Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Di-μ-chlorido-bis(chlorido{2-[(2-hydroxyphenyl)iminiomethyl]-6-methoxyphenolato-κ^2O,O'}cadium(II)) methanol disolvate

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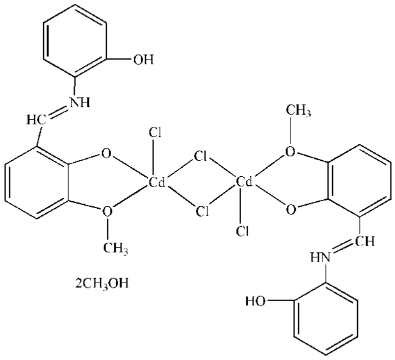
Received 2 July 2007; accepted 18 July 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.047; wR factor = 0.117; data-to-parameter ratio = 14.3.

The title centrosymmetric complex, $[Cd_2Cl_4(C_{14}H_{13}NO_3)_2]\cdot 2CH_3OH$, contains two protonated Schiff base ligands which were derived from the condensation of *o*-vanillin and 2-hydroxyaniline. The Cd^{II} ion is five-coordinated by three Cl atoms and two O atoms in a distorted square-pyramidal geometry. A basal edge containing two bridging chloride ligands is shared by both symmetry-related Cd^{II} ions. The four atoms of the Cd_2Cl_2 core are coplanar, giving a rhomboidal geometry with two short and two long Cd—Cl distances and acute Cl—Cd—Cl and obtuse Cd—Cl—Cd angles. The crystal structure is stabilized by intermolecular hydrogen bonds and weak π–π stacking interactions with a centroid-to-centroid distance of 3.710 (4) Å.

Related literature

For related literature, see: Choi & Jeon (2003); Strasdeit *et al.* (1988); Tong *et al.* (1999); Veith *et al.* (1996).



Experimental

Crystal data

$[Cd_2Cl_4(C_{14}H_{13}NO_3)_2]\cdot 2CH_4O$
M_r = 917.19
Monoclinic, $P2_1/c$
a = 9.845 (6) Å
b = 18.253 (10) Å
c = 9.792 (6) Å
β = 101.157 (6)°
V = 1726.3 (17) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.59 mm^{-1}
T = 298 (2) K
0.49 × 0.47 × 0.42 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.509, T_{max} = 0.555 (expected range = 0.471–0.512)
8174 measured reflections
3025 independent reflections
2233 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.117
S = 1.11
3025 reflections
212 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.194 (4)	Cd1—Cl1^i	2.548 (2)
Cd1—O2	2.411 (4)	Cd1—Cl1	2.563 (2)
Cd1—Cl2	2.439 (2)		
O1—Cd1—O2	69.70 (15)	O1—Cd1—Cl1	91.13 (11)
O1—Cd1—Cl2	121.20 (13)	O2—Cd1—Cl1	149.70 (12)
O2—Cd1—Cl2	98.70 (13)	Cl2—Cd1—Cl1	111.43 (7)
O1—Cd1—Cl1^i	133.60 (13)	Cl1^i—Cd1—Cl1	88.49 (6)
O2—Cd1—Cl1^i	88.49 (12)	Cd1^i—Cl1—Cd1	91.51 (6)
Cl2—Cd1—Cl1^i	101.77 (7)		

Symmetry code: (i) $-x+1, -y, -z+2$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···Cl2^{ii}	0.82	2.29	3.093 (7)	167
O3—H3···O4^{iii}	0.82	1.84	2.622 (7)	160

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors thank the Natural Science Foundation of Shandong Province (grant No. Y2004B02) for a research grant.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2451).

doi:10.1107/S1600536807035210

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supplementary materials

Acta Cryst. (2007). E**63**, m2206-m2207   [**doi:10.1107/S1600536807035210**]

Di-μ-chlorido-bis(chlorido{2-[(2-hydroxyphenyl)iminiomethyl]-6-methoxyphenolato-κ^2*O*,*O'*}cadium(II)) methanol disolvate

J.-F. Dong, L.-Z. Li, W.-J. Yu, T. Xu and D.-Q. Wang

Comment

There has been growing interest in the coordination chemistry of cadmium(II) complexes due to the increased recognition of their role in biological organisms (Strasdeit *et al.*, 1988), as well as in molecular-based materials (Veith *et al.*, 1996). As part of our ongoing studies of Schiff beses, we report herein the synthesis and crystal structure of a new bis cadmium(II) complex with Schiff base ligand derived from the condensation of *o*-vanillin and 2-hydroxyaniline.

