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Diaqua[(*N*,*N*′-dibenzylethane-1,2-diyldiimino)diacetato]cadmium(II) 2.5-hydrate

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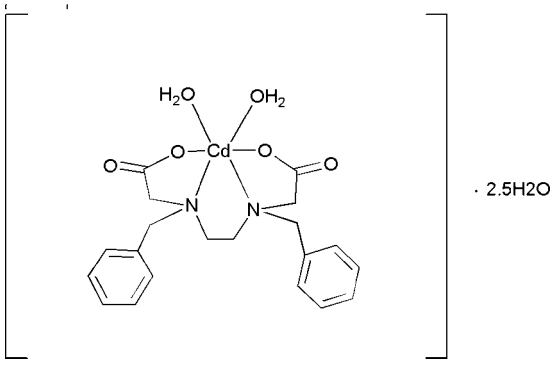
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.008 Å; R factor = 0.050; wR factor = 0.123; data-to-parameter ratio = 16.6.

In the asymmetric unit of the title compound, $[Cd(C_{20}H_{22}N_2O_4)(H_2O)_2]\cdot 2.5H_2O$, there are five water molecules and two independent mononuclear complex molecules in which the Cd^{II} ions are in distorted octahedral coordination environments, defined by N_2O_4 donor sets. In the crystal structure, extensive hydrogen bonding links molecules into one-dimensional chains along the b axis.

Related literature

For related literature, see: Xu *et al.* (2004).



Experimental

Crystal data

$[Cd(C_{20}H_{22}N_2O_4)(H_2O)_2]\cdot 2.5H_2O$
M_r = 547.87
Monoclinic, $P2_1/n$
a = 13.9704 (16) Å
b = 9.4600 (11) Å
c = 36.471 (3) Å
β = 92.273 (2)°
V = 4816.2 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.95 mm^{-1}
T = 294 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.763, T_{max} = 0.832
49413 measured reflections
9436 independent reflections
7654 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.123
S = 1.06
9436 reflections
568 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O5	2.245 (3)	Cd2—O11	2.235 (3)
Cd1—O6	2.260 (3)	Cd2—O12	2.247 (3)
Cd1—O1	2.262 (3)	Cd2—O7	2.277 (3)
Cd1—O3	2.282 (3)	Cd2—O9	2.307 (3)
Cd1—N2	2.392 (4)	Cd2—N4	2.374 (3)
Cd1—N1	2.403 (3)	Cd2—N3	2.387 (3)
O5—Cd1—O6	91.93 (11)	O11—Cd2—O12	95.76 (12)
O5—Cd1—O1	95.67 (10)	O11—Cd2—O7	95.63 (11)
O6—Cd1—O1	93.92 (12)	O12—Cd2—O7	96.35 (12)
O5—Cd1—O3	94.41 (10)	O11—Cd2—O9	96.09 (10)
O6—Cd1—O3	95.41 (11)	O12—Cd2—O9	93.47 (12)
O1—Cd1—O3	166.02 (11)	O7—Cd2—O9	163.87 (10)
O5—Cd1—N2	89.43 (11)	O11—Cd2—N4	161.46 (12)
O6—Cd1—N2	168.10 (12)	O12—Cd2—N4	99.07 (12)
O1—Cd1—N2	97.71 (12)	O7—Cd2—N4	93.74 (11)
O3—Cd1—N2	72.70 (11)	O9—Cd2—N4	72.03 (10)
O5—Cd1—N1	161.94 (12)	O11—Cd2—N3	89.20 (11)
O6—Cd1—N1	102.62 (12)	O12—Cd2—N3	168.40 (12)
O1—Cd1—N1	72.97 (11)	O7—Cd2—N3	72.68 (11)
O3—Cd1—N1	94.80 (11)	O9—Cd2—N3	96.43 (11)
N2—Cd1—N1	78.55 (12)	N4—Cd2—N3	78.37 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O9^{i}	0.82	1.90	2.717 (4)	173
O5—H5B···O8^{ii}	0.82	1.86	2.670 (4)	167
O6—H6A···O14^{iii}	0.82	1.87	2.668 (4)	162
O6—H6B···O13^{ii}	0.82	2.19	2.680 (4)	119
O6—H6B···O18	0.82	2.51	2.938 (5)	114
O11—H11A···O1^{iv}	0.83	1.83	2.654 (4)	178
O11—H11B···O4^{v}	0.82	1.84	2.651 (4)	165
O12—H12C···O18^{vi}	0.82	2.31	3.117 (5)	168
O12—H12D···O18^{iv}	0.82	2.00	2.769 (5)	155
O13—H13A···O10^{vii}	0.82	1.99	2.799 (4)	169
O13—H13B···O7	0.82	1.97	2.784 (4)	169
O14—H14A···O15	0.82	2.18	2.829 (5)	136
O14—H14B···O10^{vi}	0.82	2.01	2.774 (5)	155
O15—H15A···O2	0.82	1.90	2.704 (4)	165
O15—H15B···O3^{vii}	0.82	2.03	2.786 (4)	153
O17—H17B···O4^{viii}	0.98	2.00	2.778 (12)	134
O18—H18B···O9^{i}	0.98	2.48	3.323 (5)	144
C32—H32A···O18^{vi}	0.97	2.51	3.477 (6)	178

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997), *WinGX2003*

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(Farrugia, 1999); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2562).

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supplementary materials

Acta Cryst. (2007). E**63**, m3121-m3122 [**doi:10.1107/S1600536807058771**]

Diaqua[(*N*,*N*'-dibenzylethane-1,2-diyldiimino)diacetato]cadmium(II) 2.5-hydrate

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Comment

Previously we have synthesized the Cu(II) complex of (H_2L=[*N*,*N*'-bis(benzyl)ethane-1,2-diyldiimino]diacetate) (Xu *et al.*, 2004). Herein, we report the structure of the Cd(II) complex (1) with this ligand. In (1)(Fig 1) the asymmetric unit consists of two independent complex molecules and and five molecules of solvent water. The coordination geometry around atoms Cd1 and Cd2 is distorted octahedral defined by a N_2O_4 donor set, from two amine N atoms, two carboxyl O atoms, and two water O atoms (selected bond lengths and angles are given in Table 1). In the crystal structure (Fig. 2), extensive O—H···O hydrogen bonds (Table 2) form one-dimensional chains along the *b* axis.

Experimental

The title complex was prepared according to the literature method (Xu *et al.*, 2004). When $Cd(C_2H_3O_2)_2{\cdot}2H_2O$(0.013 g, 0.05 mmol) was added to a stirred solution (pH = 9,containing NaOH) of H_2L (0.018 g, 0.05 mmol) in H_2O(15 ml), a white precipitate formed immediately. After the pH of the solution was adjusted to 4–5 using dilute HCl, the resulting precipitete was filtered off and dried. Crystals were obtanined by slow evaporation (two weeks) of a methanol solution(15 ml) of the complex (1) (0.047 g,0.1 mmol).

