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Poly[diaqua[μ_4-2-(carboxylatomethoxy)benzoato]-[μ_2-2-(carboxylatomethoxy)benzoato]dicadmium(II)]

Gabrielle J. Gaskin and Robert L. LaDuca*

E-35 Holmes Hall, Michigan State University, Lyman Briggs College, 919 E. Shaw Lane, East Lansing, MI 48825. *Correspondence e-mail: laduca@msu.edu

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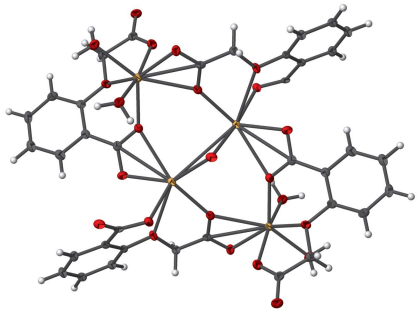
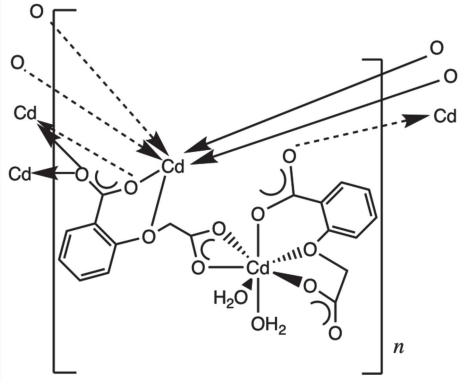
In the title compound, $[Cd_2(C_9H_6O_5)_2(H_2O)_2]_n$, the crystallographically distinct Cd^{II} cations are coordinated in pentagonal–bipyramidal and octahedral fashions. The 2-(carboxymethoxy)benzoate (cmb) ligands connect the Cd atoms into $[Cd_2(cmb)_2(H_2O)_2)]_n$ coordination polymer ribbons that are oriented along the *a*-axis direction. Supramolecular layers are formed parallel to $(01\bar{1})$ by O—H···O hydrogen bonding between the ribbons. The supramolecular three-dimensional crystal structure of the title compound is then constructed by π–π stacking interactions with a centroid–centroid distance of 3.622 (2) Å between cmb ligands in adjacent layer motifs.

3D view



Chemical scheme



Structure description

The title compound was isolated during an exploratory synthetic effort aiming to produce a cadmium coordination polymer containing both 2-(carboxymethoxy)benzoate (cmb) and 4-pyridylisonicotinamide (4-pina) ligands. Cadmium succinate coordination polymers containing the 4-pina ligands and their geometric isomers have shown intriguing self-penetrated or interpenetrated topologies (Uebler *et al.*, 2013).

The asymmetric unit of the title compound contains two crystallographically distinct Cd atoms (Cd1, Cd2), two crystallographically distinct cmb ligands (cmb-A, cmb-B) and two bound water molecules. There are no co-crystallized species in the title compound. The Cd1 atoms display a $\{CdO_7\}$ distorted pentagonal–bipyramidal geometry with one bound water molecule in an axial position and another bound water molecule in the equatorial plane. A cmb-A ligand provides three O atom donors, two in equatorial positions and one in the other axial position. A chelating carboxylate group from a cmb-B ligand occupies the final two coordination positions at Cd1. The Cd2 atoms display a

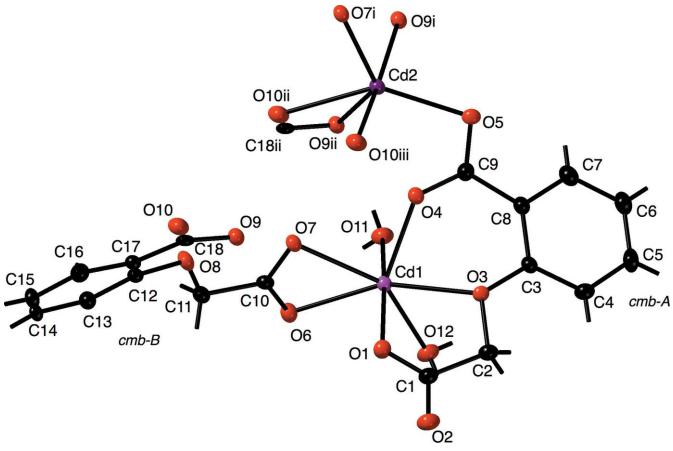


Figure 1
The coordination environments of the title compound, showing the pentagonal bipyramidal coordination at the Cd1 atom and the octahedral coordination at the Cd2 atom. Complete cmb-A and cmb-B ligands are shown. Displacement ellipsoids are drawn at the 50% probability level. Most H atoms have been omitted for clarity. Color code: Cd1, light violet; Cd2, deep purple, N, blue; O, red; C, black. H-atom positions are shown as sticks.