The complex possesses a crystallographically imposed centre of inversion, forming a bis([mu]-chlorido)-bridged binuclear structure with both cadmium centres being five-coordinated (Fig.1). In the title complex, each Cd^{II} ion is coordinated in a highly distorted square-pyramidal geometry, in which O1, O2, Cl1, and Cl1^{i}(symmetry code:(i) $-x + 1,-y,-z + 2$) lie in basal plane, and Cl2 lies in the apical position. The Cd^{II} ion lies 0.594 (3)Å above the equatorial plane, sharing the basal edge containing the bridging chloro ligands; the apical atom Cl2 is almost perpendicular the basal equatiorial plane. The four atoms of the Cd_2Cl_2 core, by virtue of the inversion center, are exactly planar, and form a rhomboidal geometry with two short Cd1—Cl1^{i} (symmetry code: (i) $-x + 1,-y,-z + 2$) distances 2.548 (2)Å and two long Cd1—Cl1 distances 2.563 (2) Å. The core bond angles of Cl1^{i}—Cd1—Cl1 and Cd1^{i}—Cl1—Cd1 are 88.49 (6)° and 91.51 (6)°, respectively and are similar to those already reported (Choi, *et al.* 2003). The ligands of Schiff base moiety related by centers of symmetry have a centroid-centroid separation of 3.710 (4)Å (perpendicular distance 3.396 (5) Å) for rings (formed by atoms C2—C7 and atoms C9—C14 at ($-x,-y,2 - z$)) and the slip angle is 23.74 (23)°, indicating significant π-π interactions (Tong *et al.*, 1999). In the crystal structure, the weak π-π stacking interactions and intermolecular hydrogen bonds resulted in the two-dimensional network structure (Fig. 2).

Experimental

2-Hydroxyaniline(1 mmol, 109.12 mg) and potassium hydroxide (1 mmol, 56.1 mg) were dissolved in hot methanol (10 ml) and added in portions to a methanol solution of *o*-vanillin (1 mmol, 152.2 mg). The mixture was then stirred at 323 K for 2 h. Subsequently, an aqueous solution(2 ml) of cadmium chloride hydrate(1 mmol, 228.35 mg) was added dropwise and stirred for another 4 h. The solution was held at room temperature for ten days, whereupon yellow blocky crystals suitable for X-ray diffraction were obtained.

Refinement

All H atoms were placed in geometrically calculated positions (C—H = 0.93 − 0.96 Å, O—H =0.82 Å, N—H =0.86 Å), and allowed to ride on their respective parent atoms, with U_{iso}(H) = 1.2–1.5U_{eq}(parent atom).

Figures

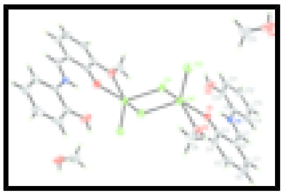

Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabeled atoms are are related by the symmetry operator ($-x + 1,-y,-z + 2$).

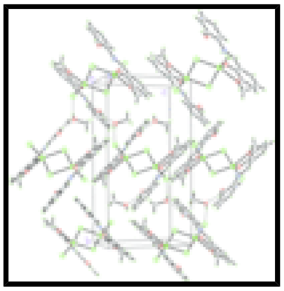

Fig. 2. The packing of the title compound. Hydrogen bond are shown as dashed lines.

