The cation and anion both lie on crystallographic twofold axes. In the crystal structure, intermolecular O—H···O hydrogen bonds form one-dimensional chains along [100] and in addition weak π–π stacking interactions connect molecules along [001]. The $Cg1$ (central fused benzene ring) and $Cg2$ (outer fused pyridine ring) centroid–centroid and perpendicular distances are 3.746 (2) and 3.623 (2) Å, respectively, with $Cg1\cdots Cg2^{i}$ = 3.602 (2) Å [symmetry code: (i) $-x, 1-y, 1-z$].

Related literature

The structure of a related Cd complex has been published (Zhang *et al.*, 2003).



$(ClO_4)^-\cdot 2H_2O$

Experimental

Crystal data

$[Cd(C_2H_4O_2)(C_{12}H_8N_2)_2]ClO_4\cdot 2H_2O$
M_r = 667.33
Monoclinic, $P2/c$
a = 9.887 (4) Å
b = 8.177 (4) Å
c = 17.791 (7) Å
β = 108.612 (19)°
V = 1363.1 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.96 mm^{-1}
T = 298 (2) K
0.32 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
8986 measured reflections
3118 independent reflections
2584 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.155
S = 1.05
3118 reflections
204 parameters
64 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N1	2.308 (4)	Cd1—O1	2.341 (4)
Cd1—N2	2.327 (4)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O5^{i}	0.84 (2)	2.34 (3)	3.165 (6)	168 (10)
O1W—H1WA···O2^{ii}	0.84 (2)	2.58 (8)	3.230 (13)	135 (9)
O1W—H1WB···O1^{iii}	0.86 (2)	1.93 (6)	2.713 (6)	152 (10)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2380).

References

Bruker (2000). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2001). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Zhang, X. J., Tian, Y. P., Li, S. L. & Jiang, M. H. (2003). *Polyhedron*, **22**, 397–402.

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supplementary materials

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(Acetato-κ^2O,O')bis(1,10-phenanthroline-κ^2N,N')cadmium(II) perchlorate dihydrate

B. Hu, M. Wang, S.-M. Lan, X.-Y. Wang and X.-T. Deng

Comment

The formula unit of (I) comprises a monnuclear $[Cd(phen)_2(CH_3COO)]^+$ cation (Fig. 1), a perchlorate anion and a hydrate. The Cd^{II} ion is in a distorted octahedral CdN_4O_2 geometry coordinated by four N atoms of phen ligands and two O atoms of a chelating bidentate acetato anion. By virtue of the twofold symmetry, atoms C13, C14, O1, O1b atoms are exactly planar (Zhang *et al.*, 2003)[symmety code: (*b*) −*x*, *y*, 1/2 − *z*]. In the crystal structure, one-dimensional chains along [100] are formed by intermolecular O_{water}—H···$O_{perchlorate}$ and O_{water} –H···O_{water} hydrogen bonds (Fig. 2. and Table 2). In addition weak π-π stacking interactions form chains along [001] as shown in Fig.3. *Cg*1 and *Cg*2 are the centroids defined by atoms C4/C5/C6/C7/C11/C12 and N2/C7/C8/C9/C10/C11, respectively. The relevant centroid–centroid and perpendicular distances defining these interactions are 3.746 (2), and 3.623 and 3.602 Å for *Cg*1··· *Cg*2^i [symmety code:(i) −*x*,1 − *y*,1 − *z*].

Experimental

$Cd(CH_3COO)_2 \cdot 2(H_2O)$(0.266 g, 1 mmol), $NaClO_4$ (0.14 g, 1 mmol) phen (0.396 g, 2 mmol) were dissolved in a water-methanol solution (40 ml, 1:1). The mixture was refluxed for 4 h, and then filtered after cooling to room temperature. Single crystals of (I) were obtained after two weeks.

