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Dichlorido[2,2′-(1,10-phenanthrolin-2-ylimino)diethanol]cadmium(II)

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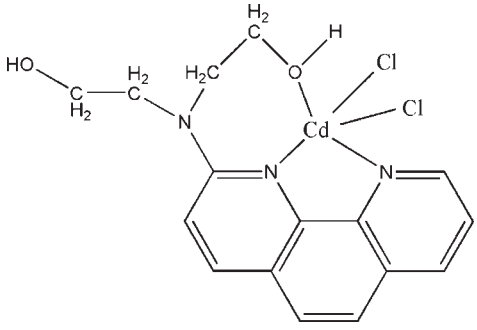
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.087; data-to-parameter ratio = 16.8.

In the title complex, $[CdCl_2(C_{16}H_{17}N_3O_2)]$, the metal atom exhibits a distorted trigonal-bipyramidal coordination geometry. O—H···O and O—H···Cl hydrogen bonds involving hydroxy groups and one of coordinated Cl atoms link complexes in the crystal packing. There is a π–π stacking interaction between adjacent 1,10-phenanthroline rings, with a distance of 3.675 (2) Å between the centroids of the pyridine and benzene rings.

Related literature

For related structures, see: Jin & Li (2009); Zhang *et al.* (2008).



Experimental

Crystal data

$[CdCl_2(C_{16}H_{17}N_3O_2)]$
M_r = 466.63
Monoclinic, $P2_1/n$
a = 7.9435 (15) Å
b = 22.548 (4) Å
c = 9.5216 (18) Å
β = 98.808 (3)°
V = 1685.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.63 mm^{-1}
T = 298 K
0.24 × 0.11 × 0.05 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.696, T_{max} = 0.923
9776 measured reflections
3641 independent reflections
2933 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.087
S = 1.03
3641 reflections
217 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N3	2.235 (3)	Cd1—Cl1	2.4752 (11)
Cd1—O2	2.279 (2)	Cd1—Cl2	2.4800 (10)
Cd1—N2	2.470 (3)		
N3—Cd1—O2	136.77 (9)	N2—Cd1—Cl1	110.02 (7)
N3—Cd1—N2	72.40 (9)	N3—Cd1—Cl2	98.90 (8)
O2—Cd1—N2	78.60 (9)	O2—Cd1—Cl2	90.69 (7)
N3—Cd1—Cl1	106.83 (7)	N2—Cd1—Cl2	150.32 (7)
O2—Cd1—Cl1	112.94 (7)	Cl1—Cd1—Cl2	99.66 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H7···O1^{i}	0.85	1.84	2.670 (4)	165
O1—H6···Cl1^{ii}	0.85	2.34	3.157 (3)	162

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2226).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Jin, X. & Li, J. M. (2009). *Acta Cryst.* E**65**, o541.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, S. G., Hu, T. Q. & Li, H. (2008). *Acta Cryst.* E**64**, m769.

supplementary materials

Acta Cryst. (2009). E**65**, m1235 [**doi:10.1107/S1600536809037465**]

Dichlorido[2,2'-(1,10-phenanthrolin-2-ylimino)diethanol]cadmium(II)

S. G. Zhang and L. M. Xie

Comment

Derivatives of 1,10-phenanthroline play an important role in modern coordination chemistry and a lot of complexes have been published with this type of ligands (see Zhang *et al.*, 2008). Although compound 2,2'-(1,10-phenanthrolin-2-ylimino)diethanol has been published (see Jin *et al.*, 2009) but its complex has not been available. Herein we report the crystal structure of Cd^{II} complex with 2,2'-(1,10-phenanthrolin-2-ylimino)diethanol as the ligand. The Cd1 atom reveals a distorted trigonal bipyramidal coordination (Fig. 1 and Table 1). O—H···O hydrogen bond between hydroxyl groups and O—H···Cl hydrogen bond connect the complexes (Fig. 2 and Table 2). There is a π–π stacking interaction involving symmetry-related 1,10-phenanthroline rings, with the relevant distances being $Cg1\cdots Cg2^{i}$ = 3.675 (2) Å and $Cg1\cdots Cg2^{i}_{perp}$ = 3.509 Å; α is 0.71° [symmetry code: (i) -*x*, -*y*, 1 - *z*; *Cg*1 and *Cg*2 are the centroids of C3—C7/N2 ring and C6C7C10C13 ring, respectively; $Cg1\cdots Cg2_{perp}$ is the perpendicular distance from ring *Cg*1 to ring $Cg2^{i}$; α is the dihedral angle between the *Cg*1 ring plane and the *Cg*2 ring plane].