{CdO_6} distorted coordination octahedron. The nominal axial positions are taken up by single carboxylate O atom donors from two different cmb-B ligands. The nominal equatorial plane at Cd2 contains a chelating carboxylate group from a third cmb-B ligand, a single carboxylate O atom donor from a fourth cmb-B ligand, and a single carboxylate O atom donor from a cmb-A ligand. A displacement ellipsoid plot of the ligand set and coordination environments is shown in Fig. 1.

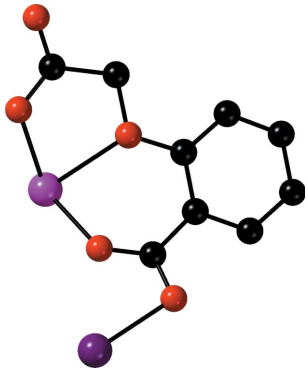


Figure 2
Exobidentate bridging mode of the cmb-A ligand.

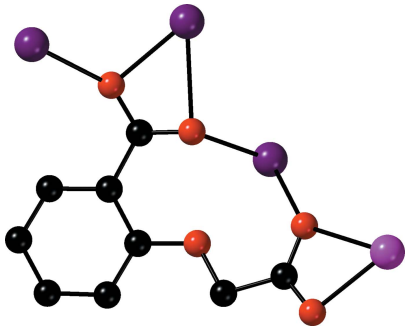


Figure 3
Exobidentate bridging mode of the cmb-B ligand.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O11—H11A···O9^{i}	0.88	2.03	2.873 (3)	162
O11—H11B···O1^{i}	0.88	1.91	2.782 (3)	178
O12—H12A···O2^{ii}	0.90	1.94	2.788 (3)	158
O12—H12B···O2^{i}	0.90	1.86	2.756 (3)	174

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

The cmb-A ligands have an exobidentate μ_2-κ^4-O:O',O'',O''' bridging mode, binding to one Cd1 atom with three donor O atoms, and binding to one Cd2 atom with only one O donor atom (Fig. 2). The cmb-A ether O atoms bind to Cd1. The cmb-B ligands have an exotetradentate μ_4-κ^5-O,O':O':O'',O''':O''' bringing mode, binding to one Cd1 atom with a chelating carboxylate group, binding to two Cd2 atoms with single carboxylate O atom donors, and binding to a third Cd2 through a chelating carboxylate group (Fig. 3). The ether O atoms of the cmb-B ligands do **not** bind to either Cd1 or Cd2.

The Cd2 atoms and cmb-B ligands form a [Cd(cmb-B)]$_n$ coordination polymer chain motif, in which *spiro*-fused {Cd_2O_2} rhomboid units construct the center of the chain (Fig. 4). The through-space Cd···Cd distance across the rhomboid units measures 3.632 (2) Å. The chain submotifs are oriented parallel to the *a* axis. These are decorated on their periphery by [Cd(cmb-A)(H_2O)$_2$] coordination fragments, resulting in one-dimensional [Cd_2(cmb)$_2$(H_2O)$_2$)]$_n$ coordination polymer ribbons (Fig. 5).

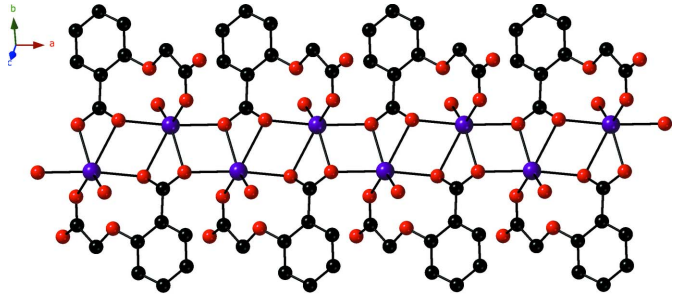


Figure 4
Inner [Cd(cmb)]$_n$ coordination polymer chain in the title compound, oriented parallel to the *a* axis. *Spiro*-fused {Cd_2O_2} rhomboid units make up the center of the chain, bracketed by cmb-B ligands

