Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(μ-2-{[3-(dimethylamino)propyl]iminomethyl}phenolato-$\kappa^4N,N',O:O$)-bis[(acetato-κ^2O,O')cadmium(II)] monohydrate

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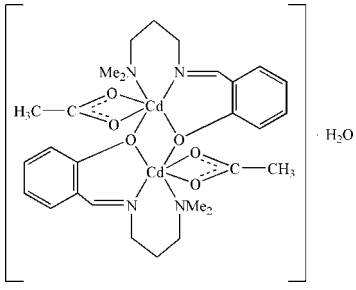
Received 5 June 2007; accepted 21 October 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.022; wR factor = 0.046; data-to-parameter ratio = 22.2.

In the crystal structure of the title compound, $[Cd_2(C_{12}H_{17}N_2O)_2(C_2H_3O_2)_2]\cdot H_2O$, the binuclear complex molecule as well as the water molecule occupy special positions on the same twofold axis. The Cd^{II} atom has a severely distorted octahedral coordination formed by two deprotonated bridging phenol O atoms, the imine and amine N atoms of the Schiff base and two O atoms of the chelating acetate group. The water H atom takes part in a hydrogen bond involving one of the acetate O atoms as an acceptor. Each water molecule forms two such bonds, thus producing isolated 1:1 complex molecule–water aggregates in the crystal structure.

Related literature

For recent studies on complexes of multidentate Schiff bases, including their application for the modeling of active sites of biological systems, see: Erxleben (2001); Ikawa *et al.* (1993); Mukherjee *et al.* (2001); Mukherjee *et al.* (2002); Ray *et al.* (2004); Saha *et al.* (2003);



Experimental

Crystal data

$[Cd_2(C_{12}H_{17}N_2O)_2(C_2H_3O_2)_2]\cdot H_2O$
M_r = 771.46
Tetragonal, $P\bar{4}b2$
a = 17.543 (3) Å
c = 10.420 (3) Å
V = 3206.8 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.37 mm^{-1}
T = 293 (2) K
0.26 × 0.18 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.716, T_{max} = 0.820
21724 measured reflections
4203 independent reflections
3543 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.046
S = 1.02
4203 reflections
189 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack (1983), 1788 Friedel pairs
Flack parameter: −0.014 (18)

Table 1
Selected geometric parameters (Å, °).

Cd1—O1^{i}	2.2685 (14)	Cd1—O3	2.2976 (19)
Cd1—O1	2.2797 (16)	Cd1—N2	2.409 (2)
Cd1—N1	2.2812 (19)	Cd1—O2	2.428 (2)
O1^{i}—Cd1—O1	78.30 (6)	N1—Cd1—N2	82.66 (7)
O1^{i}—Cd1—N1	154.63 (6)	O3—Cd1—N2	144.85 (8)
O1—Cd1—N1	80.93 (6)	O1^{i}—Cd1—O2	110.99 (6)
O1^{i}—Cd1—O3	96.99 (6)	O1—Cd1—O2	151.78 (7)
O1—Cd1—O3	99.08 (7)	N1—Cd1—O2	94.16 (7)
N1—Cd1—O3	100.53 (7)	O3—Cd1—O2	54.24 (8)
O1^{i}—Cd1—N2	93.45 (6)	N2—Cd1—O2	90.70 (8)
O1—Cd1—N2	115.91 (7)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O3	0.80	1.97	2.762 (3)	172

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

The authors thank the Foundation of the Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces (No. 0506) for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YA2057).

  doi:10.1107/S1600536807052105

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supplementary materials

Acta Cryst. (2007). E**63**, m2828-m2829 [**doi:10.1107/S1600536807052105**]

Bis(μ-2-{[3-(dimethylamino)propyl]iminomethyl}phenolato-$\kappa^4N,N',O:O$)bis[(acetato-κ^2O,O')cadmium(II)] monohydrate

W.-X. Cai, X.-Y. Zheng, H. Su and Y.-L. Feng

Comment

Recently there has been a growing interest in the synthesis of transition metal complexes with multidentate Schiff base ligands (Ray *et al.*, 2004; Saha *et al.*, 2003). Such ligands can accommodate one, two or more metal centres and thus may provide the basis for modeling of active sites of biological systems (Ikawa *et al.*, 1993; Erxleben, 2001). Up to now many Cu(II) complexes with tridentate Schiff bases have been synthesized (Mukherjee *et al.*, 2001; Mukherjee *et al.*, 2002). In this paper, we report a binuclear Cd(II) complex with tridentate Schiff base *N*-(salicylidene)-3-dimethylaminopropylamine ligand (Fig. 1).