Refinement

H atoms bonded to C atom were located at the geometrical positions with C—H =0.93Å (aromatic), 0.97Å (methylene) and U_{iso}(H) = 1.2U_{eq}(aromatic and methylene C). H atoms bonded to water O atoms were contrained at their indicative positions by using '*CALC*OH' programme in *WinGX* 2003 (Farrugia, 1999) and the U_{iso}(H) value were set 1.5 times of their carrier atoms. However, the calculated positions while sensible cause some H atoms, *e.g*. H12D, H17A, H18A, H18B and H32A, to be involved in fairly close intermolecular contacts.

Figures

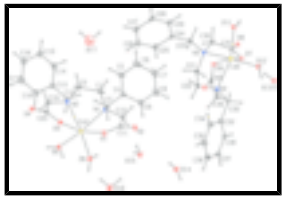


Fig. 1. The asymmetric unit showing 10% probability displacement ellipsoids.

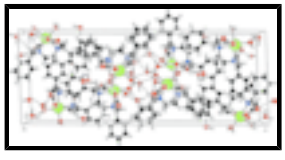


Fig. 2. Part of the crystal structure showing the formation of a one-dimensional chains. Dashed lines denote hydrogen bonds.

Diaqua[(*N*,*N*'-dibenzylethane-1,2-diyldiimino)diacetato]cadmium(II) 2.5-hydrate

Crystal data

$[Cd(C_{20}H_{22}N_2O_4)(H_2O_1)_2]\cdot 2.5H_2O$	$F_{000} = 2248$
$M_r = 547.87$	$D_x = 1.511$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 5870 reflections
$a = 13.9704$ (16) Å	$\theta = 2.2$–23.7^o
$b = 9.4600$ (11) Å	$\mu = 0.95$ mm^{-1}
$c = 36.471$ (3) Å	$T = 294$ (2) K
$\beta = 92.273$ (2)^o	Block, colorless
$V = 4816.2$ (9) Å^3	0.30 × 0.20 × 0.20 mm
$Z = 8$	

Data collection

Bruker SMART-CCD diffractometer	9436 independent reflections
Radiation source: fine-focus sealed tube	7654 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.075$
$T = 294$(2) K	$\theta_{max} = 26.0^o$
φ and ω scans	$\theta_{min} = 1.1^o$
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -16\rightarrow17$
$T_{min} = 0.763$, $T_{max} = 0.832$	$k = -11\rightarrow11$
49413 measured reflections	$l = -44\rightarrow43$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.123$	$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
9436 reflections	$\Delta\rho_{max} = 0.70$ e Å^{-3}
568 parameters	$\Delta\rho_{min} = -0.85$ 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.14816 (2)	0.07448 (3)	0.123273 (9)	0.03309 (11)
Cd2	0.92890 (2)	0.51568 (3)	0.096232 (8)	0.03220 (11)
C1	0.3374 (3)	0.1193 (5)	0.16963 (13)	0.0399 (11)
H1A	0.3235	0.2176	0.1748	0.048*
H1B	0.4047	0.1031	0.1759	0.048*
C2	0.2773 (3)	0.0261 (5)	0.19337 (13)	0.0399 (11)
H2A	0.2892	−0.0722	0.1875	0.048*
H2B	0.2967	0.0407	0.2189	0.048*
C3	0.3710 (3)	−0.0346 (5)	0.11676 (14)	0.0395 (11)
H3A	0.3466	−0.0571	0.0922	0.047*
H3B	0.3558	−0.1135	0.1325	0.047*
C4	0.4789 (3)	−0.0217 (4)	0.11599 (15)	0.0428 (12)
C5	0.5373 (4)	−0.0648 (5)	0.14582 (17)	0.0604 (15)
H5	0.5105	−0.1022	0.1666	0.073*
C6	0.6385 (5)	−0.0509 (7)	0.1440 (2)	0.083 (2)
H6	0.6780	−0.0791	0.1638	0.099*
C7	0.6783 (4)	0.0040 (7)	0.1131 (3)	0.082 (2)
H7	0.7444	0.0141	0.1121	0.098*
C8	0.6208 (4)	0.0428 (6)	0.0845 (2)	0.074 (2)
H8	0.6481	0.0785	0.0636	0.088*
C9	0.5230 (4)	0.0313 (5)	0.08524 (17)	0.0552 (14)
H9	0.4855	0.0594	0.0649	0.066*
C10	0.3432 (3)	0.2185 (4)	0.10856 (13)	0.0399 (11)
H10A	0.3483	0.1918	0.0830	0.048*
H10B	0.4055	0.2528	0.1172	0.048*
C11	0.2706 (3)	0.3398 (5)	0.11076 (12)	0.0386 (10)
C12	0.1427 (3)	0.1846 (5)	0.20828 (13)	0.0425 (11)
H12A	0.0867	0.2236	0.1953	0.051*
H12B	0.1934	0.2544	0.2074	0.051*
C13	0.1190 (3)	0.1623 (5)	0.24803 (13)	0.0434 (11)
C14	0.1891 (4)	0.1407 (5)	0.27534 (14)	0.0545 (13)
H14	0.2532	0.1462	0.2696	0.065*
C15	0.1660 (5)	0.1116 (6)	0.31056 (17)	0.0727 (18)