Experimental

10 ml methanol solution of 2,2'-(1,10-phenanthrolin-2-ylimino)diethanol (0.0439 g, 0.155 mmol) was added into 10 ml H_2O solution containing $CdCl_2.2.5\ H_2O$ (0.0354 g, 0.155 mmol) and the mixture was stirred for a few m. The colourless single crystals were obtained after the filtrate had been allowed to stand at room temperature for two weeks.

Refinement

HO-bound H atoms were located in a difference Fourier map, and placed in idealised positions with O—H = 0.85 Å and with $U_{iso}(H) = 1.5U_{eq}(O)$; other H atoms were placed in calculated positions with C—H = 0.97 Å for methylene group and C—H = 0.93 Å for 1,10-phenanthroline ring with $U_{iso}(H) = 1.2U_{eq}(C)$. All H atoms were refined as riding entities.

Figures

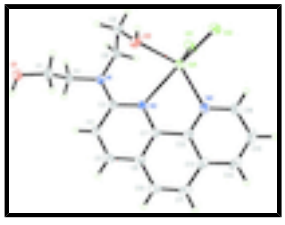

Fig. 1. Structure of title complex with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

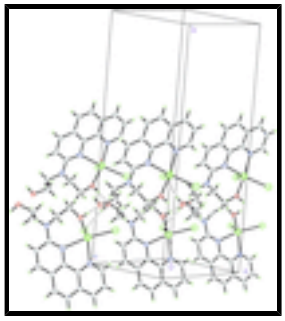

Fig. 2. The crystal structure with hydrogen bonds shown as dashed lines.

Dichlorido[2,2'-(1,10-phenanthrolin-2-ylimino)diethanol]cadmium(II)

Crystal data

$[CdCl_2(C_{16}H_{17}N_3O_2)]$	F_{000} = 928
M_r = 466.63	D_x = 1.839 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2277 reflections
a = 7.9435 (15) Å	θ = 2.4–24.0º
b = 22.548 (4) Å	μ = 1.63 mm^{-1}
c = 9.5216 (18) Å	T = 298 K
β = 98.808 (3)º	Prism, colourless
V = 1685.3 (5) Å^3	0.24 × 0.11 × 0.05 mm
Z = 4	

Data collection

Bruker SMART APEX CCD diffractometer	3641 independent reflections
Radiation source: fine-focus sealed tube	2933 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.040
T = 298 K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→9
T_{min} = 0.696, T_{max} = 0.923	k = −28→24
9776 measured reflections	l = −11→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H-atom parameters constrained
$wR(F^2)$ = 0.087	$w = 1/[\sigma^2(F_o^2) + (0.0368P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.003

3641 reflections	$\Delta\rho_{max}$ = 0.54 e Å^{-3}
217 parameters	$\Delta\rho_{min}$ = −0.40 e Å^{-3}
2 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}
C1	0.1374 (5)	0.21631 (17)	0.8042 (4)	0.0422 (9)
H1A	0.2248	0.1869	0.8330	0.051*
H1B	0.1863	0.2473	0.7526	0.051*
C2	−0.0096 (5)	0.18806 (15)	0.7096 (3)	0.0349 (8)
H2A	−0.0637	0.1594	0.7641	0.042*
H2B	−0.0931	0.2183	0.6761	0.042*
C3	0.1122 (4)	0.10255 (14)	0.5974 (3)	0.0289 (7)
C4	0.1161 (5)	0.07105 (15)	0.7281 (4)	0.0368 (9)
H4	0.0798	0.0894	0.8057	0.044*
C5	0.1724 (5)	0.01476 (16)	0.7386 (4)	0.0386 (9)
H5	0.1720	−0.0059	0.8231	0.046*
C6	0.2315 (4)	−0.01327 (14)	0.6243 (4)	0.0316 (8)
C7	0.2289 (4)	0.02028 (14)	0.4999 (3)	0.0272 (7)
C8	0.0074 (5)	0.19041 (15)	0.4534 (4)	0.0386 (9)
H8A	−0.0969	0.2128	0.4539	0.046*
H8B	−0.0132	0.1620	0.3761	0.046*
C9	0.1446 (5)	0.23235 (16)	0.4243 (4)	0.0483 (10)
H9A	0.1064	0.2550	0.3388	0.058*
H9B	0.1724	0.2598	0.5030	0.058*
C10	0.2929 (5)	−0.07252 (15)	0.6327 (4)	0.0418 (9)
H10	0.2950	−0.0934	0.7172	0.050*
C11	0.3475 (5)	−0.09907 (16)	0.5234 (4)	0.0426 (10)
H11	0.3859	−0.1381	0.5319	0.051*
C12	0.2908 (4)	−0.00865 (14)	0.3824 (4)	0.0298 (8)
C13	0.3472 (4)	−0.06791 (14)	0.3938 (4)	0.0351 (8)
C14	0.4001 (5)	−0.09367 (17)	0.2731 (5)	0.0476 (10)
H14	0.4379	−0.1327	0.2769	0.057*