The crystal structure of (I) is built of binuclear neutral cadmium complexes and lattice water molecules. The complex dimeric molecule $[Cd(C_{12}H_{17}N_2O)(CH_3COO)]_2$ occupies a special position on the twofold axis. Each Cd^{II} atom has a severely distorted octahedral coordination formed by two deprotonated bridging phenolic O atoms, imine and amine N atoms of the Schiff base, and two oxygen atoms of the chelate acetato group. The Cd1···$Cd1^i$ separation is 3.519 (6) Å and the Cd1—O1—$Cd1^i$ angle is equal to 101.40 (6)° [symmetry code (i): 0.5 − *y*, 0.5 − *x*, 1 − *z*].

The water H atom takes part in the H-bond involving one of the acetate oxygen atoms, O3, as an acceptor (Table 2). The water molecule, therefore, participates in two such H-bonds with one and the same complex molecule, thus producing isolated 1:1 complex molecule-water molecule aggregates in crystal.

Experimental

The Schiff base ligand *N*-(salicylidene)-3-dimethylaminopropylamine was prepared by refluxing 3-dimethylamino-1-propylamine (1.0 mmol) and salicyladehyde (1.0 mmol) in ethyl alcohol (10 ml) for half an hour. $Cd(CH_3COO)_2{\cdot}2H_2O$ (1.0 mmol) in 10 ml of ethyl alcohol was added to the ethyl alcohol solution of the ligand (1.0 mmol). A yellow mixture was obtained by refluxing for about an hour, then allowed to stand at room temperature. After several weeks yellow crystals suitable for X-ray diffraction were collected (yield 51%).

Refinement

All H atoms bonded to C atoms were positioned geometrically [aromatic C—H 0.93 Å and aliphatic C—H = 0.97(methyl), 0.96(methylene) or 0.93(methylidyne) Å], and the water H atom was located in the difference Fourier map. All H atoms were included in the refinement in the riding motion approximation with U_{iso}(H) = 1.5U_{eq}(C,*O*) for methyl and water H atoms and U_{iso}(H) = 1.2U_{eq}(C)] for all other H atoms.

Figures

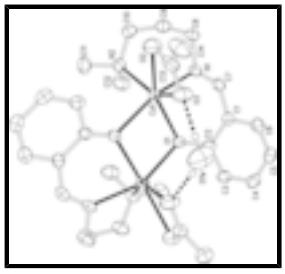

Fig. 1. The complex molecule-water molecule aggregate in the structure of the title compound; the unlabeled atoms are derived by the (−*y* + 1/2, −*x* + 1/2, −*z* + 1) symmetry transformation. Displacement ellipsoids are drawn at the 30% probability level. The H atoms with the exception of that of the water molecule are omitted for clarity; the H-bonds are represented as dashed lines.

Bis(μ-2-{[3-(dimethylamino)propyl]iminomethyl}phenolato- $\kappa^4N,N',O:O$)bis[(acetato-κ^2O,O')cadmium(II)] monohydrate

Crystal data

$[Cd_2(C_{12}H_{17}N_2O)_2(C_2H_3O_2)_2]\cdot H_2O$	$Z = 4$
$M_r = 771.46$	$F_{000} = 1560$
Tetragonal, $P\bar{4}b2$	$D_x = 1.598$ Mg m^{-3}
Hall symbol: P -4 -2ab	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 17.543$ (3) Å	Cell parameters from 5789 reflections
$b = 17.543$ (3) Å	$\theta = 1.9$–29.3º
$c = 10.420$ (3) Å	$\mu = 1.37$ mm^{-1}
$\alpha = 90$º	$T = 293$ (2) K
$\beta = 90$º	Block, yellow
$\gamma = 90$º	0.26 × 0.18 × 0.15 mm
$V = 3206.8$ (11) Å^3	

Data collection

Bruker APEXII area-detector diffractometer	4203 independent reflections
Radiation source: fine-focus sealed tube	3543 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.030$
$T = 293(2)$ K	$\theta_{max} = 29.3$º
ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -23\rightarrow24$
$T_{min} = 0.716$, $T_{max} = 0.820$	$k = -23\rightarrow24$
21724 measured reflections	$l = -14\rightarrow10$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.022$	$w = 1/[\sigma^2(F_o^2) + (0.0216P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.046$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.23$ e Å^{-3}
4203 reflections	$\Delta\rho_{min} = -0.24$ e Å^{-3}
189 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1788 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.014 (18)