Refinement

H atoms bonded to O atoms were located in difference maps and then included in the refinement with bond-length restraints of O – H = 0.82 (2) Å, with 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—0.96 Å and U_{iso}(H) = 1.2U_{eq} (C of aromatic) or 1.5U_{eq}(C of methyl). Atoms O2/O3/O4 of the perchlorate anion are disordered over a twofold axis with equal occupancies. The largest peak of 1.18 $Å^{-3}$ in the final differnce Fourier is close to atom Cl1.

Figures

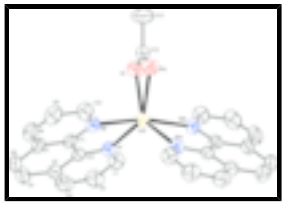

Fig. 1. The cation of (I), with displacement ellipsoids drawn at the 50% probability level. The H atoms, disordered perchlorate and water molecules have been omitted for clarity. [symmetry code:(*b*) −*x*, *y*, 1/2 − *z*]

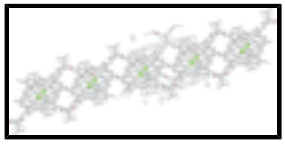

Fig. 2. Part of the crystal structure of (I), showing the formation of hydrogen-bonded (dashed lines) one-dimensional chains.

Fig. 3. Part of the crystal structure of (I), showing the formation of π-π stacking (dashed lines) interactions.

(Acetato-κ^2*O*,*O*')bis(1,10-phenanthroline-κ^2*N*,*N*')cadmium(II) perchlorate dihydrate

Crystal data

$[Cd(C_2H_4O_2)(C_{12}H_8N_2)_2]ClO_4{\cdot}2H_2O$	F_{000} = 672
M_r = 667.33	D_x = 1.626 Mg m^{-3}
Monoclinic, *P*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yc	Cell parameters from 3241 reflections
a = 9.887 (4) Å	θ = 2.2–23.0º
b = 8.177 (4) Å	μ = 0.96 mm^{-1}
c = 17.791 (7) Å	*T* = 298 (2) K
β = 108.612 (19)º	Block, colorless
V = 1363.1 (10) Å^3	0.32 × 0.30 × 0.30 mm
Z = 2	

Data collection

Bruker SMART CCD diffractometer	2584 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.058
Monochromator: graphite	θ_{max} = 27.5º
T = 298(2) K	θ_{min} = 2.2º
φ and ω scans	*h* = −12→12
Absorption correction: none	*k* = −10→10
8986 measured reflections	*l* = −23→17