C15	0.3964 (5)	−0.06231 (18)	0.1520 (5)	0.0523 (11)
H15	0.4297	−0.0796	0.0719	0.063*
C16	0.3424 (5)	−0.00404 (17)	0.1491 (4)	0.0452 (10)
H16	0.3409	0.0176	0.0658	0.054*
Cd1	0.22860 (3)	0.118861 (11)	0.25829 (3)	0.03483 (11)
Cl1	−0.04098 (14)	0.13138 (5)	0.09231 (11)	0.0546 (3)
Cl2	0.43311 (13)	0.15483 (4)	0.10510 (10)	0.0440 (2)
N1	0.0451 (4)	0.15814 (11)	0.5862 (3)	0.0301 (6)
N2	0.1698 (3)	0.07740 (11)	0.4860 (3)	0.0267 (6)
N3	0.2925 (4)	0.02232 (13)	0.2602 (3)	0.0335 (7)
O1	0.0806 (3)	0.24096 (10)	0.9274 (2)	0.0452 (7)
H6	0.0645	0.2146	0.9874	0.068*
O2	0.2902 (3)	0.19779 (11)	0.4069 (3)	0.0488 (7)
H7	0.3766	0.2187	0.3977	0.073*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.045 (2)	0.042 (2)	0.038 (2)	0.0009 (18)	0.0019 (18)	−0.0076 (17)
C2	0.037 (2)	0.037 (2)	0.0319 (19)	0.0038 (16)	0.0070 (16)	−0.0047 (15)
C3	0.0278 (18)	0.0306 (18)	0.0274 (18)	−0.0018 (14)	0.0010 (14)	−0.0002 (14)
C4	0.047 (2)	0.038 (2)	0.0260 (18)	−0.0003 (17)	0.0101 (16)	−0.0003 (15)
C5	0.043 (2)	0.041 (2)	0.031 (2)	−0.0045 (18)	0.0050 (16)	0.0087 (16)
C6	0.0280 (19)	0.0268 (18)	0.037 (2)	−0.0029 (14)	−0.0034 (15)	0.0027 (14)
C7	0.0239 (18)	0.0242 (17)	0.0321 (18)	−0.0029 (14)	0.0001 (14)	0.0000 (13)
C8	0.045 (2)	0.037 (2)	0.034 (2)	0.0105 (17)	0.0083 (17)	0.0059 (16)
C9	0.068 (3)	0.034 (2)	0.047 (2)	0.010 (2)	0.022 (2)	0.0033 (17)
C10	0.037 (2)	0.034 (2)	0.052 (2)	0.0017 (17)	0.0003 (19)	0.0122 (17)
C11	0.037 (2)	0.0249 (19)	0.064 (3)	0.0020 (16)	0.003 (2)	0.0088 (18)
C12	0.0255 (18)	0.0251 (17)	0.037 (2)	−0.0037 (14)	−0.0007 (15)	−0.0024 (14)
C13	0.0260 (19)	0.0278 (19)	0.051 (2)	−0.0035 (15)	0.0043 (16)	−0.0070 (16)
C14	0.042 (2)	0.031 (2)	0.071 (3)	−0.0002 (18)	0.013 (2)	−0.016 (2)
C15	0.058 (3)	0.048 (3)	0.055 (3)	−0.006 (2)	0.025 (2)	−0.023 (2)
C16	0.056 (3)	0.045 (2)	0.037 (2)	−0.005 (2)	0.0134 (19)	−0.0097 (17)
Cd1	0.04436 (19)	0.03078 (16)	0.03027 (16)	0.00004 (12)	0.00864 (12)	0.00178 (11)
Cl1	0.0468 (6)	0.0775 (8)	0.0375 (6)	−0.0090 (5)	0.0002 (5)	0.0155 (5)
Cl2	0.0523 (6)	0.0405 (5)	0.0431 (5)	0.0007 (4)	0.0191 (5)	0.0054 (4)
N1	0.0351 (17)	0.0281 (15)	0.0280 (15)	0.0048 (12)	0.0076 (12)	−0.0010 (12)
N2	0.0291 (16)	0.0244 (14)	0.0262 (15)	−0.0020 (12)	0.0026 (12)	0.0003 (11)
N3	0.0387 (17)	0.0314 (16)	0.0307 (16)	−0.0009 (13)	0.0061 (13)	−0.0043 (12)
O1	0.0655 (19)	0.0362 (14)	0.0326 (15)	0.0092 (13)	0.0034 (13)	−0.0036 (11)
O2	0.0503 (17)	0.0341 (14)	0.0693 (19)	−0.0079 (13)	0.0323 (14)	−0.0100 (13)