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	0.231751 (8)	0.354386 (8)	0.634193 (16)	0.04198 (5)
O1	0.22984 (9)	0.36177 (8)	0.41579 (14)	0.0451 (3)
O2	0.29307 (13)	0.32036 (13)	0.83507 (19)	0.0755 (6)
O3	0.32810 (12)	0.26684 (11)	0.6582 (2)	0.0729 (6)
O1W	0.35631 (13)	0.14369 (13)	0.5000	0.1164 (15)
H1W	0.3524	0.1783	0.5489	0.175*
N1	0.30084 (11)	0.46347 (10)	0.60836 (19)	0.0480 (5)
N2	0.14606 (12)	0.43888 (13)	0.74563 (19)	0.0531 (5)
C1	0.32474 (12)	0.45900 (11)	0.3765 (2)	0.0428 (5)
C2	0.27952 (12)	0.39507 (12)	0.3380 (2)	0.0409 (5)
C3	0.28801 (14)	0.37069 (13)	0.2108 (3)	0.0472 (6)
H3A	0.2610	0.3280	0.1838	0.057*
C4	0.33442 (13)	0.40717 (14)	0.1246 (3)	0.0529 (6)
H4A	0.3378	0.3891	0.0409	0.063*
C5	0.37623 (15)	0.47056 (14)	0.1605 (3)	0.0568 (7)
H5A	0.4067	0.4962	0.1016	0.068*
C6	0.37144 (13)	0.49453 (15)	0.2855 (2)	0.0543 (6)
H6A	0.4005	0.5362	0.3109	0.065*
C7	0.32879 (13)	0.49019 (14)	0.5056 (3)	0.0488 (6)
H7A	0.3554	0.5358	0.5138	0.059*
C8	0.31653 (15)	0.50458 (18)	0.7280 (2)	0.0630 (8)
H8A	0.3549	0.5432	0.7120	0.076*
H8B	0.3369	0.4692	0.7909	0.076*
C9	0.24522 (17)	0.54242 (17)	0.7824 (3)	0.0687 (8)

H9A	0.2212	0.5718	0.7147	0.082*
H9B	0.2605	0.5778	0.8491	0.082*
C10	0.18630 (15)	0.48761 (16)	0.8382 (2)	0.0650 (8)
H10A	0.2117	0.4550	0.9000	0.078*
H10B	0.1487	0.5173	0.8847	0.078*
C11	0.08785 (16)	0.39618 (17)	0.8156 (3)	0.0764 (9)
H11A	0.0521	0.4311	0.8533	0.115*
H11B	0.1116	0.3666	0.8821	0.115*
H11C	0.0616	0.3628	0.7576	0.115*
C12	0.10697 (15)	0.48511 (18)	0.6487 (3)	0.0777 (8)
H12A	0.0741	0.5211	0.6904	0.116*
H12B	0.0772	0.4526	0.5941	0.116*
H12C	0.1440	0.5119	0.5981	0.116*
C13	0.33258 (17)	0.27384 (17)	0.7767 (3)	0.0612 (7)
C14	0.38725 (18)	0.22233 (18)	0.8470 (4)	0.0854 (10)
H14A	0.4368	0.2454	0.8489	0.128*
H14B	0.3902	0.1741	0.8038	0.128*
H14C	0.3696	0.2147	0.9333	0.128*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04226 (9)	0.04557 (9)	0.03810 (8)	−0.00513 (7)	−0.00350 (8)	−0.00795 (8)
O1	0.0479 (10)	0.0484 (10)	0.0390 (7)	−0.0141 (7)	−0.0023 (7)	−0.0046 (7)
O2	0.0807 (13)	0.0862 (15)	0.0596 (14)	0.0015 (12)	−0.0111 (11)	−0.0070 (11)
O3	0.0770 (13)	0.0799 (14)	0.0617 (14)	0.0208 (10)	−0.0223 (11)	−0.0109 (11)
O1W	0.126 (2)	0.126 (2)	0.096 (3)	0.060 (2)	−0.010 (2)	−0.010 (2)
N1	0.0443 (10)	0.0502 (10)	0.0495 (13)	−0.0073 (8)	−0.0016 (9)	−0.0160 (9)
N2	0.0466 (12)	0.0550 (13)	0.0577 (13)	−0.0027 (9)	0.0051 (9)	−0.0113 (10)
C1	0.0417 (10)	0.0389 (11)	0.0477 (12)	0.0012 (8)	0.0027 (11)	0.0012 (11)
C2	0.0401 (11)	0.0407 (12)	0.0420 (14)	0.0019 (9)	−0.0041 (9)	−0.0015 (9)
C3	0.0491 (13)	0.0496 (14)	0.0429 (14)	0.0043 (10)	−0.0050 (11)	−0.0025 (11)
C4	0.0545 (13)	0.0636 (15)	0.0405 (13)	0.0120 (11)	−0.0002 (12)	0.0050 (13)
C5	0.0582 (14)	0.0570 (15)	0.0553 (17)	0.0029 (12)	0.0090 (12)	0.0120 (12)
C6	0.0554 (15)	0.0452 (14)	0.0623 (15)	−0.0043 (11)	0.0012 (12)	0.0029 (13)
C7	0.0456 (14)	0.0402 (13)	0.0604 (15)	−0.0063 (11)	0.0027 (11)	−0.0089 (12)
C8	0.0590 (16)	0.0711 (19)	0.0590 (16)	−0.0209 (14)	0.0052 (13)	−0.0311 (15)
C9	0.0747 (19)	0.0615 (17)	0.0698 (19)	−0.0139 (13)	0.0097 (16)	−0.0324 (15)
C10	0.0618 (16)	0.0729 (18)	0.0603 (18)	−0.0035 (13)	0.0069 (13)	−0.0263 (14)
C11	0.0646 (17)	0.0703 (19)	0.094 (2)	−0.0121 (15)	0.0305 (17)	−0.0211 (16)
C12	0.0677 (17)	0.0829 (19)	0.0824 (19)	0.0123 (15)	−0.0164 (17)	−0.0101 (19)
C13	0.0589 (17)	0.0632 (19)	0.0614 (19)	−0.0164 (14)	−0.0203 (14)	0.0033 (15)
C14	0.087 (2)	0.0793 (19)	0.090 (3)	−0.0130 (16)	−0.036 (2)	0.0237 (19)