3118 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.059	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.155	$w = 1/[\sigma^2(F_o^2) + (0.0965P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
3118 reflections	$\Delta\rho_{max}$ = 1.27 e Å^{-3}
204 parameters	$\Delta\rho_{min}$ = −0.59 e Å^{-3}
64 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}	Occ. (<1)
Cd1	0.0000	0.53861 (6)	0.2500	0.0522 (2)	
O1	−0.1072 (4)	0.2850 (5)	0.2079 (2)	0.0759 (10)	
N1	−0.1344 (4)	0.6807 (5)	0.1392 (2)	0.0553 (9)	
N2	0.1397 (4)	0.5700 (5)	0.1676 (2)	0.0551 (9)	
C1	−0.2671 (6)	0.7337 (7)	0.1252 (3)	0.0695 (13)	
H1	−0.3124	0.7125	0.1626	0.083*	
C2	−0.3405 (7)	0.8187 (8)	0.0577 (4)	0.0831 (16)	
H2	−0.4324	0.8569	0.0504	0.100*	
C3	−0.2761 (7)	0.8454 (7)	0.0025 (4)	0.0840 (17)	
H3	−0.3252	0.9008	−0.0439	0.101*	
C4	−0.1383 (6)	0.7917 (6)	0.0134 (3)	0.0657 (13)	
C5	−0.0647 (8)	0.8114 (8)	−0.0436 (3)	0.0844 (17)	
H5	−0.1112	0.8633	−0.0914	0.101*	
C6	0.0664 (8)	0.7584 (8)	−0.0305 (3)	0.0829 (18)	
H6	0.1110	0.7770	−0.0685	0.099*	
C7	0.1428 (6)	0.6720 (7)	0.0411 (3)	0.0663 (13)	
C8	0.2802 (7)	0.6092 (8)	0.0557 (4)	0.0798 (17)	
H8	0.3280	0.6230	0.0189	0.096*	
C9	0.3412 (7)	0.5300 (9)	0.1227 (5)	0.0847 (19)	
H9	0.4324	0.4875	0.1324	0.102*	
C10	0.2714 (6)	0.5085 (8)	0.1795 (4)	0.0730 (14)	
H10	0.3166	0.4511	0.2258	0.088*	
C11	0.0762 (5)	0.6493 (5)	0.0986 (3)	0.0531 (10)	
C12	−0.0698 (5)	0.7090 (5)	0.0842 (2)	0.0519 (10)	
C13	0.0000	0.2084 (9)	0.2500	0.0667 (19)	
C14	0.0000	0.0252 (12)	0.2500	0.130 (5)	
H14A	−0.0764	−0.0139	0.2053	0.195*	0.50
H14B	−0.0130	−0.0139	0.2981	0.195*	0.50
H14C	0.0894	−0.0139	0.2466	0.195*	0.50
O1W	0.6176 (5)	0.2737 (11)	0.1119 (3)	0.130 (2)	
O2	0.487 (2)	0.9428 (11)	0.3240 (6)	0.155 (6)	0.50
O3	0.6310 (13)	0.9327 (13)	0.2453 (14)	0.280 (14)	0.50
O4	0.3858 (18)	0.9310 (14)	0.1877 (9)	0.68 (6)	0.50