H15	0.2142	0.0974	0.3285	0.087*
C16	0.0723 (6)	0.1034 (7)	0.31944 (18)	0.084 (2)
H16	0.0567	0.0827	0.3434	0.101*
C17	0.0019 (5)	0.1252 (7)	0.2935 (2)	0.084 (2)
H17	−0.0618	0.1196	0.2999	0.100*
C18	0.0238 (4)	0.1562 (6)	0.25756 (16)	0.0658 (16)
H18	−0.0249	0.1726	0.2400	0.079*
C19	0.1158 (3)	−0.0682 (4)	0.19762 (12)	0.0391 (10)
H19A	0.0499	−0.0383	0.1999	0.047*
H19B	0.1384	−0.1037	0.2214	0.047*
C20	0.1181 (3)	−0.1894 (4)	0.16968 (12)	0.0359 (10)
C21	0.7233 (3)	0.5532 (4)	0.12492 (12)	0.0347 (10)
H21A	0.7162	0.6526	0.1189	0.042*
H21B	0.6731	0.5285	0.1414	0.042*
C22	0.7104 (3)	0.4670 (4)	0.09019 (12)	0.0345 (10)
H22A	0.7169	0.3676	0.0962	0.041*
H22B	0.6462	0.4819	0.0798	0.041*
C23	0.8227 (3)	0.3971 (4)	0.16563 (13)	0.0402 (11)
H23A	0.8866	0.3896	0.1768	0.048*
H23B	0.8143	0.3186	0.1487	0.048*
C24	0.7520 (3)	0.3804 (5)	0.19530 (12)	0.0382 (10)
C25	0.6727 (4)	0.2952 (5)	0.18932 (15)	0.0572 (14)
H25	0.6624	0.2515	0.1667	0.069*
C26	0.6077 (4)	0.2739 (7)	0.21691 (18)	0.0701 (17)
H26	0.5549	0.2153	0.2128	0.084*
C27	0.6218 (4)	0.3390 (7)	0.24973 (16)	0.0652 (16)
H27	0.5779	0.3258	0.2679	0.078*
C28	0.6994 (5)	0.4238 (7)	0.25645 (15)	0.0663 (17)
H28	0.7089	0.4680	0.2791	0.080*
C29	0.7637 (4)	0.4430 (6)	0.22915 (14)	0.0541 (13)
H29	0.8169	0.5004	0.2338	0.065*
C30	0.8477 (3)	0.6557 (4)	0.16554 (12)	0.0362 (10)
H30A	0.8977	0.6278	0.1833	0.043*
H30B	0.7938	0.6897	0.1790	0.043*
C31	0.8850 (3)	0.7769 (4)	0.14203 (12)	0.0330 (9)
C32	0.7600 (3)	0.6413 (4)	0.04399 (13)	0.0378 (10)
H32A	0.8104	0.6594	0.0270	0.045*
H32B	0.7634	0.7151	0.0625	0.045*
C33	0.6642 (3)	0.6535 (4)	0.02302 (13)	0.0394 (11)
C34	0.5872 (3)	0.7167 (5)	0.03930 (16)	0.0562 (14)
H34	0.5933	0.7479	0.0635	0.067*
C35	0.5012 (4)	0.7336 (6)	0.0197 (2)	0.0722 (18)
H35	0.4502	0.7778	0.0306	0.087*
C36	0.4905 (4)	0.6864 (6)	−0.0153 (2)	0.0695 (18)
H36	0.4320	0.6973	−0.0280	0.083*
C37	0.5650 (4)	0.6230 (6)	−0.03202 (15)	0.0590 (15)
H37	0.5573	0.5908	−0.0560	0.071*
C38	0.6524 (4)	0.6072 (5)	−0.01280 (14)	0.0494 (12)
H38	0.7034	0.5649	−0.0242	0.059*

C39	0.7928 (3)	0.3874 (4)	0.03638 (12)	0.0355 (10)
H39A	0.8291	0.4212	0.0160	0.043*
H39B	0.7304	0.3575	0.0267	0.043*
C40	0.8448 (3)	0.2595 (4)	0.05404 (12)	0.0337 (10)
N1	0.3196 (2)	0.0923 (3)	0.12969 (10)	0.0332 (8)
N2	0.1734 (2)	0.0553 (3)	0.18834 (10)	0.0338 (8)
N3	0.8172 (2)	0.5310 (3)	0.14395 (10)	0.0323 (8)
N4	0.7803 (2)	0.5037 (3)	0.06244 (10)	0.0326 (8)
O1	0.1857 (2)	0.3060 (3)	0.11787 (9)	0.0479 (8)
O2	0.2997 (2)	0.4583 (3)	0.10453 (10)	0.0505 (9)
O3	0.1434 (2)	−0.1601 (3)	0.13766 (8)	0.0389 (7)
O4	0.0931 (2)	−0.3067 (3)	0.18056 (9)	0.0473 (8)
O5	−0.0086 (2)	0.1096 (3)	0.13117 (8)	0.0409 (7)
H5A	−0.0358	0.1668	0.1175	0.061*
H5B	−0.0472	0.0522	0.1388	0.061*
O6	0.1234 (2)	0.0431 (3)	0.06219 (8)	0.0467 (8)
H6A	0.1720	0.0060	0.0545	0.070*
H6B	0.0814	0.0475	0.0459	0.070*
O7	0.9119 (2)	0.7488 (3)	0.11012 (8)	0.0393 (7)
O8	0.8889 (2)	0.8951 (3)	0.15652 (9)	0.0440 (8)
O9	0.8997 (2)	0.2819 (3)	0.08162 (8)	0.0377 (7)
O10	0.8308 (2)	0.1429 (3)	0.03897 (9)	0.0455 (8)
O11	1.0454 (2)	0.4736 (3)	0.13859 (8)	0.0409 (7)
H11A	1.0896	0.4215	0.1326	0.061*
H11B	1.0675	0.5445	0.1490	0.061*
O12	1.0267 (2)	0.5476 (4)	0.04948 (9)	0.0505 (8)
H12C	0.9959	0.5922	0.0338	0.076*
H12D	1.0535	0.4824	0.0392	0.076*
O13	0.9549 (2)	0.9130 (3)	0.04959 (9)	0.0491 (8)
H13A	0.9154	0.9745	0.0440	0.074*
H13B	0.9410	0.8746	0.0689	0.074*
O14	0.2542 (2)	0.8830 (4)	0.03073 (9)	0.0566 (9)
H14A	0.2619	0.8041	0.0397	0.085*
H14B	0.2466	0.8736	0.0085	0.085*
O15	0.1875 (2)	0.6709 (3)	0.07808 (9)	0.0483 (8)
H15A	0.2135	0.6036	0.0886	0.072*
H15B	0.1561	0.7131	0.0931	0.072*
O17	0.4568 (8)	0.0413 (13)	0.2579 (3)	0.271 (6)
H17A	0.5273	0.0413	0.2579	0.406*
H17B	0.4361	0.0413	0.2833	0.406*
O18	0.0625 (3)	0.2882 (4)	0.01765 (10)	0.0739 (12)
H18A	0.1329	0.2881	0.0176	0.111*
H18B	0.0417	0.2881	0.0431	0.111*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03149 (18)	0.03535 (18)	0.0322 (2)	0.00266 (12)	−0.00139 (13)	−0.00107 (13)