Geometric parameters (Å, °)

Cd1—O1^{i}	2.2685 (14)	C4—H4A	0.9300
Cd1—O1	2.2797 (16)	C5—C6	1.371 (3)

Cd1—N1	2.2812 (19)	C5—H5A	0.9300
Cd1—O3	2.2976 (19)	C6—H6A	0.9300
Cd1—N2	2.409 (2)	C7—H7A	0.9300
Cd1—O2	2.428 (2)	C8—C9	1.525 (4)
Cd1—C13	2.707 (3)	C8—H8A	0.9700
O1—C2	1.326 (3)	C8—H8B	0.9700
O1—Cd1^{i}	2.2685 (14)	C9—C10	1.527 (4)
O2—C13	1.232 (4)	C9—H9A	0.9700
O3—C13	1.243 (4)	C9—H9B	0.9700
O1W—H1W	0.7950	C10—H10A	0.9700
N1—C7	1.268 (3)	C10—H10B	0.9700
N1—C8	1.466 (3)	C11—H11A	0.9600
N2—C11	1.462 (3)	C11—H11B	0.9600
N2—C12	1.466 (3)	C11—H11C	0.9600
N2—C10	1.470 (3)	C12—H12A	0.9600
C1—C6	1.400 (3)	C12—H12B	0.9600
C1—C2	1.431 (3)	C12—H12C	0.9600
C1—C7	1.454 (3)	C13—C14	1.508 (4)
C2—C3	1.400 (3)	C14—H14A	0.9600
C3—C4	1.371 (4)	C14—H14B	0.9600
C3—H3A	0.9300	C14—H14C	0.9600
C4—C5	1.384 (3)		
O1^{i}—Cd1—O1	78.30 (6)	C4—C5—H5A	121.0
O1^{i}—Cd1—N1	154.63 (6)	C5—C6—C1	122.9 (2)
O1—Cd1—N1	80.93 (6)	C5—C6—H6A	118.6
O1^{i}—Cd1—O3	96.99 (6)	C1—C6—H6A	118.6
O1—Cd1—O3	99.08 (7)	N1—C7—C1	128.6 (2)
N1—Cd1—O3	100.53 (7)	N1—C7—H7A	115.7
O1^{i}—Cd1—N2	93.45 (6)	C1—C7—H7A	115.7
O1—Cd1—N2	115.91 (7)	N1—C8—C9	112.1 (2)
N1—Cd1—N2	82.66 (7)	N1—C8—H8A	109.2
O3—Cd1—N2	144.85 (8)	C9—C8—H8A	109.2
O1^{i}—Cd1—O2	110.99 (6)	N1—C8—H8B	109.2
O1—Cd1—O2	151.78 (7)	C9—C8—H8B	109.2
N1—Cd1—O2	94.16 (7)	H8A—C8—H8B	107.9
O3—Cd1—O2	54.24 (8)	C8—C9—C10	115.0 (2)
N2—Cd1—O2	90.70 (8)	C8—C9—H9A	108.5
O1^{i}—Cd1—C13	104.98 (7)	C10—C9—H9A	108.5
O1—Cd1—C13	125.93 (9)	C8—C9—H9B	108.5
N1—Cd1—C13	98.94 (7)	C10—C9—H9B	108.5
O3—Cd1—C13	27.20 (9)	H9A—C9—H9B	107.5
N2—Cd1—C13	117.67 (9)	N2—C10—C9	116.2 (2)
O2—Cd1—C13	27.06 (8)	N2—C10—H10A	108.2
C2—O1—Cd1^{i}	127.33 (13)	C9—C10—H10A	108.2
C2—O1—Cd1	128.73 (13)	N2—C10—H10B	108.2
Cd1^{i}—O1—Cd1	101.40 (6)	C9—C10—H10B	108.2
C13—O2—Cd1	89.22 (17)	H10A—C10—H10B	107.4