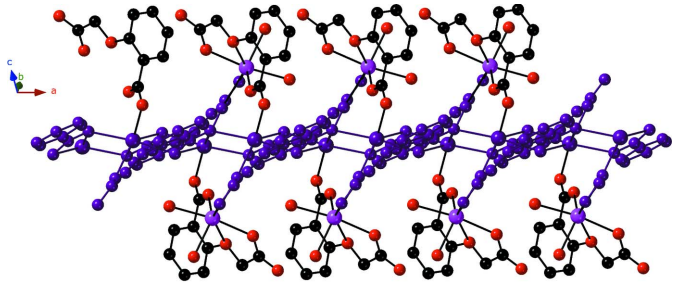


Figure 5
[Cd_2(cmb)$_2$(H_2O)$_2$)]$_n$ coordination polymer ribbon in the title compound, oriented parallel to the *a* axis. The inner chain sub-motif is shown in purple.

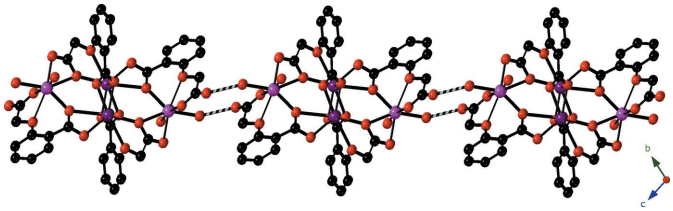


Figure 6
Supramolecular layer in the title compound, oriented parallel to $(01\bar{1})$. O—H···O hydrogen-bonding interactions (Table 1) between neighboring ribbons are shown as dashed lines.

Supramolecular interactions

Adjacent $[Cd_2(cmb)_2(H_2O)_2)]_n$ coordination polymer ribbons interact by means of O–H···O hydrogen-bonding interactions (Table 1) between the bound water molecules and unligated cmb-A carboxylate O atoms, thereby constructing supramolecular layer motifs coincident with $(01\bar{1})$ (Fig. 6). The O···O distance measures 2.788 (1) Å. In turn, the two-dimensional supramolecular layer motifs form the three-dimensional crystal structure of the title compound (Fig. 7) by means of π–π stacking mechanisms involving the aromatic rings of the cmb-A ligands on the ribbon periphery [centroid–centroid distance = 3.622 (2) Å]. The stacking occurs along the *c*-axis direction, in an *AAA* pattern.

Synthesis and crystallization

$Cd(NO_3)_2{\cdot}4H_2O$ (115 mg, 0.37 mmol), 2-(carboxymethoxy)benzoic acid (73 mg, 0.37 mmol), 4-pyridylisonicotinamide (79 mg, 0.37 mmol) and 0.75 ml of a 1.0 *M* NaOH solution were placed into 10 ml distilled H_2O in a Teflon-lined acid digestion bomb. The bomb was sealed and heated in an oven at 393 K for 2 d, and then cooled slowly to 273 K. Colorless crystals of the title complex (75 mg, 62% yield based on Cd) were isolated after washing with distilled water and acetone, and drying in air.