Geometric parameters (Å, °)

C1—O1	1.431 (4)	C9—H9A	0.9700
C1—C2	1.503 (5)	C9—H9B	0.9700
C1—H1A	0.9700	C10—C11	1.329 (5)
C1—H1B	0.9700	C10—H10	0.9300

C2—N1	1.476 (4)	C11—C13	1.420 (5)
C2—H2A	0.9700	C11—H11	0.9300
C2—H2B	0.9700	C12—N3	1.359 (4)
C3—N2	1.344 (4)	C12—C13	1.408 (4)
C3—N1	1.360 (4)	C13—C14	1.408 (5)
C3—C4	1.429 (4)	C14—C15	1.349 (6)
C4—C5	1.344 (5)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.381 (5)
C5—C6	1.400 (5)	C15—H15	0.9300
C5—H5	0.9300	C16—N3	1.325 (4)
C6—C7	1.403 (4)	C16—H16	0.9300
C6—C10	1.420 (4)	Cd1—N3	2.235 (3)
C7—N2	1.370 (4)	Cd1—O2	2.279 (2)
C7—C12	1.445 (5)	Cd1—N2	2.470 (3)
C8—N1	1.450 (4)	Cd1—Cl1	2.4752 (11)
C8—C9	1.500 (5)	Cd1—Cl2	2.4800 (10)
C8—H8A	0.9700	O1—H6	0.8482
C8—H8B	0.9700	O2—H7	0.8481
C9—O2	1.425 (4)		
O1—C1—C2	110.0 (3)	C10—C11—C13	120.0 (3)
O1—C1—H1A	109.7	C10—C11—H11	120.0
C2—C1—H1A	109.7	C13—C11—H11	120.0
O1—C1—H1B	109.7	N3—C12—C13	120.6 (3)
C2—C1—H1B	109.7	N3—C12—C7	118.7 (3)
H1A—C1—H1B	108.2	C13—C12—C7	120.7 (3)
N1—C2—C1	112.0 (3)	C14—C13—C12	117.4 (3)
N1—C2—H2A	109.2	C14—C13—C11	123.0 (3)
C1—C2—H2A	109.2	C12—C13—C11	119.6 (3)
N1—C2—H2B	109.2	C15—C14—C13	120.7 (4)
C1—C2—H2B	109.2	C15—C14—H14	119.6
H2A—C2—H2B	107.9	C13—C14—H14	119.6
N2—C3—N1	120.2 (3)	C14—C15—C16	118.8 (4)
N2—C3—C4	120.9 (3)	C14—C15—H15	120.6
N1—C3—C4	118.8 (3)	C16—C15—H15	120.6
C5—C4—C3	119.7 (3)	N3—C16—C15	122.8 (4)
C5—C4—H4	120.1	N3—C16—H16	118.6
C3—C4—H4	120.1	C15—C16—H16	118.6
C4—C5—C6	121.1 (3)	N3—Cd1—O2	136.77 (9)
C4—C5—H5	119.5	N3—Cd1—N2	72.40 (9)
C6—C5—H5	119.5	O2—Cd1—N2	78.60 (9)
C5—C6—C7	116.7 (3)	N3—Cd1—Cl1	106.83 (7)
C5—C6—C10	122.3 (3)	O2—Cd1—Cl1	112.94 (7)
C7—C6—C10	121.0 (3)	N2—Cd1—Cl1	110.02 (7)
N2—C7—C6	123.3 (3)	N3—Cd1—Cl2	98.90 (8)
N2—C7—C12	120.1 (3)	O2—Cd1—Cl2	90.69 (7)
C6—C7—C12	116.6 (3)	N2—Cd1—Cl2	150.32 (7)
N1—C8—C9	114.7 (3)	Cl1—Cd1—Cl2	99.66 (4)
N1—C8—H8A	108.6	C3—N1—C8	123.9 (3)
C9—C8—H8A	108.6	C3—N1—C2	121.2 (3)