Cd2	0.02739 (17)	0.03698 (18)	0.0323 (2)	0.00211 (12)	0.00186 (13)	−0.00149 (13)
C1	0.034 (2)	0.034 (2)	0.051 (3)	−0.0021 (18)	−0.004 (2)	−0.006 (2)
C2	0.046 (3)	0.038 (2)	0.035 (3)	0.003 (2)	−0.007 (2)	−0.002 (2)
C3	0.033 (2)	0.035 (2)	0.051 (3)	0.0056 (18)	0.001 (2)	−0.004 (2)
C4	0.035 (2)	0.027 (2)	0.066 (4)	0.0105 (18)	−0.007 (2)	−0.008 (2)
C5	0.052 (3)	0.048 (3)	0.080 (4)	0.017 (2)	−0.011 (3)	−0.002 (3)
C6	0.061 (4)	0.060 (4)	0.123 (7)	0.027 (3)	−0.042 (4)	−0.025 (4)
C7	0.041 (3)	0.054 (4)	0.150 (8)	0.007 (3)	0.000 (4)	−0.020 (4)
C8	0.049 (3)	0.049 (3)	0.125 (6)	0.007 (3)	0.031 (4)	−0.001 (4)
C9	0.046 (3)	0.046 (3)	0.075 (4)	0.013 (2)	0.010 (3)	0.000 (3)
C10	0.035 (2)	0.032 (2)	0.053 (3)	0.0050 (18)	0.007 (2)	0.005 (2)
C11	0.040 (3)	0.037 (2)	0.039 (3)	0.004 (2)	−0.001 (2)	−0.003 (2)
C12	0.045 (3)	0.037 (2)	0.046 (3)	0.005 (2)	0.001 (2)	−0.009 (2)
C13	0.051 (3)	0.038 (2)	0.041 (3)	−0.005 (2)	0.006 (2)	−0.014 (2)
C14	0.073 (4)	0.054 (3)	0.036 (3)	−0.013 (3)	0.004 (3)	−0.011 (2)
C15	0.109 (5)	0.060 (4)	0.049 (4)	−0.019 (4)	−0.001 (4)	−0.013 (3)
C16	0.124 (6)	0.084 (5)	0.046 (4)	−0.041 (4)	0.021 (4)	−0.019 (3)
C17	0.079 (4)	0.100 (5)	0.074 (5)	−0.027 (4)	0.039 (4)	−0.036 (4)
C18	0.066 (4)	0.081 (4)	0.051 (4)	−0.004 (3)	0.008 (3)	−0.030 (3)
C19	0.048 (3)	0.035 (2)	0.034 (3)	−0.0018 (19)	0.002 (2)	−0.0057 (19)
C20	0.034 (2)	0.036 (2)	0.037 (3)	0.0086 (18)	−0.007 (2)	−0.004 (2)
C21	0.032 (2)	0.036 (2)	0.037 (3)	0.0044 (18)	0.0097 (19)	0.0029 (19)
C22	0.027 (2)	0.034 (2)	0.043 (3)	−0.0012 (17)	0.0058 (19)	0.002 (2)
C23	0.047 (3)	0.033 (2)	0.041 (3)	0.0050 (19)	0.006 (2)	0.004 (2)
C24	0.048 (3)	0.037 (2)	0.029 (3)	0.002 (2)	0.002 (2)	0.008 (2)
C25	0.075 (4)	0.052 (3)	0.045 (3)	−0.020 (3)	0.008 (3)	0.004 (3)
C26	0.060 (4)	0.076 (4)	0.076 (5)	−0.017 (3)	0.015 (3)	0.021 (4)
C27	0.068 (4)	0.080 (4)	0.050 (4)	0.018 (3)	0.025 (3)	0.025 (3)
C28	0.089 (5)	0.078 (4)	0.032 (3)	0.015 (4)	0.011 (3)	0.016 (3)
C29	0.065 (3)	0.061 (3)	0.036 (3)	−0.007 (3)	0.001 (3)	0.010 (3)
C30	0.041 (2)	0.038 (2)	0.030 (2)	0.0013 (19)	0.0041 (19)	0.0007 (19)
C31	0.027 (2)	0.035 (2)	0.037 (3)	0.0012 (17)	0.0014 (19)	0.005 (2)
C32	0.037 (2)	0.035 (2)	0.041 (3)	−0.0020 (18)	0.000 (2)	0.007 (2)
C33	0.036 (2)	0.034 (2)	0.048 (3)	0.0012 (18)	−0.005 (2)	0.012 (2)
C34	0.051 (3)	0.048 (3)	0.069 (4)	0.012 (2)	−0.008 (3)	−0.005 (3)
C35	0.044 (3)	0.062 (4)	0.110 (6)	0.017 (3)	−0.007 (3)	0.008 (4)
C36	0.049 (3)	0.064 (4)	0.092 (5)	−0.009 (3)	−0.028 (3)	0.032 (4)
C37	0.058 (3)	0.066 (3)	0.052 (3)	−0.016 (3)	−0.019 (3)	0.021 (3)
C38	0.052 (3)	0.053 (3)	0.043 (3)	−0.003 (2)	−0.002 (2)	0.014 (2)
C39	0.033 (2)	0.039 (2)	0.035 (3)	0.0023 (18)	0.0026 (19)	0.001 (2)
C40	0.029 (2)	0.037 (2)	0.035 (3)	0.0016 (18)	0.0046 (19)	0.001 (2)
N1	0.0298 (18)	0.0297 (18)	0.040 (2)	0.0057 (14)	0.0031 (16)	0.0033 (16)
N2	0.039 (2)	0.0314 (18)	0.031 (2)	−0.0004 (15)	0.0013 (16)	−0.0031 (15)
N3	0.0331 (19)	0.0297 (17)	0.034 (2)	0.0001 (14)	0.0045 (16)	0.0036 (16)
N4	0.0302 (18)	0.0365 (19)	0.031 (2)	0.0048 (14)	0.0012 (16)	0.0024 (16)
O1	0.0391 (17)	0.0316 (16)	0.073 (2)	0.0073 (14)	0.0055 (16)	−0.0013 (16)
O2	0.053 (2)	0.0289 (16)	0.071 (3)	0.0011 (14)	0.0105 (18)	0.0000 (16)
O3	0.0528 (19)	0.0358 (16)	0.0282 (17)	0.0025 (14)	0.0024 (14)	−0.0035 (14)
O4	0.063 (2)	0.0323 (17)	0.046 (2)	−0.0073 (15)	−0.0024 (16)	0.0007 (15)

O5	0.0328 (16)	0.0400 (16)	0.050 (2)	0.0018 (13)	0.0012 (14)	0.0115 (15)
O6	0.053 (2)	0.0544 (19)	0.0327 (19)	0.0056 (16)	−0.0027 (15)	−0.0052 (15)
O7	0.0449 (17)	0.0385 (16)	0.0348 (18)	−0.0021 (14)	0.0061 (14)	0.0048 (14)
O8	0.0524 (19)	0.0312 (16)	0.049 (2)	−0.0008 (14)	0.0080 (16)	−0.0058 (15)
O9	0.0386 (16)	0.0372 (16)	0.0364 (18)	0.0076 (13)	−0.0120 (14)	−0.0024 (14)
O10	0.0518 (19)	0.0351 (17)	0.049 (2)	0.0034 (14)	−0.0083 (16)	−0.0030 (15)
O11	0.0346 (16)	0.0401 (16)	0.047 (2)	0.0077 (13)	−0.0069 (14)	−0.0119 (15)
O12	0.050 (2)	0.065 (2)	0.037 (2)	0.0072 (17)	0.0081 (16)	0.0054 (17)
O13	0.055 (2)	0.0491 (19)	0.044 (2)	0.0048 (16)	0.0049 (16)	0.0056 (16)
O14	0.063 (2)	0.061 (2)	0.045 (2)	0.0034 (18)	−0.0025 (17)	−0.0042 (18)
O15	0.061 (2)	0.0407 (17)	0.044 (2)	0.0095 (15)	0.0061 (16)	0.0031 (15)
O17	0.225 (11)	0.413 (17)	0.175 (9)	−0.078 (11)	0.034 (8)	−0.037 (10)
O18	0.086 (3)	0.080 (3)	0.057 (3)	0.010 (2)	0.027 (2)	0.005 (2)