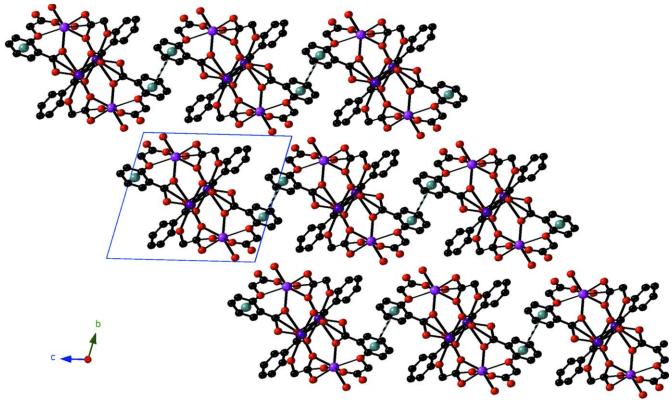


Figure 7
AAA pattern stacking of supramolecular layer motifs along the *c*-axis direction in the title compound, mediated by interlayer π–π stacking interactions, which are shown as dashed lines. Ring centroids of the cmb ligands are shown as teal spheres.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd_2(C_9H_6O_5)_2(H_2O)_2]$
M_r	649.11
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	173
a, *b*, *c* (Å)	6.3966 (9), 11.7504 (16), 13.3579 (19)
α, β, γ (°)	104.407 (1), 96.978 (1), 93.267 (1)
V (Å^3)	961.3 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.28
Crystal size (mm)	0.19 × 0.18 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014/5)
T_{min}, T_{max}	0.663, 0.745
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	10335, 3536, 3172
R_{int}	0.028
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.604
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.057, 1.06
No. of reflections	3536
No. of parameters	291
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.96, −0.46

Computer programs: *COSMO* (Bruker, 2009), *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

GJG thanks her mother for serving as a constant, unconditional positive influence in her life.

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full crystallographic data

IUCrData (2019). **4**, x190953 [https://doi.org/10.1107/S2414314619009532]

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Poly[diaqua[μ_4-2-(carboxylatomethoxy)benzoato][μ_2-2-(carboxylatomethoxy)benzoato]dicadmium(II)]

Crystal data

$[Cd_2(C_9H_6O_5)_2(H_2O)_2]$
M_r = 649.11
Triclinic, $P\overline{1}$
a = 6.3966 (9) Å
b = 11.7504 (16) Å
c = 13.3579 (19) Å
α = 104.407 (1)°
β = 96.978 (1)°
γ = 93.267 (1)°
V = 961.3 (2) Å^3
Z = 2
$F(000)$ = 632
D_x = 2.243 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7284 reflections
θ = 3.2–25.4°
μ = 2.28 mm^{-1}
T = 173 K
Block, colourless
0.19 × 0.18 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8.36 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014/5)
T_{min} = 0.663, T_{max} = 0.745
10335 measured reflections
3536 independent reflections
3172 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.4°, θ_{min} = 1.6°
h = −7→7
k = −14→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.057
S = 1.06
3536 reflections
291 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0194P)^2 + 1.6836P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