N1—C8—H8B	108.6	C8—N1—C2	114.7 (3)
C9—C8—H8B	108.6	C3—N2—C7	118.2 (3)
H8A—C8—H8B	107.6	C3—N2—Cd1	131.8 (2)
O2—C9—C8	107.6 (3)	C7—N2—Cd1	109.5 (2)
O2—C9—H9A	110.2	C16—N3—C12	119.7 (3)
C8—C9—H9A	110.2	C16—N3—Cd1	121.7 (3)
O2—C9—H9B	110.2	C12—N3—Cd1	118.4 (2)
C8—C9—H9B	110.2	C1—O1—H6	112.3
H9A—C9—H9B	108.5	C9—O2—Cd1	113.5 (2)
C11—C10—C6	122.0 (4)	C9—O2—H7	113.0
C11—C10—H10	119.0	Cd1—O2—H7	118.1
C6—C10—H10	119.0		
O1—C1—C2—N1	−175.8 (3)	N1—C3—N2—C7	−176.9 (3)
N2—C3—C4—C5	−2.4 (5)	C4—C3—N2—C7	1.4 (5)
N1—C3—C4—C5	176.0 (3)	N1—C3—N2—Cd1	12.5 (5)
C3—C4—C5—C6	1.6 (5)	C4—C3—N2—Cd1	−169.2 (2)
C4—C5—C6—C7	0.1 (5)	C6—C7—N2—C3	0.3 (5)
C4—C5—C6—C10	179.5 (3)	C12—C7—N2—C3	179.5 (3)
C5—C6—C7—N2	−1.0 (5)	C6—C7—N2—Cd1	172.9 (2)
C10—C6—C7—N2	179.5 (3)	C12—C7—N2—Cd1	−7.9 (3)
C5—C6—C7—C12	179.7 (3)	N3—Cd1—N2—C3	179.4 (3)
C10—C6—C7—C12	0.2 (5)	O2—Cd1—N2—C3	31.8 (3)
N1—C8—C9—O2	65.3 (4)	Cl1—Cd1—N2—C3	−78.6 (3)
C5—C6—C10—C11	179.4 (4)	Cl2—Cd1—N2—C3	102.6 (3)
C7—C6—C10—C11	−1.2 (5)	N3—Cd1—N2—C7	8.15 (19)
C6—C10—C11—C13	0.6 (6)	O2—Cd1—N2—C7	−139.4 (2)
N2—C7—C12—N3	1.4 (5)	Cl1—Cd1—N2—C7	110.14 (19)
C6—C7—C12—N3	−179.3 (3)	Cl2—Cd1—N2—C7	−68.6 (2)
N2—C7—C12—C13	−178.1 (3)	C15—C16—N3—C12	−1.1 (6)
C6—C7—C12—C13	1.2 (5)	C15—C16—N3—Cd1	174.3 (3)
N3—C12—C13—C14	−1.7 (5)	C13—C12—N3—C16	2.2 (5)
C7—C12—C13—C14	177.8 (3)	C7—C12—N3—C16	−177.3 (3)
N3—C12—C13—C11	178.7 (3)	C13—C12—N3—Cd1	−173.3 (2)
C7—C12—C13—C11	−1.7 (5)	C7—C12—N3—Cd1	7.1 (4)
C10—C11—C13—C14	−178.7 (4)	O2—Cd1—N3—C16	−133.4 (3)
C10—C11—C13—C12	0.8 (5)	N2—Cd1—N3—C16	176.4 (3)
C12—C13—C14—C15	0.1 (5)	Cl1—Cd1—N3—C16	70.2 (3)
C11—C13—C14—C15	179.6 (4)	Cl2—Cd1—N3—C16	−32.8 (3)
C13—C14—C15—C16	1.0 (6)	O2—Cd1—N3—C12	42.1 (3)
C14—C15—C16—N3	−0.6 (6)	N2—Cd1—N3—C12	−8.1 (2)
N2—C3—N1—C8	9.4 (5)	Cl1—Cd1—N3—C12	−114.3 (2)
C4—C3—N1—C8	−169.0 (3)	Cl2—Cd1—N3—C12	142.7 (2)
N2—C3—N1—C2	−176.3 (3)	C8—C9—O2—Cd1	47.5 (3)
C4—C3—N1—C2	5.3 (5)	N3—Cd1—O2—C9	−133.1 (2)
C9—C8—N1—C3	−95.7 (4)	N2—Cd1—O2—C9	−84.7 (2)
C9—C8—N1—C2	89.6 (4)	Cl1—Cd1—O2—C9	22.3 (2)
C1—C2—N1—C3	82.0 (4)	Cl2—Cd1—O2—C9	123.1 (2)
C1—C2—N1—C8	−103.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H7···O1^{i}	0.85	1.84	2.670 (4)	165
O1—H6···Cl1^{ii}	0.85	2.34	3.157 (3)	162