Geometric parameters (Å, °)

Cd1—O5	2.245 (3)	C21—H21B	0.9700
Cd1—O6	2.260 (3)	C22—N4	1.475 (5)
Cd1—O1	2.262 (3)	C22—H22A	0.9700
Cd1—O3	2.282 (3)	C22—H22B	0.9700
Cd1—N2	2.392 (4)	C23—N3	1.493 (5)
Cd1—N1	2.403 (3)	C23—C24	1.501 (6)
Cd2—O11	2.235 (3)	C23—H23A	0.9700
Cd2—O12	2.247 (3)	C23—H23B	0.9700
Cd2—O7	2.277 (3)	C24—C29	1.374 (7)
Cd2—O9	2.307 (3)	C24—C25	1.381 (6)
Cd2—N4	2.374 (3)	C25—C26	1.396 (7)
Cd2—N3	2.387 (3)	C25—H25	0.9300
C1—N1	1.490 (6)	C26—C27	1.354 (8)
C1—C2	1.514 (6)	C26—H26	0.9300
C1—H1A	0.9700	C27—C28	1.363 (8)
C1—H1B	0.9700	C27—H27	0.9300
C2—N2	1.482 (5)	C28—C29	1.379 (7)
C2—H2A	0.9700	C28—H28	0.9300
C2—H2B	0.9700	C29—H29	0.9300
C3—N1	1.485 (5)	C30—N3	1.472 (5)
C3—C4	1.514 (6)	C30—C31	1.535 (6)
C3—H3A	0.9700	C30—H30A	0.9700
C3—H3B	0.9700	C30—H30B	0.9700
C4—C9	1.394 (7)	C31—O8	1.237 (5)
C4—C5	1.395 (7)	C31—O7	1.265 (5)
C5—C6	1.425 (8)	C32—N4	1.488 (5)
C5—H5	0.9300	C32—C33	1.519 (6)
C6—C7	1.376 (10)	C32—H32A	0.9700
C6—H6	0.9300	C32—H32B	0.9700
C7—C8	1.343 (9)	C33—C38	1.382 (7)
C7—H7	0.9300	C33—C34	1.385 (7)
C8—C9	1.373 (7)	C34—C35	1.383 (7)
C8—H8	0.9300	C34—H34	0.9300

C9—H9	0.9300	C35—C36	1.354 (9)
C10—N1	1.466 (5)	C35—H35	0.9300
C10—C11	1.535 (6)	C36—C37	1.365 (8)
C10—H10A	0.9700	C36—H36	0.9300
C10—H10B	0.9700	C37—C38	1.392 (7)
C11—O2	1.217 (5)	C37—H37	0.9300
C11—O1	1.265 (5)	C38—H38	0.9300
C12—N2	1.495 (5)	C39—N4	1.469 (5)
C12—C13	1.514 (6)	C39—C40	1.539 (6)
C12—H12A	0.9700	C39—H39A	0.9700
C12—H12B	0.9700	C39—H39B	0.9700
C13—C14	1.384 (7)	C40—O10	1.244 (5)
C13—C18	1.388 (7)	C40—O9	1.259 (5)
C14—C15	1.365 (7)	O5—H5A	0.8190
C14—H14	0.9300	O5—H5B	0.8211
C15—C16	1.363 (9)	O6—H6A	0.8236
C15—H15	0.9300	O6—H6B	0.8177
C16—C17	1.352 (10)	O11—H11A	0.8264
C16—H16	0.9300	O11—H11B	0.8238
C17—C18	1.391 (8)	O12—H12C	0.8201
C17—H17	0.9300	O12—H12D	0.8201
C18—H18	0.9300	O13—H13A	0.8224
C19—N2	1.466 (5)	O13—H13B	0.8215
C19—C20	1.535 (6)	O14—H14A	0.8201
C19—H19A	0.9700	O14—H14B	0.8200
C19—H19B	0.9700	O15—H15A	0.8200
C20—O4	1.233 (5)	O15—H15B	0.8200
C20—O3	1.264 (5)	O17—H17A	0.9840
C21—N3	1.476 (5)	O17—H17B	0.9827
C21—C22	1.511 (6)	O18—H18A	0.9835
C21—H21A	0.9700	O18—H18B	0.9839
O5—Cd1—O6	91.93 (11)	C21—C22—H22A	109.0
O5—Cd1—O1	95.67 (10)	N4—C22—H22B	109.0
O6—Cd1—O1	93.92 (12)	C21—C22—H22B	109.0
O5—Cd1—O3	94.41 (10)	H22A—C22—H22B	107.8
O6—Cd1—O3	95.41 (11)	N3—C23—C24	116.7 (3)
O1—Cd1—O3	166.02 (11)	N3—C23—H23A	108.1
O5—Cd1—N2	89.43 (11)	C24—C23—H23A	108.1
O6—Cd1—N2	168.10 (12)	N3—C23—H23B	108.1
O1—Cd1—N2	97.71 (12)	C24—C23—H23B	108.1
O3—Cd1—N2	72.70 (11)	H23A—C23—H23B	107.3
O5—Cd1—N1	161.94 (12)	C29—C24—C25	117.4 (5)
O6—Cd1—N1	102.62 (12)	C29—C24—C23	123.0 (4)
O1—Cd1—N1	72.97 (11)	C25—C24—C23	119.6 (4)
O3—Cd1—N1	94.80 (11)	C24—C25—C26	120.7 (5)
N2—Cd1—N1	78.55 (12)	C24—C25—H25	119.6
O11—Cd2—O12	95.76 (12)	C26—C25—H25	119.6
O11—Cd2—O7	95.63 (11)	C27—C26—C25	119.7 (6)
O12—Cd2—O7	96.35 (12)	C27—C26—H26	120.2