Experimental. Data was collected using a BRUKER CCD (charge coupled device) based diffractometer equipped with an Oxford low-temperature apparatus operating at 173 K. A suitable crystal was chosen and mounted on a nylon loop using Paratone oil. Data were measured using omega scans of 0.5° per frame for 30 s. The total number of images were based on results from the program COSMO where redundancy was expected to be 4 and completeness to 0.83Å to 100%. Cell parameters were retrieved using APEX II software and refined using SAINT on all observed reflections.Data reduction was performed using the SAINT software which corrects for Lp. Scaling and absorption corrections were applied using SADABS6 multi-scan technique, supplied by George Sheldrick. The structure was solved by the direct method using the SHELXT program and refined by least squares method on F2, SHELXL, incorporated in OLEX2.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The structure was refined by Least Squares using version 2018/3 of XL (Sheldrick, 2015) incorporated in Olex2 (Dolomanov *et al.*, 2009). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model, except for the Hydrogen atom on the nitrogen atom which was found by difference Fourier methods and refined isotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.30111 (3)	0.18731 (2)	0.26320 (2)	0.01372 (8)
Cd2	0.26261 (3)	0.56335 (2)	0.45843 (2)	0.01311 (7)
O1	0.6054 (4)	0.1503 (2)	0.19000 (17)	0.0199 (5)
O2	0.7503 (4)	0.0924 (2)	0.04417 (18)	0.0223 (5)
O3	0.3239 (4)	0.2625 (2)	0.10350 (17)	0.0192 (5)
O4	0.2524 (3)	0.37691 (19)	0.29797 (17)	0.0174 (5)
O5	0.1116 (4)	0.54112 (19)	0.29333 (17)	0.0206 (5)
O6	0.4298 (3)	0.08315 (19)	0.37674 (17)	0.0178 (5)
O7	0.5650 (3)	0.26916 (19)	0.42704 (17)	0.0165 (5)
O8	0.8603 (3)	0.22913 (18)	0.56197 (17)	0.0171 (5)
O9	1.0690 (3)	0.38854 (19)	0.49607 (16)	0.0154 (5)
O10	1.3856 (3)	0.45670 (19)	0.57865 (17)	0.0171 (5)
O11	−0.0206 (4)	0.1786 (2)	0.32737 (18)	0.0202 (5)
H11A	−0.0207	0.2381	0.3820	0.030*
H11B	−0.1387	0.1714	0.2845	0.030*
O12	0.1160 (4)	0.0302 (2)	0.14044 (17)	0.0215 (5)
H12A	0.1920	0.0021	0.0887	0.032*
H12B	0.0020	0.0533	0.1071	0.032*
C1	0.6117 (5)	0.1404 (3)	0.0939 (2)	0.0169 (7)
C2	0.4371 (5)	0.1873 (3)	0.0318 (2)	0.0173 (7)
H2A	0.4989	0.2321	−0.0129	0.021*
H2B	0.3400	0.1209	−0.0137	0.021*
C3	0.1492 (5)	0.3093 (3)	0.0643 (2)	0.0146 (7)
C4	0.0711 (5)	0.2810 (3)	−0.0415 (3)	0.0197 (7)
H4	0.1405	0.2289	−0.0905	0.024*
C5	−0.1080 (5)	0.3293 (3)	−0.0751 (3)	0.0223 (8)
H5	−0.1606	0.3105	−0.1475	0.027*
C6	−0.2112 (6)	0.4042 (3)	−0.0051 (3)	0.0224 (8)