Di-μ-chlorido-bis(chlorido{2-[(2-hydroxyphenyl)iminiomethyl]-6- methoxyphenolato-κ^2*O*,*O*'}cadium(II)) dimethanol solvate

Crystal data

$[Cd_2Cl_4(C_{14}H_{13}NO_3)_2]\cdot 2CH_4O$	F_{000} = 912
M_r = 917.19	D_x = 1.764 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3509 reflections
a = 9.845 (6) Å	θ = 2.4–27.6°
b = 18.253 (10) Å	μ = 1.59 mm^{-1}
c = 9.792 (6) Å	*T* = 298 (2) K
β = 101.157 (6)°	Block, yellow
V = 1726.3 (17) Å^3	0.49 × 0.47 × 0.42 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	3025 independent reflections
Radiation source: fine-focus sealed tube	2233 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.061
T = 298(2) K	θ_{max} = 25.0°
φ and ω scans	θ_{min} = 2.1°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11\rightarrow 11$
T_{min} = 0.509, T_{max} = 0.555	$k = -21\rightarrow 15$
8174 measured reflections	$l = -11\rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.117$	$w = 1/[\sigma^2(F_o^2) + (0.0233P)^2 + 6.6242P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} < 0.001$
3025 reflections	$\Delta\rho_{max} = 1.00$ e Å^{-3}
212 parameters	$\Delta\rho_{min} = -0.69$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Cd1	0.38169 (5)	0.02721 (3)	0.84003 (5)	0.03929 (18)
Cl1	0.43742 (18)	0.07287 (10)	1.09219 (17)	0.0434 (4)
Cl2	0.4903 (2)	0.10392 (10)	0.68766 (19)	0.0523 (5)
N1	−0.0539 (5)	0.0914 (3)	0.9234 (5)	0.0298 (11)
H1	0.0340	0.0896	0.9268	0.036*
O1	0.1587 (4)	0.0338 (2)	0.8376 (4)	0.0375 (10)
O2	0.2568 (5)	−0.0548 (3)	0.6671 (4)	0.0416 (11)
O3	0.1336 (5)	0.1781 (3)	1.0652 (6)	0.0556 (14)
H3	0.1841	0.2111	1.1020	0.083*
O4	0.3157 (8)	0.2598 (4)	0.2280 (7)	0.093 (2)
H4	0.3600	0.2937	0.2035	0.139*
C1	−0.1286 (7)	0.0454 (3)	0.8386 (6)	0.0328 (14)
H1A	−0.2236	0.0444	0.8355	0.039*
C2	−0.0730 (7)	−0.0028 (3)	0.7516 (6)	0.0341 (15)
C3	0.0706 (7)	−0.0063 (3)	0.7523 (6)	0.0304 (14)
C4	0.1171 (7)	−0.0553 (3)	0.6572 (6)	0.0337 (14)
C5	0.0252 (8)	−0.0975 (3)	0.5681 (7)	0.0403 (16)
H5	0.0571	−0.1290	0.5065	0.048*