O5	0.5000	1.1640 (7)	0.2500	0.414 (15)
Cl1	0.5000	0.9901 (4)	0.2500	0.1092 (10)
H1WA	0.593 (9)	0.231 (12)	0.148 (4)	0.164*
H1WB	0.700 (6)	0.312 (12)	0.138 (4)	0.164*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0537 (3)	0.0570 (3)	0.0476 (3)	0.000	0.0184 (2)	0.000
O1	0.078 (2)	0.070 (2)	0.071 (2)	−0.0126 (19)	0.0116 (19)	−0.0031 (19)
N1	0.053 (2)	0.057 (2)	0.055 (2)	−0.0023 (17)	0.0175 (17)	−0.0029 (17)
N2	0.048 (2)	0.061 (2)	0.057 (2)	−0.0040 (16)	0.0187 (17)	−0.0046 (17)
C1	0.058 (3)	0.075 (3)	0.073 (3)	0.007 (2)	0.018 (3)	0.001 (3)
C2	0.072 (4)	0.081 (4)	0.086 (4)	0.014 (3)	0.011 (3)	0.010 (3)
C3	0.089 (4)	0.075 (4)	0.070 (4)	0.010 (3)	0.000 (3)	0.009 (3)
C4	0.081 (3)	0.058 (3)	0.052 (3)	−0.008 (2)	0.012 (2)	−0.001 (2)
C5	0.113 (5)	0.084 (4)	0.053 (3)	−0.013 (4)	0.022 (3)	0.006 (3)
C6	0.117 (5)	0.087 (4)	0.058 (3)	−0.026 (4)	0.047 (3)	−0.011 (3)
C7	0.082 (3)	0.067 (3)	0.059 (3)	−0.022 (3)	0.035 (3)	−0.018 (2)
C8	0.080 (4)	0.093 (4)	0.082 (4)	−0.024 (3)	0.049 (3)	−0.027 (4)
C9	0.057 (3)	0.101 (5)	0.105 (5)	−0.004 (3)	0.038 (3)	−0.024 (4)
C10	0.056 (3)	0.085 (3)	0.081 (4)	0.002 (3)	0.026 (3)	−0.004 (3)
C11	0.058 (3)	0.052 (2)	0.050 (2)	−0.0127 (19)	0.019 (2)	−0.0140 (19)
C12	0.063 (3)	0.046 (2)	0.045 (2)	−0.0106 (19)	0.0150 (19)	−0.0072 (17)
C13	0.098 (6)	0.052 (4)	0.055 (4)	0.000	0.032 (4)	0.000
C14	0.194 (16)	0.055 (5)	0.131 (11)	0.000	0.039 (11)	0.000
O1W	0.069 (3)	0.202 (7)	0.113 (4)	0.007 (4)	0.020 (3)	0.048 (4)
O2	0.145 (9)	0.180 (10)	0.145 (9)	−0.008 (7)	0.050 (7)	0.058 (7)
O3	0.285 (16)	0.296 (17)	0.277 (16)	0.038 (10)	0.114 (11)	−0.010 (10)
O4	0.68 (6)	0.69 (6)	0.68 (6)	−0.009 (11)	0.22 (2)	−0.015 (11)
O5	0.424 (17)	0.394 (17)	0.439 (17)	0.000	0.158 (11)	0.000
Cl1	0.155 (3)	0.0983 (16)	0.101 (2)	0.000	0.078 (2)	0.000