C13—O3—Cd1	95.09 (19)	N2—C11—H11A	109.5
C7—N1—C8	117.6 (2)	N2—C11—H11B	109.5
C7—N1—Cd1	127.97 (16)	H11A—C11—H11B	109.5
C8—N1—Cd1	114.34 (16)	N2—C11—H11C	109.5
C11—N2—C12	107.5 (2)	H11A—C11—H11C	109.5
C11—N2—C10	107.8 (2)	H11B—C11—H11C	109.5
C12—N2—C10	110.8 (2)	N2—C12—H12A	109.5
C11—N2—Cd1	111.17 (16)	N2—C12—H12B	109.5
C12—N2—Cd1	107.47 (15)	H12A—C12—H12B	109.5
C10—N2—Cd1	112.01 (16)	N2—C12—H12C	109.5
C6—C1—C2	118.9 (2)	H12A—C12—H12C	109.5
C6—C1—C7	115.5 (2)	H12B—C12—H12C	109.5
C2—C1—C7	125.5 (2)	O2—C13—O3	121.4 (3)
O1—C2—C3	120.9 (2)	O2—C13—C14	121.0 (3)
O1—C2—C1	122.6 (2)	O3—C13—C14	117.6 (3)
C3—C2—C1	116.4 (2)	O2—C13—Cd1	63.73 (15)
C4—C3—C2	122.7 (2)	O3—C13—Cd1	57.70 (15)
C4—C3—H3A	118.6	C14—C13—Cd1	174.2 (2)
C2—C3—H3A	118.6	C13—C14—H14A	109.5
C3—C4—C5	120.8 (3)	C13—C14—H14B	109.5
C3—C4—H4A	119.6	H14A—C14—H14B	109.5
C5—C4—H4A	119.6	C13—C14—H14C	109.5
C6—C5—C4	118.1 (2)	H14A—C14—H14C	109.5
C6—C5—H5A	121.0	H14B—C14—H14C	109.5
$O1^{i}$—Cd1—O1—C2	−168.64 (14)	$O1^{i}$—Cd1—N2—C10	157.39 (17)
N1—Cd1—O1—C2	26.00 (17)	O1—Cd1—N2—C10	−123.95 (16)
O3—Cd1—O1—C2	−73.32 (17)	N1—Cd1—N2—C10	−47.79 (17)
N2—Cd1—O1—C2	103.21 (17)	O3—Cd1—N2—C10	50.1 (2)
O2—Cd1—O1—C2	−55.8 (2)	O2—Cd1—N2—C10	46.31 (17)
C13—Cd1—O1—C2	−68.51 (19)	C13—Cd1—N2—C10	48.49 (19)
$O1^{i}$—Cd1—O1—$Cd1^{i}$	−5.94 (8)	$Cd1^{i}$—O1—C2—C3	−4.0 (3)
N1—Cd1—O1—$Cd1^{i}$	−171.30 (8)	Cd1—O1—C2—C3	154.54 (16)
O3—Cd1—O1—$Cd1^{i}$	89.38 (8)	$Cd1^{i}$—O1—C2—C1	173.45 (14)
N2—Cd1—O1—$Cd1^{i}$	−94.09 (8)	Cd1—O1—C2—C1	−28.1 (3)
O2—Cd1—O1—$Cd1^{i}$	106.87 (13)	C6—C1—C2—O1	−175.0 (2)
C13—Cd1—O1—$Cd1^{i}$	94.19 (9)	C7—C1—C2—O1	7.0 (3)
$O1^{i}$—Cd1—O2—C13	81.80 (18)	C6—C1—C2—C3	2.5 (3)
O1—Cd1—O2—C13	−23.0 (2)	C7—C1—C2—C3	−175.5 (2)
N1—Cd1—O2—C13	−101.55 (17)	O1—C2—C3—C4	174.9 (2)
O3—Cd1—O2—C13	−1.56 (17)	C1—C2—C3—C4	−2.6 (3)
N2—Cd1—O2—C13	175.76 (17)	C2—C3—C4—C5	0.5 (4)
$O1^{i}$—Cd1—O3—C13	−109.33 (18)	C3—C4—C5—C6	1.7 (4)
O1—Cd1—O3—C13	171.47 (17)	C4—C5—C6—C1	−1.8 (4)
N1—Cd1—O3—C13	89.09 (18)	C2—C1—C6—C5	−0.3 (4)
N2—Cd1—O3—C13	−3.1 (3)	C7—C1—C6—C5	177.8 (2)
O2—Cd1—O3—C13	1.55 (16)	C8—N1—C7—C1	177.0 (2)
$O1^{i}$—Cd1—N1—C7	−47.2 (3)	Cd1—N1—C7—C1	−0.1 (4)