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

Fig. 1

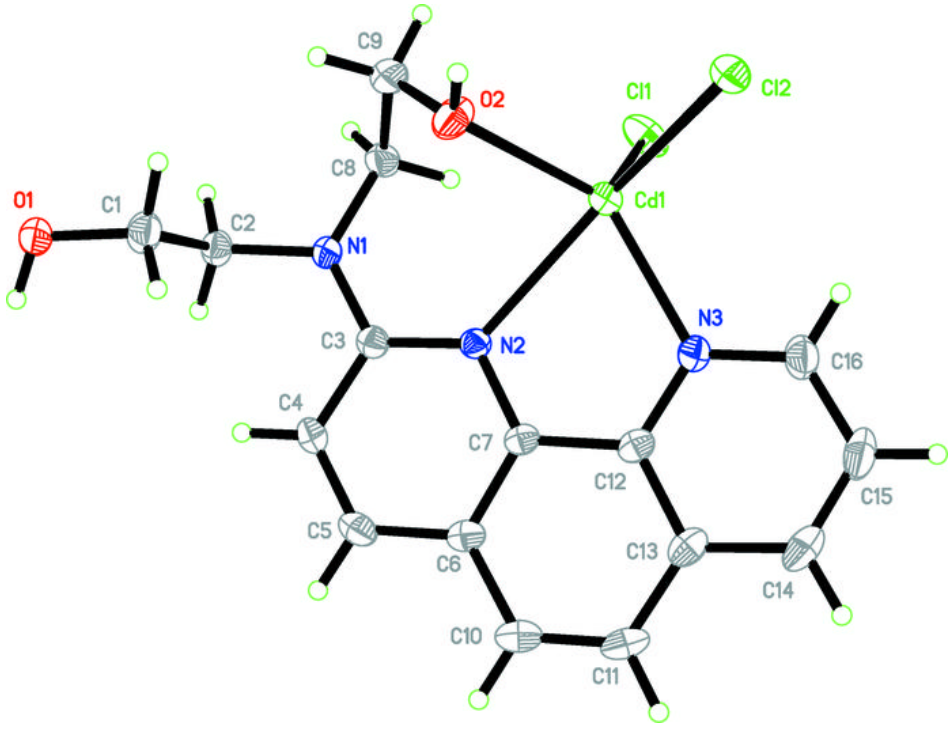
C9
O2
Cl1
Cl2
C8
Cd1
O1
C1
C2
N1
N3
C3
N2
C16
C4
C7
C12
C15
C5
C6
C13
C14
C10
C11

Fig. 2