Geometric parameters (Å, °)

Cd1—N1^{i}	2.308 (4)	C8—C9	1.320 (10)
Cd1—N1	2.308 (4)	C8—H8	0.9300
Cd1—N2^{i}	2.327 (4)	C9—C10	1.405 (9)
Cd1—N2	2.327 (4)	C9—H9	0.9300
Cd1—O1	2.341 (4)	C10—H10	0.9300
Cd1—O1^{i}	2.341 (4)	C11—C12	1.467 (6)
Cd1—C13	2.700 (7)	C13—O1^{i}	1.253 (5)
O1—C13	1.253 (5)	C13—C14	1.498 (11)
N1—C1	1.328 (6)	C14—H14A	0.9600
N1—C12	1.348 (6)	C14—H14B	0.9600
N2—C10	1.348 (7)	C14—H14C	0.9600
N2—C11	1.352 (6)	O1W—H1WA	0.84 (2)
C1—C2	1.376 (8)	O1W—H1WB	0.86 (2)

C1—H1	0.9300	O2—O4^{ii}	1.345 (17)
C2—C3	1.349 (9)	O2—O3^{ii}	1.403 (15)
C2—H2	0.9300	O2—Cl1	1.419 (5)
C3—C4	1.385 (8)	O3—O4^{ii}	1.254 (16)
C3—H3	0.9300	O3—O2^{ii}	1.403 (15)
C4—C12	1.399 (7)	O3—Cl1	1.405 (6)
C4—C5	1.434 (8)	O4—O3^{ii}	1.254 (16)
C5—C6	1.315 (9)	O4—O2^{ii}	1.345 (17)
C5—H5	0.9300	O4—Cl1	1.392 (6)
C6—C7	1.442 (9)	O5—Cl1	1.422 (6)
C6—H6	0.9300	Cl1—O4^{ii}	1.392 (6)
C7—C11	1.395 (6)	Cl1—O3^{ii}	1.405 (6)
C7—C8	1.397 (9)	Cl1—O2^{ii}	1.419 (5)
N1^{i}—Cd1—N1	119.55 (19)	C10—C9—H9	119.2
N1^{i}—Cd1—N2^{i}	72.68 (14)	N2—C10—C9	120.8 (6)
N1—Cd1—N2^{i}	100.75 (14)	N2—C10—H10	119.6
N1^{i}—Cd1—N2	100.75 (14)	C9—C10—H10	119.6
N1—Cd1—N2	72.68 (14)	N2—C11—C7	122.5 (5)
N2^{i}—Cd1—N2	167.32 (19)	N2—C11—C12	117.7 (4)
N1^{i}—Cd1—O1	142.90 (14)	C7—C11—C12	119.8 (5)
N1—Cd1—O1	95.42 (14)	N1—C12—C4	122.1 (5)
N2^{i}—Cd1—O1	89.99 (14)	N1—C12—C11	118.9 (4)
N2—Cd1—O1	101.29 (13)	C4—C12—C11	119.0 (4)
N1^{i}—Cd1—O1^{i}	95.42 (14)	O1^{i}—C13—O1	120.0 (7)
N1—Cd1—O1^{i}	142.90 (14)	O1^{i}—C13—C14	120.0 (3)
N2^{i}—Cd1—O1^{i}	101.29 (13)	O1—C13—C14	120.0 (3)
N2—Cd1—O1^{i}	89.99 (14)	O1^{i}—C13—Cd1	60.0 (3)
O1—Cd1—O1^{i}	55.2 (2)	O1—C13—Cd1	60.0 (3)
N1^{i}—Cd1—C13	120.22 (10)	C14—C13—Cd1	180.000 (1)
N1—Cd1—C13	120.22 (10)	C13—C14—H14A	109.5
N2^{i}—Cd1—C13	96.34 (9)	C13—C14—H14B	109.5
N2—Cd1—C13	96.34 (9)	H14A—C14—H14B	109.5
O1—Cd1—C13	27.62 (10)	C13—C14—H14C	109.5
O1^{i}—Cd1—C13	27.62 (10)	H14A—C14—H14C	109.5
C13—O1—Cd1	92.4 (4)	H14B—C14—H14C	109.5
C1—N1—C12	118.4 (4)	H1WA—O1W—H1WB	100 (3)
C1—N1—Cd1	126.2 (3)	O4^{ii}—O2—O3^{ii}	114.5 (10)
C12—N1—Cd1	115.5 (3)	O4^{ii}—O2—Cl1	60.4 (5)
C10—N2—C11	117.9 (4)	O3^{ii}—O2—Cl1	59.7 (4)
C10—N2—Cd1	126.7 (4)	O4^{ii}—O3—O2^{ii}	120.8 (10)
C11—N2—Cd1	115.3 (3)	O4^{ii}—O3—Cl1	62.8 (5)
N1—C1—C2	122.9 (5)	O2^{ii}—O3—Cl1	60.7 (4)