O11—Cd2—O9	96.09 (10)	C25—C26—H26	120.2
O12—Cd2—O9	93.47 (12)	C26—C27—C28	120.9 (5)
O7—Cd2—O9	163.87 (10)	C26—C27—H27	119.5
O11—Cd2—N4	161.46 (12)	C28—C27—H27	119.5
O12—Cd2—N4	99.07 (12)	C27—C28—C29	118.9 (6)
O7—Cd2—N4	93.74 (11)	C27—C28—H28	120.5
O9—Cd2—N4	72.03 (10)	C29—C28—H28	120.5
O11—Cd2—N3	89.20 (11)	C24—C29—C28	122.3 (5)
O12—Cd2—N3	168.40 (12)	C24—C29—H29	118.9
O7—Cd2—N3	72.68 (11)	C28—C29—H29	118.9
O9—Cd2—N3	96.43 (11)	N3—C30—C31	113.4 (3)
N4—Cd2—N3	78.37 (12)	N3—C30—H30A	108.9
N1—C1—C2	112.6 (3)	C31—C30—H30A	108.9
N1—C1—H1A	109.1	N3—C30—H30B	108.9
C2—C1—H1A	109.1	C31—C30—H30B	108.9
N1—C1—H1B	109.1	H30A—C30—H30B	107.7
C2—C1—H1B	109.1	O8—C31—O7	125.0 (4)
H1A—C1—H1B	107.8	O8—C31—C30	116.5 (4)
N2—C2—C1	112.6 (4)	O7—C31—C30	118.5 (4)
N2—C2—H2A	109.1	N4—C32—C33	116.3 (3)
C1—C2—H2A	109.1	N4—C32—H32A	108.2
N2—C2—H2B	109.1	C33—C32—H32A	108.2
C1—C2—H2B	109.1	N4—C32—H32B	108.2
H2A—C2—H2B	107.8	C33—C32—H32B	108.2
N1—C3—C4	115.8 (4)	H32A—C32—H32B	107.4
N1—C3—H3A	108.3	C38—C33—C34	118.5 (4)
C4—C3—H3A	108.3	C38—C33—C32	121.5 (4)
N1—C3—H3B	108.3	C34—C33—C32	120.0 (4)
C4—C3—H3B	108.3	C35—C34—C33	120.1 (5)
H3A—C3—H3B	107.4	C35—C34—H34	119.9
C9—C4—C5	118.0 (5)	C33—C34—H34	119.9
C9—C4—C3	121.0 (4)	C36—C35—C34	120.7 (6)
C5—C4—C3	120.9 (5)	C36—C35—H35	119.7
C4—C5—C6	119.2 (6)	C34—C35—H35	119.7
C4—C5—H5	120.4	C35—C36—C37	120.6 (5)
C6—C5—H5	120.4	C35—C36—H36	119.7
C7—C6—C5	120.5 (6)	C37—C36—H36	119.7
C7—C6—H6	119.8	C36—C37—C38	119.4 (6)
C5—C6—H6	119.8	C36—C37—H37	120.3
C8—C7—C6	119.4 (6)	C38—C37—H37	120.3
C8—C7—H7	120.3	C33—C38—C37	120.8 (5)
C6—C7—H7	120.3	C33—C38—H38	119.6
C7—C8—C9	121.9 (7)	C37—C38—H38	119.6
C7—C8—H8	119.0	N4—C39—C40	112.6 (3)
C9—C8—H8	119.0	N4—C39—H39A	109.1
C8—C9—C4	121.0 (6)	C40—C39—H39A	109.1
C8—C9—H9	119.5	N4—C39—H39B	109.1
C4—C9—H9	119.5	C40—C39—H39B	109.1
N1—C10—C11	114.7 (3)	H39A—C39—H39B	107.8

N1—C10—H10A	108.6	O10—C40—O9	125.6 (4)
C11—C10—H10A	108.6	O10—C40—C39	116.7 (4)
N1—C10—H10B	108.6	O9—C40—C39	117.7 (4)
C11—C10—H10B	108.6	C10—N1—C3	111.7 (3)
H10A—C10—H10B	107.6	C10—N1—C1	110.0 (3)
O2—C11—O1	126.4 (4)	C3—N1—C1	112.6 (3)
O2—C11—C10	116.9 (4)	C10—N1—Cd1	104.5 (2)
O1—C11—C10	116.7 (4)	C3—N1—Cd1	113.9 (2)
N2—C12—C13	115.4 (4)	C1—N1—Cd1	103.6 (2)
N2—C12—H12A	108.4	C19—N2—C2	111.5 (3)
C13—C12—H12A	108.4	C19—N2—C12	111.6 (3)
N2—C12—H12B	108.4	C2—N2—C12	113.0 (3)
C13—C12—H12B	108.4	C19—N2—Cd1	103.2 (3)
H12A—C12—H12B	107.5	C2—N2—Cd1	104.0 (3)
C14—C13—C18	118.1 (5)	C12—N2—Cd1	112.8 (3)
C14—C13—C12	122.3 (4)	C30—N3—C21	111.7 (3)
C18—C13—C12	119.6 (5)	C30—N3—C23	112.9 (3)
C15—C14—C13	121.3 (6)	C21—N3—C23	113.3 (3)
C15—C14—H14	119.3	C30—N3—Cd2	104.8 (2)
C13—C14—H14	119.3	C21—N3—Cd2	105.1 (2)
C16—C15—C14	120.0 (6)	C23—N3—Cd2	108.3 (2)
C16—C15—H15	120.0	C39—N4—C22	111.5 (3)
C14—C15—H15	120.0	C39—N4—C32	112.8 (3)
C17—C16—C15	120.3 (6)	C22—N4—C32	113.4 (3)
C17—C16—H16	119.9	C39—N4—Cd2	104.4 (2)
C15—C16—H16	119.9	C22—N4—Cd2	104.1 (2)
C16—C17—C18	120.6 (6)	C32—N4—Cd2	109.9 (2)
C16—C17—H17	119.7	C11—O1—Cd1	119.0 (3)
C18—C17—H17	119.7	C20—O3—Cd1	115.9 (3)
C13—C18—C17	119.6 (6)	Cd1—O5—H5A	116.8
C13—C18—H18	120.2	Cd1—O5—H5B	127.1
C17—C18—H18	120.2	H5A—O5—H5B	110.3
N2—C19—C20	114.6 (4)	Cd1—O6—H6A	107.1
N2—C19—H19A	108.6	Cd1—O6—H6B	141.7
C20—C19—H19A	108.6	H6A—O6—H6B	110.7
N2—C19—H19B	108.6	C31—O7—Cd2	116.5 (3)
C20—C19—H19B	108.6	C40—O9—Cd2	116.3 (3)
H19A—C19—H19B	107.6	Cd2—O11—H11A	117.1
O4—C20—O3	126.0 (4)	Cd2—O11—H11B	115.0
O4—C20—C19	116.4 (4)	H11A—O11—H11B	109.6
O3—C20—C19	117.6 (4)	Cd2—O12—H12C	106.3
N3—C21—C22	113.0 (3)	Cd2—O12—H12D	123.3
N3—C21—H21A	109.0	H12C—O12—H12D	107.7
C22—C21—H21A	109.0	H13A—O13—H13B	110.2
N3—C21—H21B	109.0	H14A—O14—H14B	107.7
C22—C21—H21B	109.0	H15A—O15—H15B	107.7
H21A—C21—H21B	107.8	H17A—O17—H17B	109.4
N4—C22—C21	112.9 (3)	H18A—O18—H18B	109.5
N4—C22—H22A	109.0		