C6	−0.1167 (8)	−0.0936 (4)	0.5690 (8)	0.0510 (19)
H6	−0.1782	−0.1224	0.5075	0.061*
C7	−0.1655 (7)	−0.0486 (4)	0.6574 (7)	0.0429 (17)
H7	−0.2600	−0.0472	0.6573	0.051*
C8	0.3163 (9)	−0.1007 (5)	0.5748 (8)	0.058 (2)
H8A	0.3018	−0.1512	0.5953	0.086*
H8B	0.4138	−0.0912	0.5873	0.086*
H8C	0.2730	−0.0904	0.4803	0.086*
C9	−0.1002 (6)	0.1441 (3)	1.0108 (6)	0.0309 (14)
C10	0.0041 (7)	0.1893 (3)	1.0857 (7)	0.0359 (15)
C11	−0.0332 (9)	0.2426 (4)	1.1743 (7)	0.0461 (18)
H11	0.0338	0.2731	1.2248	0.055*
C12	−0.1690 (9)	0.2495 (4)	1.1863 (8)	0.053 (2)
H12	−0.1928	0.2847	1.2462	0.064*
C13	−0.2719 (8)	0.2054 (4)	1.1114 (7)	0.0463 (18)
H13	−0.3637	0.2113	1.1200	0.056*
C14	−0.2356 (7)	0.1525 (4)	1.0239 (7)	0.0379 (15)
H14	−0.3035	0.1225	0.9734	0.046*
C15	0.3774 (12)	0.2377 (5)	0.3610 (10)	0.088 (3)
H15A	0.4742	0.2496	0.3775	0.132*
H15B	0.3664	0.1858	0.3697	0.132*
H15C	0.3344	0.2626	0.4280	0.132*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0293 (3)	0.0492 (3)	0.0400 (3)	0.0012 (2)	0.00819 (19)	0.0026 (3)
Cl1	0.0392 (10)	0.0491 (10)	0.0412 (9)	0.0107 (8)	0.0059 (7)	−0.0046 (8)
Cl2	0.0546 (12)	0.0552 (11)	0.0531 (10)	0.0044 (9)	0.0255 (9)	0.0120 (9)
N1	0.022 (3)	0.032 (3)	0.036 (3)	−0.001 (2)	0.005 (2)	0.000 (2)
O1	0.030 (2)	0.041 (3)	0.040 (2)	0.000 (2)	0.0047 (19)	−0.011 (2)
O2	0.035 (3)	0.052 (3)	0.038 (2)	0.006 (2)	0.010 (2)	−0.010 (2)
O3	0.042 (3)	0.058 (3)	0.066 (3)	−0.014 (3)	0.007 (3)	−0.020 (3)
O4	0.098 (6)	0.088 (5)	0.078 (4)	−0.050 (4)	−0.017 (4)	0.001 (4)
C1	0.023 (3)	0.041 (4)	0.035 (3)	−0.002 (3)	0.008 (3)	−0.002 (3)
C2	0.034 (4)	0.030 (3)	0.038 (4)	−0.003 (3)	0.006 (3)	0.001 (3)
C3	0.036 (4)	0.032 (3)	0.024 (3)	−0.001 (3)	0.005 (3)	0.005 (3)
C4	0.041 (4)	0.032 (3)	0.030 (3)	0.003 (3)	0.009 (3)	0.001 (3)
C5	0.053 (5)	0.032 (4)	0.034 (4)	−0.004 (3)	0.006 (3)	−0.006 (3)
C6	0.055 (5)	0.042 (4)	0.054 (4)	−0.013 (4)	0.005 (4)	−0.009 (4)
C7	0.033 (4)	0.049 (4)	0.047 (4)	−0.013 (3)	0.007 (3)	−0.006 (3)
C8	0.054 (5)	0.074 (6)	0.048 (4)	0.009 (4)	0.019 (4)	−0.012 (4)
C9	0.032 (4)	0.031 (3)	0.029 (3)	0.004 (3)	0.004 (3)	0.005 (3)
C10	0.039 (4)	0.030 (4)	0.039 (4)	−0.005 (3)	0.010 (3)	0.007 (3)
C11	0.063 (5)	0.031 (4)	0.042 (4)	−0.006 (3)	0.004 (4)	0.000 (3)
C12	0.076 (6)	0.036 (4)	0.049 (4)	0.007 (4)	0.018 (4)	−0.007 (3)
C13	0.040 (4)	0.054 (5)	0.045 (4)	0.009 (3)	0.010 (3)	0.003 (4)
C14	0.034 (4)	0.042 (4)	0.038 (4)	0.000 (3)	0.007 (3)	0.000 (3)

C15	0.109 (9)	0.066 (6)	0.083 (7)	−0.022 (6)	0.004 (6)	−0.002 (5)

Geometric parameters (Å, °)