H6	−0.3374	0.4343	−0.0286	0.027*
C7	−0.1298 (5)	0.4356 (3)	0.1002 (3)	0.0210 (7)
H7	−0.1995	0.4886	0.1483	0.025*
C8	0.0528 (5)	0.3903 (3)	0.1362 (2)	0.0149 (7)
C9	0.1449 (5)	0.4362 (3)	0.2489 (2)	0.0152 (7)
C10	0.5591 (5)	0.1631 (3)	0.4348 (2)	0.0140 (7)
C11	0.7138 (5)	0.1291 (3)	0.5142 (2)	0.0153 (7)
H11C	0.6386	0.1052	0.5673	0.018*
H11D	0.7889	0.0619	0.4798	0.018*
C12	1.0460 (5)	0.2124 (3)	0.6169 (2)	0.0130 (6)
C13	1.0573 (5)	0.1223 (3)	0.6671 (2)	0.0154 (7)
H13	0.9365	0.0691	0.6617	0.018*
C14	1.2463 (5)	0.1105 (3)	0.7252 (2)	0.0172 (7)
H14	1.2563	0.0473	0.7577	0.021*
C15	1.4200 (5)	0.1906 (3)	0.7360 (3)	0.0189 (7)
H15	1.5481	0.1835	0.7772	0.023*
C16	1.4071 (5)	0.2806 (3)	0.6867 (2)	0.0172 (7)
H16	1.5262	0.3362	0.6960	0.021*
C17	1.2230 (5)	0.2919 (3)	0.6235 (2)	0.0140 (7)
C18	1.2237 (5)	0.3837 (3)	0.5635 (2)	0.0132 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01275 (13)	0.01489 (13)	0.01405 (12)	0.00280 (9)	0.00192 (9)	0.00434 (9)
Cd2	0.01108 (13)	0.01325 (12)	0.01568 (12)	0.00162 (9)	0.00207 (9)	0.00483 (9)
O1	0.0175 (12)	0.0270 (13)	0.0167 (12)	0.0076 (10)	0.0049 (9)	0.0059 (10)
O2	0.0186 (12)	0.0241 (13)	0.0225 (12)	0.0048 (10)	0.0077 (10)	−0.0004 (10)
O3	0.0222 (13)	0.0228 (12)	0.0136 (11)	0.0109 (10)	0.0050 (9)	0.0036 (9)
O4	0.0178 (12)	0.0172 (11)	0.0167 (11)	0.0041 (9)	−0.0005 (9)	0.0041 (9)
O5	0.0260 (13)	0.0169 (12)	0.0182 (12)	0.0067 (10)	0.0034 (10)	0.0018 (9)
O6	0.0166 (12)	0.0152 (11)	0.0203 (12)	−0.0024 (9)	−0.0036 (9)	0.0058 (9)
O7	0.0176 (12)	0.0155 (11)	0.0172 (11)	0.0037 (9)	0.0002 (9)	0.0060 (9)
O8	0.0125 (11)	0.0141 (11)	0.0242 (12)	−0.0011 (9)	−0.0044 (9)	0.0079 (9)
O9	0.0139 (11)	0.0163 (11)	0.0170 (11)	0.0024 (9)	0.0021 (9)	0.0061 (9)
O10	0.0150 (12)	0.0136 (11)	0.0242 (12)	0.0002 (9)	0.0069 (9)	0.0059 (9)
O11	0.0151 (12)	0.0232 (12)	0.0201 (12)	0.0011 (10)	0.0050 (9)	0.0002 (10)
O12	0.0172 (12)	0.0246 (13)	0.0185 (12)	0.0015 (10)	0.0036 (10)	−0.0025 (10)
C1	0.0169 (17)	0.0137 (15)	0.0183 (16)	−0.0014 (13)	0.0027 (13)	0.0016 (12)
C2	0.0165 (17)	0.0186 (16)	0.0176 (16)	0.0035 (13)	0.0076 (13)	0.0030 (13)
C3	0.0171 (17)	0.0115 (15)	0.0170 (16)	0.0006 (12)	0.0034 (13)	0.0069 (12)
C4	0.0237 (19)	0.0148 (16)	0.0192 (17)	0.0005 (14)	0.0040 (14)	0.0019 (13)
C5	0.0231 (19)	0.0214 (18)	0.0213 (17)	−0.0045 (14)	−0.0070 (14)	0.0098 (14)
C6	0.0183 (18)	0.0228 (18)	0.0267 (18)	0.0002 (14)	−0.0034 (14)	0.0110 (15)
C7	0.0176 (18)	0.0199 (17)	0.0273 (18)	0.0023 (14)	0.0026 (14)	0.0098 (14)
C8	0.0143 (16)	0.0128 (15)	0.0184 (16)	−0.0013 (12)	0.0015 (13)	0.0068 (12)
C9	0.0123 (16)	0.0181 (16)	0.0158 (15)	−0.0009 (13)	0.0031 (13)	0.0057 (13)
C10	0.0142 (16)	0.0139 (16)	0.0157 (15)	0.0036 (13)	0.0076 (13)	0.0039 (12)