N1—C1—C2—N2	−64.9 (5)	N1—Cd1—N2—C19	−131.6 (3)
N1—C3—C4—C9	−88.1 (5)	O5—Cd1—N2—C2	178.6 (2)
N1—C3—C4—C5	93.0 (5)	O6—Cd1—N2—C2	81.9 (6)
C9—C4—C5—C6	1.1 (7)	O1—Cd1—N2—C2	−85.8 (2)
C3—C4—C5—C6	−180.0 (4)	O3—Cd1—N2—C2	83.8 (2)
C4—C5—C6—C7	−0.2 (8)	N1—Cd1—N2—C2	−15.0 (2)
C5—C6—C7—C8	−0.8 (9)	O5—Cd1—N2—C12	−58.6 (3)
C6—C7—C8—C9	1.0 (9)	O6—Cd1—N2—C12	−155.3 (5)
C7—C8—C9—C4	−0.1 (9)	O1—Cd1—N2—C12	37.0 (3)
C5—C4—C9—C8	−1.0 (7)	O3—Cd1—N2—C12	−153.4 (3)
C3—C4—C9—C8	−179.9 (5)	N1—Cd1—N2—C12	107.8 (3)
N1—C10—C11—O2	156.5 (4)	C31—C30—N3—C21	−76.4 (4)
N1—C10—C11—O1	−25.4 (6)	C31—C30—N3—C23	154.5 (3)
N2—C12—C13—C14	74.1 (6)	C31—C30—N3—Cd2	36.9 (4)
N2—C12—C13—C18	−102.7 (5)	C22—C21—N3—C30	152.5 (3)
C18—C13—C14—C15	1.2 (8)	C22—C21—N3—C23	−78.6 (4)
C12—C13—C14—C15	−175.7 (5)	C22—C21—N3—Cd2	39.4 (4)
C13—C14—C15—C16	−0.1 (9)	C24—C23—N3—C30	69.2 (5)
C14—C15—C16—C17	−0.6 (10)	C24—C23—N3—C21	−59.0 (5)
C15—C16—C17—C18	0.1 (10)	C24—C23—N3—Cd2	−175.2 (3)
C14—C13—C18—C17	−1.7 (8)	O11—Cd2—N3—C30	64.9 (2)
C12—C13—C18—C17	175.3 (5)	O12—Cd2—N3—C30	−50.7 (7)
C16—C17—C18—C13	1.1 (10)	O7—Cd2—N3—C30	−31.3 (2)
N2—C19—C20—O4	161.2 (4)	O9—Cd2—N3—C30	160.9 (2)
N2—C19—C20—O3	−20.1 (5)	N4—Cd2—N3—C30	−129.0 (3)
N3—C21—C22—N4	−62.1 (5)	O11—Cd2—N3—C21	−177.2 (2)
N3—C23—C24—C29	−79.8 (6)	O12—Cd2—N3—C21	67.2 (7)
N3—C23—C24—C25	102.3 (5)	O7—Cd2—N3—C21	86.6 (2)
C29—C24—C25—C26	−0.3 (8)	O9—Cd2—N3—C21	−81.2 (2)
C23—C24—C25—C26	177.7 (5)	N4—Cd2—N3—C21	−11.1 (2)
C24—C25—C26—C27	1.0 (9)	O11—Cd2—N3—C23	−55.9 (3)
C25—C26—C27—C28	−0.9 (9)	O12—Cd2—N3—C23	−171.4 (5)
C26—C27—C28—C29	0.2 (9)	O7—Cd2—N3—C23	−152.0 (3)
C25—C24—C29—C28	−0.4 (7)	O9—Cd2—N3—C23	40.2 (3)
C23—C24—C29—C28	−178.3 (5)	N4—Cd2—N3—C23	110.3 (3)
C27—C28—C29—C24	0.4 (8)	C40—C39—N4—C22	−69.7 (4)
N3—C30—C31—O8	162.4 (4)	C40—C39—N4—C32	161.4 (3)
N3—C30—C31—O7	−19.6 (5)	C40—C39—N4—Cd2	42.1 (4)
N4—C32—C33—C38	−84.9 (5)	C21—C22—N4—C39	157.3 (3)
N4—C32—C33—C34	97.4 (5)	C21—C22—N4—C32	−74.0 (4)
C38—C33—C34—C35	−0.6 (7)	C21—C22—N4—Cd2	45.4 (4)
C32—C33—C34—C35	177.1 (5)	C33—C32—N4—C39	67.5 (5)
C33—C34—C35—C36	1.3 (9)	C33—C32—N4—C22	−60.4 (5)
C34—C35—C36—C37	−0.9 (9)	C33—C32—N4—Cd2	−176.5 (3)
C35—C36—C37—C38	0.0 (8)	O11—Cd2—N4—C39	−85.7 (4)
C34—C33—C38—C37	−0.3 (7)	O12—Cd2—N4—C39	57.0 (3)
C32—C33—C38—C37	−178.0 (4)	O7—Cd2—N4—C39	154.1 (2)
C36—C37—C38—C33	0.6 (8)	O9—Cd2—N4—C39	−33.7 (2)
N4—C39—C40—O10	156.5 (4)	N3—Cd2—N4—C39	−134.5 (3)