Cd1—O1	2.194 (4)	C5—C6	1.401 (11)
Cd1—O2	2.411 (4)	C5—H5	0.9300
Cd1—Cl2	2.439 (2)	C6—C7	1.348 (10)
Cd1—Cl1^{i}	2.548 (2)	C6—H6	0.9300
Cd1—Cl1	2.563 (2)	C7—H7	0.9300
Cl1—Cd1^{i}	2.548 (2)	C8—H8A	0.9600
N1—C1	1.303 (7)	C8—H8B	0.9600
N1—C9	1.420 (8)	C8—H8C	0.9600
N1—H1	0.8600	C9—C14	1.372 (9)
O1—C3	1.307 (7)	C9—C10	1.408 (9)
O2—C4	1.360 (8)	C10—C11	1.398 (10)
O2—C8	1.438 (8)	C11—C12	1.371 (11)
O3—C10	1.345 (8)	C11—H11	0.9300
O3—H3	0.8200	C12—C13	1.387 (10)
O4—C15	1.386 (11)	C12—H12	0.9300
O4—H4	0.8200	C13—C14	1.383 (10)
C1—C2	1.407 (9)	C13—H13	0.9300
C1—H1A	0.9300	C14—H14	0.9300
C2—C3	1.414 (9)	C15—H15A	0.9600
C2—C7	1.433 (9)	C15—H15B	0.9600
C3—C4	1.429 (9)	C15—H15C	0.9600
C4—C5	1.366 (9)		
O1—Cd1—O2	69.70 (15)	C7—C6—H6	119.5
O1—Cd1—Cl2	121.20 (13)	C5—C6—H6	119.5
O2—Cd1—Cl2	98.70 (13)	C6—C7—C2	120.5 (7)
O1—Cd1—Cl1^{i}	133.60 (13)	C6—C7—H7	119.7
O2—Cd1—Cl1^{i}	88.49 (12)	C2—C7—H7	119.7
Cl2—Cd1—Cl1^{i}	101.77 (7)	O2—C8—H8A	109.5
O1—Cd1—Cl1	91.13 (11)	O2—C8—H8B	109.5
O2—Cd1—Cl1	149.70 (12)	H8A—C8—H8B	109.5
Cl2—Cd1—Cl1	111.43 (7)	O2—C8—H8C	109.5
Cl1^{i}—Cd1—Cl1	88.49 (6)	H8A—C8—H8C	109.5
Cd1^{i}—Cl1—Cd1	91.51 (6)	H8B—C8—H8C	109.5
C1—N1—C9	127.8 (5)	C14—C9—C10	120.6 (6)
C1—N1—H1	116.1	C14—C9—N1	124.3 (6)
C9—N1—H1	116.1	C10—C9—N1	115.1 (6)
C3—O1—Cd1	121.0 (4)	O3—C10—C11	124.7 (6)
C4—O2—C8	118.7 (5)	O3—C10—C9	116.7 (6)
C4—O2—Cd1	115.2 (4)	C11—C10—C9	118.6 (7)
C8—O2—Cd1	126.1 (4)	C12—C11—C10	119.7 (7)
C10—O3—H3	109.5	C12—C11—H11	120.2
C15—O4—H4	109.5	C10—C11—H11	120.2
N1—C1—C2	123.4 (6)	C11—C12—C13	121.7 (7)

N1—C1—H1A	118.3	C11—C12—H12	119.2
C2—C1—H1A	118.3	C13—C12—H12	119.2
C1—C2—C3	122.1 (6)	C14—C13—C12	118.9 (7)
C1—C2—C7	118.8 (6)	C14—C13—H13	120.6
C3—C2—C7	119.1 (6)	C12—C13—H13	120.6
O1—C3—C2	121.1 (5)	C9—C14—C13	120.6 (6)
O1—C3—C4	120.7 (6)	C9—C14—H14	119.7
C2—C3—C4	118.1 (6)	C13—C14—H14	119.7
O2—C4—C5	125.8 (6)	O4—C15—H15A	109.5
O2—C4—C3	113.3 (5)	O4—C15—H15B	109.5
C5—C4—C3	120.9 (6)	H15A—C15—H15B	109.5
C4—C5—C6	120.3 (6)	O4—C15—H15C	109.5
C4—C5—H5	119.9	H15A—C15—H15C	109.5
C6—C5—H5	119.9	H15B—C15—H15C	109.5
C7—C6—C5	121.0 (7)		