N1—C1—H1	118.5	$O3^{ii}$—O4—$O2^{ii}$	124.2 (10)
C2—C1—H1	118.5	$O3^{ii}$—O4—Cl1	63.9 (5)
C3—C2—C1	118.5 (6)	$O2^{ii}$—O4—Cl1	62.4 (5)
C3—C2—H2	120.7	$O4^{ii}$—Cl1—O4	139.3 (10)
C1—C2—H2	120.7	$O4^{ii}$—Cl1—O3	53.3 (7)
C2—C3—C4	121.2 (5)	O4—Cl1—O3	111.5 (5)
C2—C3—H3	119.4	$O4^{ii}$—Cl1—$O3^{ii}$	111.5 (5)
C4—C3—H3	119.4	O4—Cl1—$O3^{ii}$	53.3 (7)
C3—C4—C12	116.8 (5)	O3—Cl1—$O3^{ii}$	141.0 (10)
C3—C4—C5	124.3 (5)	$O4^{ii}$—Cl1—$O2^{ii}$	110.6 (5)
C12—C4—C5	118.8 (5)	O4—Cl1—$O2^{ii}$	57.2 (7)
C6—C5—C4	122.1 (5)	O3—Cl1—$O2^{ii}$	59.6 (6)
C6—C5—H5	118.9	$O3^{ii}$—Cl1—$O2^{ii}$	108.9 (5)
C4—C5—H5	118.9	$O4^{ii}$—Cl1—O2	57.2 (7)
C5—C6—C7	121.8 (5)	O4—Cl1—O2	110.6 (5)
C5—C6—H6	119.1	O3—Cl1—O2	108.9 (5)
C7—C6—H6	119.1	$O3^{ii}$—Cl1—O2	59.6 (6)
C11—C7—C8	118.3 (5)	$O2^{ii}$—Cl1—O2	148.3 (8)
C11—C7—C6	118.5 (5)	$O4^{ii}$—Cl1—O5	110.3 (5)
C8—C7—C6	123.2 (5)	O4—Cl1—O5	110.3 (5)
C9—C8—C7	119.0 (5)	O3—Cl1—O5	109.5 (5)
C9—C8—H8	120.5	$O3^{ii}$—Cl1—O5	109.5 (5)
C7—C8—H8	120.5	$O2^{ii}$—Cl1—O5	105.8 (4)
C8—C9—C10	121.5 (6)	O2—Cl1—O5	105.8 (4)
C8—C9—H9	119.2		
$N1^{i}$—Cd1—O1—C13	−43.4 (3)	C1—N1—C12—C4	−0.1 (7)
N1—Cd1—O1—C13	155.4 (2)	Cd1—N1—C12—C4	179.1 (3)
$N2^{i}$—Cd1—O1—C13	−103.8 (2)	C1—N1—C12—C11	−179.3 (4)
N2—Cd1—O1—C13	82.0 (2)	Cd1—N1—C12—C11	0.0 (5)
$O1^{i}$—Cd1—O1—C13	0.0	C3—C4—C12—N1	0.7 (7)
$N1^{i}$—Cd1—N1—C1	−87.6 (4)	C5—C4—C12—N1	−177.5 (5)
$N2^{i}$—Cd1—N1—C1	−11.5 (4)	C3—C4—C12—C11	179.8 (4)
N2—Cd1—N1—C1	179.7 (4)	C5—C4—C12—C11	1.7 (7)
O1—Cd1—N1—C1	79.5 (4)	N2—C11—C12—N1	−0.9 (6)
$O1^{i}$—Cd1—N1—C1	114.1 (4)	C7—C11—C12—N1	177.6 (4)
C13—Cd1—N1—C1	92.4 (4)	N2—C11—C12—C4	179.9 (4)
$N1^{i}$—Cd1—N1—C12	93.3 (3)	C7—C11—C12—C4	−1.6 (6)
$N2^{i}$—Cd1—N1—C12	169.3 (3)	Cd1—O1—C13—$O1^{i}$	0.0
N2—Cd1—N1—C12	0.5 (3)	Cd1—O1—C13—C14	180.0
O1—Cd1—N1—C12	−99.7 (3)	$N1^{i}$—Cd1—C13—$O1^{i}$	−28.7 (2)
$O1^{i}$—Cd1—N1—C12	−65.1 (4)	N1—Cd1—C13—$O1^{i}$	151.3 (2)
C13—Cd1—N1—C12	−86.7 (3)	$N2^{i}$—Cd1—C13—$O1^{i}$	−102.3 (2)
$N1^{i}$—Cd1—N2—C10	65.9 (5)	N2—Cd1—C13—$O1^{i}$	77.7 (2)