N4—C39—C40—O9	−25.5 (5)	O11—Cd2—N4—C22	31.3 (5)
C11—C10—N1—C3	160.3 (4)	O12—Cd2—N4—C22	174.1 (2)
C11—C10—N1—C1	−73.9 (5)	O7—Cd2—N4—C22	−88.9 (2)
C11—C10—N1—Cd1	36.7 (4)	O9—Cd2—N4—C22	83.3 (2)
C4—C3—N1—C10	54.9 (5)	N3—Cd2—N4—C22	−17.5 (2)
C4—C3—N1—C1	−69.5 (5)	O11—Cd2—N4—C32	153.1 (3)
C4—C3—N1—Cd1	173.0 (3)	O12—Cd2—N4—C32	−64.2 (3)
C2—C1—N1—C10	154.9 (3)	O7—Cd2—N4—C32	32.8 (3)
C2—C1—N1—C3	−79.8 (4)	O9—Cd2—N4—C32	−155.0 (3)
C2—C1—N1—Cd1	43.7 (4)	N3—Cd2—N4—C32	104.3 (3)
O5—Cd1—N1—C10	−80.5 (5)	O2—C11—O1—Cd1	174.4 (4)
O6—Cd1—N1—C10	62.5 (3)	C10—C11—O1—Cd1	−3.4 (5)
O1—Cd1—N1—C10	−27.8 (3)	O5—Cd1—O1—C11	−176.2 (3)
O3—Cd1—N1—C10	159.1 (3)	O6—Cd1—O1—C11	−83.8 (3)
N2—Cd1—N1—C10	−129.6 (3)	O3—Cd1—O1—C11	47.9 (6)
O5—Cd1—N1—C3	157.4 (3)	N2—Cd1—O1—C11	93.6 (3)
O6—Cd1—N1—C3	−59.7 (3)	N1—Cd1—O1—C11	18.2 (3)
O1—Cd1—N1—C3	−149.9 (3)	O4—C20—O3—Cd1	165.0 (3)
O3—Cd1—N1—C3	37.0 (3)	C19—C20—O3—Cd1	−13.5 (5)
N2—Cd1—N1—C3	108.2 (3)	O5—Cd1—O3—C20	−61.3 (3)
O5—Cd1—N1—C1	34.7 (5)	O6—Cd1—O3—C20	−153.7 (3)
O6—Cd1—N1—C1	177.6 (2)	O1—Cd1—O3—C20	74.7 (5)
O1—Cd1—N1—C1	87.4 (2)	N2—Cd1—O3—C20	26.7 (3)
O3—Cd1—N1—C1	−85.7 (2)	N1—Cd1—O3—C20	103.1 (3)
N2—Cd1—N1—C1	−14.5 (2)	O8—C31—O7—Cd2	166.0 (3)
C20—C19—N2—C2	−72.4 (5)	C30—C31—O7—Cd2	−11.8 (5)
C20—C19—N2—C12	160.1 (4)	O11—Cd2—O7—C31	−62.8 (3)
C20—C19—N2—Cd1	38.7 (4)	O12—Cd2—O7—C31	−159.3 (3)
C1—C2—N2—C19	154.9 (4)	O9—Cd2—O7—C31	73.6 (5)
C1—C2—N2—C12	−78.3 (5)	N4—Cd2—O7—C31	101.2 (3)
C1—C2—N2—Cd1	44.3 (4)	N3—Cd2—O7—C31	24.6 (3)
C13—C12—N2—C19	41.0 (5)	O10—C40—O9—Cd2	169.7 (3)
C13—C12—N2—C2	−85.7 (5)	C39—C40—O9—Cd2	−8.1 (5)
C13—C12—N2—Cd1	156.7 (3)	O11—Cd2—O9—C40	−170.6 (3)
O5—Cd1—N2—C19	62.0 (3)	O12—Cd2—O9—C40	−74.4 (3)
O6—Cd1—N2—C19	−34.7 (7)	O7—Cd2—O9—C40	53.1 (5)
O1—Cd1—N2—C19	157.6 (2)	N4—Cd2—O9—C40	24.0 (3)
O3—Cd1—N2—C19	−32.8 (2)	N3—Cd2—O9—C40	99.6 (3)

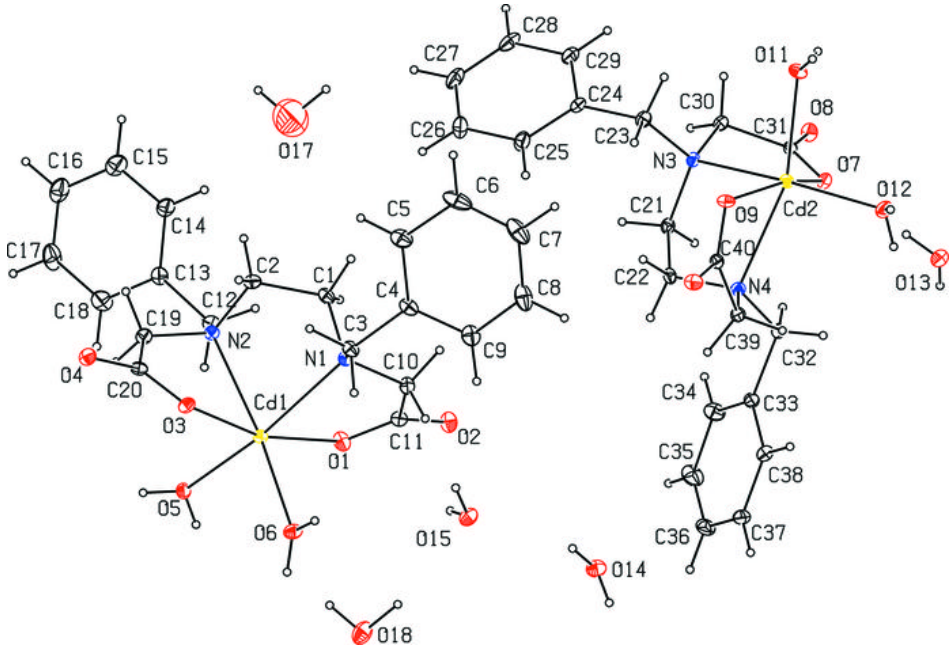
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5A···O9^{i}	0.82	1.90	2.717 (4)	173
O5—H5B···O8^{ii}	0.82	1.86	2.670 (4)	167
O6—H6A···O14^{iii}	0.82	1.87	2.668 (4)	162
O6—H6B···O13^{ii}	0.82	2.19	2.680 (4)	119
O6—H6B···O18	0.82	2.51	2.938 (5)	114
O11—H11A···O1^{iv}	0.83	1.83	2.654 (4)	178

O11—H11B···O4^{v}	0.82	1.84	2.651 (4)	165
O12—H12C···O18^{vi}	0.82	2.31	3.117 (5)	168
O12—H12D···O18^{iv}	0.82	2.00	2.769 (5)	155
O13—H13A···O10^{vii}	0.82	1.99	2.799 (4)	169
O13—H13B···O7	0.82	1.97	2.784 (4)	169
O14—H14A···O15	0.82	2.18	2.829 (5)	136
O14—H14B···O10^{vi}	0.82	2.01	2.774 (5)	155
O15—H15A···O2	0.82	1.90	2.704 (4)	165
O15—H15B···O3^{vii}	0.82	2.03	2.786 (4)	153
O17—H17B···O4^{viii}	0.98	2.00	2.778 (12)	134
O18—H18B···O9^{i}	0.98	2.48	3.323 (5)	144
C32—H32A···O18^{vi}	0.97	2.51	3.477 (6)	178

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

Fig. 1


C28
C27
C29
O11
C24
C30
O8
C26
C25
C23
C31
N3
O7
O17
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C16
C15
C5
C21
O9
Cd2
O12
C14
C7
C17
C2
C1
C40
C22
N4
O13
C13
C4
C8
C18
C12
C3
C19
N2
C39
C32
O4
N1
C10
C9
C20
Cd1
C34
C33
O3
C11
O2
C35
O1
C38
O5
O15
C36
C37
O6
O14
O18

Fig. 2