O1—Cd1—Cl1—Cd1^{i}	133.59 (13)	Cd1—O2—C4—C5	−179.4 (5)
O2—Cd1—Cl1—Cd1^{i}	84.4 (2)	C8—O2—C4—C3	−178.8 (6)
Cl2—Cd1—Cl1—Cd1^{i}	−102.05 (8)	Cd1—O2—C4—C3	0.1 (6)
Cl1^{i}—Cd1—Cl1—Cd1^{i}	0.0	O1—C3—C4—O2	0.2 (8)
O2—Cd1—O1—C3	0.4 (4)	C2—C3—C4—O2	−179.6 (5)
Cl2—Cd1—O1—C3	88.4 (4)	O1—C3—C4—C5	179.8 (6)
Cl1^{i}—Cd1—O1—C3	−66.6 (5)	C2—C3—C4—C5	0.0 (9)
Cl1—Cd1—O1—C3	−155.6 (4)	O2—C4—C5—C6	179.3 (6)
O1—Cd1—O2—C4	−0.3 (4)	C3—C4—C5—C6	−0.2 (10)
Cl2—Cd1—O2—C4	−120.4 (4)	C4—C5—C6—C7	−0.2 (11)
Cl1^{i}—Cd1—O2—C4	137.9 (4)	C5—C6—C7—C2	0.9 (11)
Cl1—Cd1—O2—C4	53.5 (5)	C1—C2—C7—C6	177.7 (7)
O1—Cd1—O2—C8	178.5 (6)	C3—C2—C7—C6	−1.1 (10)
Cl2—Cd1—O2—C8	58.4 (5)	C1—N1—C9—C14	3.1 (10)
Cl1^{i}—Cd1—O2—C8	−43.3 (5)	C1—N1—C9—C10	−176.5 (6)
Cl1—Cd1—O2—C8	−127.7 (5)	C14—C9—C10—O3	−179.0 (6)
C9—N1—C1—C2	177.2 (6)	N1—C9—C10—O3	0.6 (8)
N1—C1—C2—C3	1.8 (10)	C14—C9—C10—C11	0.5 (9)
N1—C1—C2—C7	−177.0 (6)	N1—C9—C10—C11	−179.9 (5)
Cd1—O1—C3—C2	179.3 (4)	O3—C10—C11—C12	179.5 (7)
Cd1—O1—C3—C4	−0.5 (7)	C9—C10—C11—C12	0.0 (10)
C1—C2—C3—O1	2.1 (9)	C10—C11—C12—C13	−0.7 (11)
C7—C2—C3—O1	−179.2 (6)	C11—C12—C13—C14	0.8 (11)
C1—C2—C3—C4	−178.1 (6)	C10—C9—C14—C13	−0.3 (10)
C7—C2—C3—C4	0.7 (9)	N1—C9—C14—C13	−179.9 (6)
C8—O2—C4—C5	1.7 (9)	C12—C13—C14—C9	−0.3 (10)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···Cl2^{ii}	0.82	2.29	3.093 (7)	167

O3—H3···O4^{iii}	0.82	1.84	2.622 (7)	160

Symmetry codes: (ii) x, $-y+1/2$, $z-1/2$; (iii) x, y, $z+1$.

Fig. 1

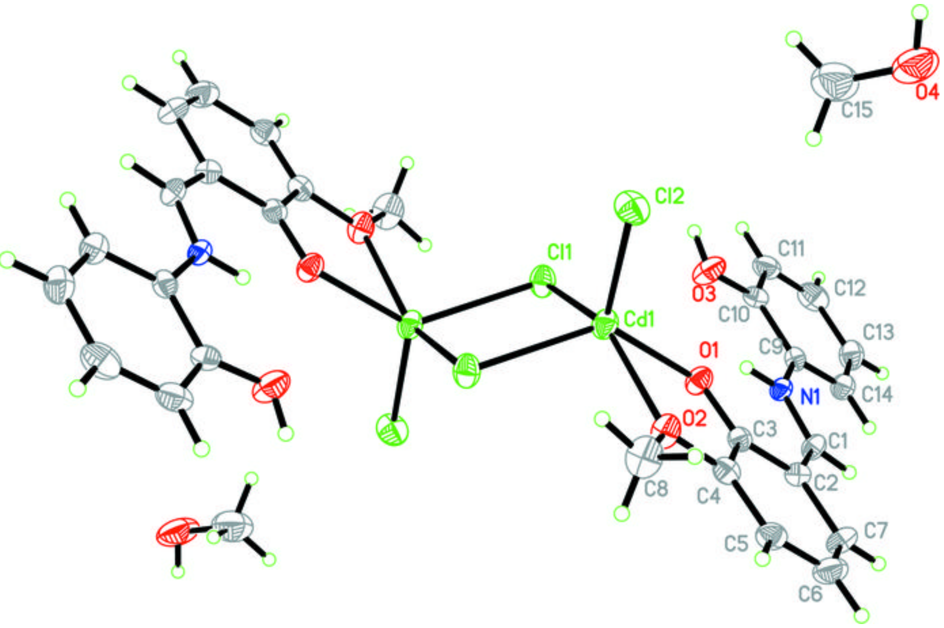

Fig. 2