N1—Cd1—N2—C10	−176.3 (5)	O1—Cd1—C13—O1^{i}	180.0
N2^{i}—Cd1—N2—C10	123.5 (4)	N1^{i}—Cd1—C13—O1	151.3 (2)
O1—Cd1—N2—C10	−84.0 (4)	N1—Cd1—C13—O1	−28.7 (2)
O1^{i}—Cd1—N2—C10	−29.6 (4)	N2^{i}—Cd1—C13—O1	77.7 (2)
C13—Cd1—N2—C10	−56.5 (4)	N2—Cd1—C13—O1	−102.3 (2)
N1^{i}—Cd1—N2—C11	−118.8 (3)	O1^{i}—Cd1—C13—O1	180.0
N1—Cd1—N2—C11	−1.0 (3)	O3^{ii}—O4—Cl1—O4^{ii}	80.3 (7)
N2^{i}—Cd1—N2—C11	−61.3 (3)	O2^{ii}—O4—Cl1—O4^{ii}	−83.8 (6)
O1—Cd1—N2—C11	91.2 (3)	O3^{ii}—O4—Cl1—O3	138.4 (12)
O1^{i}—Cd1—N2—C11	145.7 (3)	O2^{ii}—O4—Cl1—O3	−25.7 (10)
C13—Cd1—N2—C11	118.7 (3)	O2^{ii}—O4—Cl1—O3^{ii}	−164.2 (12)
C12—N1—C1—C2	−1.2 (8)	O3^{ii}—O4—Cl1—O2^{ii}	164.2 (12)
Cd1—N1—C1—C2	179.7 (5)	O3^{ii}—O4—Cl1—O2	17.1 (12)
N1—C1—C2—C3	1.9 (10)	O2^{ii}—O4—Cl1—O2	−147.1 (9)
C1—C2—C3—C4	−1.2 (10)	O3^{ii}—O4—Cl1—O5	−99.7 (7)
C2—C3—C4—C12	0.0 (9)	O2^{ii}—O4—Cl1—O5	96.2 (6)
C2—C3—C4—C5	178.1 (6)	O2^{ii}—O3—Cl1—O4^{ii}	161.4 (12)
C3—C4—C5—C6	180.0 (6)	O4^{ii}—O3—Cl1—O4	−136.3 (12)
C12—C4—C5—C6	−2.0 (9)	O2^{ii}—O3—Cl1—O4	25.0 (10)
C4—C5—C6—C7	2.1 (10)	O4^{ii}—O3—Cl1—O3^{ii}	−78.7 (8)
C5—C6—C7—C11	−2.0 (9)	O2^{ii}—O3—Cl1—O3^{ii}	82.7 (6)
C5—C6—C7—C8	177.8 (6)	O4^{ii}—O3—Cl1—O2^{ii}	−161.4 (12)
C11—C7—C8—C9	0.6 (8)	O4^{ii}—O3—Cl1—O2	−14.0 (11)
C6—C7—C8—C9	−179.2 (6)	O2^{ii}—O3—Cl1—O2	147.4 (9)
C7—C8—C9—C10	−0.4 (10)	O4^{ii}—O3—Cl1—O5	101.3 (8)
C11—N2—C10—C9	1.6 (8)	O2^{ii}—O3—Cl1—O5	−97.3 (6)
Cd1—N2—C10—C9	176.7 (4)	O3^{ii}—O2—Cl1—O4^{ii}	−152.0 (10)
C8—C9—C10—N2	−0.7 (10)	O4^{ii}—O2—Cl1—O4	136.2 (12)
C10—N2—C11—C7	−1.4 (7)	O3^{ii}—O2—Cl1—O4	−15.9 (11)
Cd1—N2—C11—C7	−177.1 (3)	O4^{ii}—O2—Cl1—O3	13.4 (11)
C10—N2—C11—C12	177.1 (4)	O3^{ii}—O2—Cl1—O3	−138.7 (11)
Cd1—N2—C11—C12	1.3 (5)	O4^{ii}—O2—Cl1—O3^{ii}	152.0 (10)
C8—C7—C11—N2	0.3 (7)	O4^{ii}—O2—Cl1—O2^{ii}	75.7 (7)
C6—C7—C11—N2	−179.9 (5)	O3^{ii}—O2—Cl1—O2^{ii}	−76.3 (6)
C8—C7—C11—C12	−178.1 (5)	O4^{ii}—O2—Cl1—O5	−104.3 (7)
C6—C7—C11—C12	1.7 (7)	O3^{ii}—O2—Cl1—O5	103.7 (6)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O5^{iii}	0.84 (2)	2.34 (3)	3.165 (6)	168 (10)