O1—Cd1—N1—C7	−11.9 (2)	C6—C1—C7—N1	−170.0 (2)
O3—Cd1—N1—C7	85.7 (2)	C2—C1—C7—N1	8.0 (4)
N2—Cd1—N1—C7	−129.7 (2)	C7—N1—C8—C9	111.1 (3)
O2—Cd1—N1—C7	140.1 (2)	Cd1—N1—C8—C9	−71.4 (3)
C13—Cd1—N1—C7	113.3 (2)	N1—C8—C9—C10	71.1 (3)
O1^{i}—Cd1—N1—C8	135.62 (19)	C11—N2—C10—C9	−174.9 (3)
O1—Cd1—N1—C8	170.92 (19)	C12—N2—C10—C9	−57.5 (3)
O3—Cd1—N1—C8	−91.45 (18)	Cd1—N2—C10—C9	62.5 (3)
N2—Cd1—N1—C8	53.10 (18)	C8—C9—C10—N2	−69.1 (3)
O2—Cd1—N1—C8	−37.07 (19)	Cd1—O2—C13—O3	2.7 (3)
C13—Cd1—N1—C8	−63.89 (19)	Cd1—O2—C13—C14	−176.2 (2)
O1^{i}—Cd1—N2—C11	36.70 (19)	Cd1—O3—C13—O2	−2.9 (3)
O1—Cd1—N2—C11	115.36 (18)	Cd1—O3—C13—C14	176.1 (2)
N1—Cd1—N2—C11	−168.48 (19)	O1^{i}—Cd1—C13—O2	−106.95 (17)
O3—Cd1—N2—C11	−70.6 (2)	O1—Cd1—C13—O2	166.80 (15)
O2—Cd1—N2—C11	−74.38 (19)	N1—Cd1—C13—O2	81.57 (17)
C13—Cd1—N2—C11	−72.2 (2)	O3—Cd1—C13—O2	177.2 (3)
O1^{i}—Cd1—N2—C12	−80.67 (17)	N2—Cd1—C13—O2	−4.79 (19)
O1—Cd1—N2—C12	−2.01 (18)	O1^{i}—Cd1—C13—O3	75.83 (18)
N1—Cd1—N2—C12	74.14 (17)	O1—Cd1—C13—O3	−10.4 (2)
O3—Cd1—N2—C12	172.03 (16)	N1—Cd1—C13—O3	−95.66 (18)
O2—Cd1—N2—C12	168.25 (17)	N2—Cd1—C13—O3	177.98 (17)
C13—Cd1—N2—C12	170.43 (16)	O2—Cd1—C13—O3	−177.2 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W···O3	0.80	1.97	2.762 (3)	172

Fig. 1