O1W—H1WA···O2^{iv}	0.84 (2)	2.58 (8)	3.230 (13)	135 (9)
O1W—H1WB···O1^{v}	0.86 (2)	1.93 (6)	2.713 (6)	152 (10)

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

Fig. 1

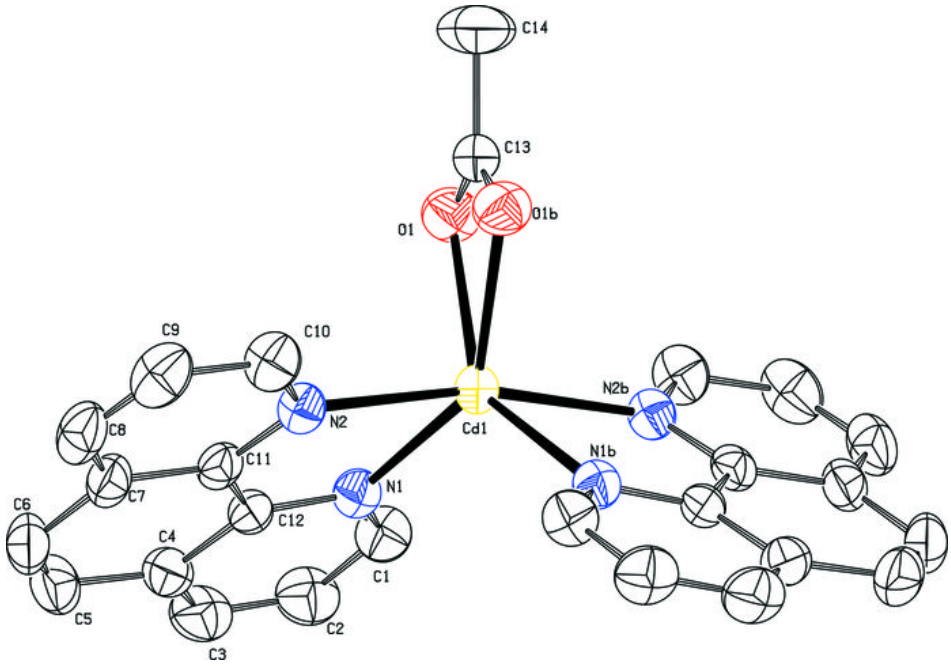
C14
C13
O1
O1b
C9
C10
N2
C8
C11
C7
C6
C12
N1
C4
C1
C5
C2
C3
Cd1
N2b
N1b

Fig. 2

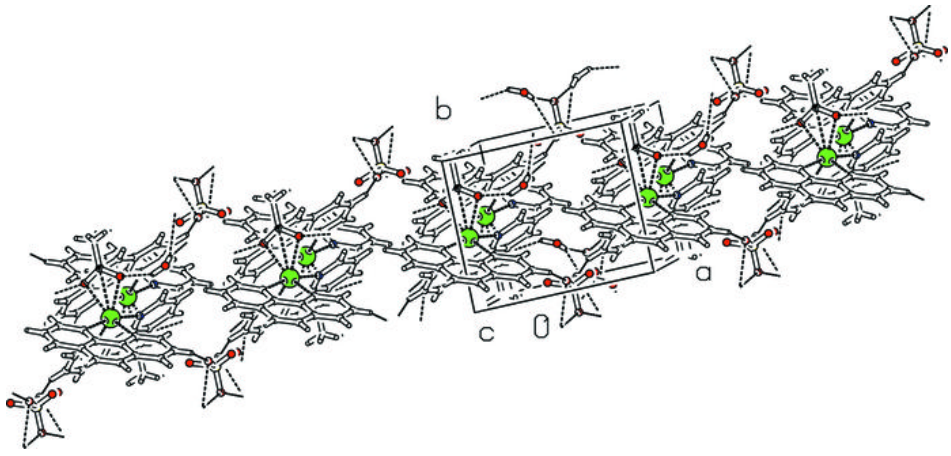

Fig. 3