C11	0.0136 (16)	0.0125 (15)	0.0193 (16)	−0.0012 (13)	0.0001 (13)	0.0049 (12)
C12	0.0102 (15)	0.0135 (15)	0.0143 (15)	0.0024 (12)	0.0010 (12)	0.0018 (12)
C13	0.0136 (16)	0.0155 (16)	0.0175 (16)	−0.0006 (13)	0.0019 (13)	0.0055 (12)
C14	0.0255 (18)	0.0144 (16)	0.0142 (15)	0.0062 (13)	0.0022 (13)	0.0078 (12)
C15	0.0172 (17)	0.0220 (17)	0.0189 (16)	0.0046 (14)	−0.0019 (13)	0.0090 (13)
C16	0.0115 (16)	0.0203 (17)	0.0185 (16)	−0.0013 (13)	0.0012 (13)	0.0036 (13)
C17	0.0164 (17)	0.0118 (15)	0.0143 (15)	0.0025 (12)	0.0022 (13)	0.0037 (12)
C18	0.0134 (16)	0.0113 (15)	0.0147 (15)	0.0041 (12)	0.0065 (13)	0.0001 (12)

Geometric parameters (Å, º)

Cd1—O1	2.298 (2)	O11—H11A	0.8766
Cd1—O3	2.520 (2)	O11—H11B	0.8772
Cd1—O4	2.208 (2)	O12—H12A	0.8993
Cd1—O6	2.283 (2)	O12—H12B	0.8991
Cd1—O7	2.537 (2)	C1—C2	1.520 (5)
Cd1—O11	2.330 (2)	C2—H2A	0.9900
Cd1—O12	2.296 (2)	C2—H2B	0.9900
Cd1—C10	2.742 (3)	C3—C4	1.391 (4)
Cd2—O4	2.648 (2)	C3—C8	1.401 (4)
Cd2—O5	2.243 (2)	C4—H4	0.9500
Cd2—O7^{i}	2.297 (2)	C4—C5	1.383 (5)
Cd2—O9^{ii}	2.526 (2)	C5—H5	0.9500
Cd2—O9^{i}	2.338 (2)	C5—C6	1.375 (5)
Cd2—O10^{ii}	2.361 (2)	C6—H6	0.9500
Cd2—O10^{iii}	2.374 (2)	C6—C7	1.388 (5)
O1—C1	1.266 (4)	C7—H7	0.9500
O2—C1	1.248 (4)	C7—C8	1.393 (5)
O3—C2	1.429 (4)	C8—C9	1.500 (4)
O3—C3	1.377 (4)	C10—C11	1.505 (4)
O4—C9	1.249 (4)	C11—H11C	0.9900
O5—C9	1.270 (4)	C11—H11D	0.9900
O6—C10	1.249 (4)	C12—C13	1.387 (4)
O7—Cd2^{i}	2.297 (2)	C12—C17	1.405 (4)
O7—C10	1.275 (4)	C13—H13	0.9500
O8—C11	1.422 (3)	C13—C14	1.388 (5)
O8—C12	1.370 (4)	C14—H14	0.9500
O9—Cd2^{iv}	2.526 (2)	C14—C15	1.385 (5)
O9—Cd2^{i}	2.338 (2)	C15—H15	0.9500
O9—C18	1.268 (4)	C15—C16	1.378 (5)
O10—Cd2^{iii}	2.374 (2)	C16—H16	0.9500
O10—Cd2^{iv}	2.361 (2)	C16—C17	1.397 (4)
O10—C18	1.269 (4)	C17—C18	1.496 (4)
O1—Cd1—O3	65.56 (8)	Cd1—O11—H11B	119.2
O1—Cd1—O7	81.95 (8)	H11A—O11—H11B	110.1
O1—Cd1—O11	167.04 (8)	Cd1—O12—H12A	111.1
O1—Cd1—C10	80.86 (8)	Cd1—O12—H12B	110.7

O3—Cd1—O7	120.43 (7)	H12A—O12—H12B	103.0
O3—Cd1—C10	139.43 (9)	O1—C1—C2	118.9 (3)
O4—Cd1—O1	111.25 (8)	O2—C1—O1	124.9 (3)
O4—Cd1—O3	69.81 (8)	O2—C1—C2	116.3 (3)
O4—Cd1—O6	127.85 (8)	O3—C2—C1	108.5 (3)
O4—Cd1—O7	78.68 (7)	O3—C2—H2A	110.0
O4—Cd1—O11	81.56 (8)	O3—C2—H2B	110.0
O4—Cd1—O12	130.05 (8)	C1—C2—H2A	110.0
O4—Cd1—C10	104.76 (8)	C1—C2—H2B	110.0
O6—Cd1—O1	85.47 (8)	H2A—C2—H2B	108.4
O6—Cd1—O3	150.85 (8)	O3—C3—C4	122.7 (3)
O6—Cd1—O7	54.31 (7)	O3—C3—C8	117.0 (3)
O6—Cd1—O11	88.00 (8)	C4—C3—C8	120.3 (3)
O6—Cd1—O12	96.77 (8)	C3—C4—H4	120.2
O6—Cd1—C10	26.85 (8)	C5—C4—C3	119.6 (3)
O7—Cd1—C10	27.60 (8)	C5—C4—H4	120.2
O11—Cd1—O3	119.67 (8)	C4—C5—H5	119.6
O11—Cd1—O7	103.23 (8)	C6—C5—C4	120.8 (3)
O11—Cd1—C10	98.15 (9)	C6—C5—H5	119.6
O12—Cd1—O1	91.10 (8)	C5—C6—H6	120.2
O12—Cd1—O3	81.33 (8)	C5—C6—C7	119.6 (3)
O12—Cd1—O7	150.54 (8)	C7—C6—H6	120.2
O12—Cd1—O11	78.55 (8)	C6—C7—H7	119.6
O12—Cd1—C10	123.09 (9)	C6—C7—C8	120.8 (3)
O5—Cd2—O4	52.32 (7)	C8—C7—H7	119.6
O5—Cd2—O7^{i}	128.03 (8)	C3—C8—C9	122.9 (3)
O5—Cd2—O9^{i}	85.48 (8)	C7—C8—C3	118.6 (3)
O5—Cd2—O9^{ii}	98.88 (8)	C7—C8—C9	118.4 (3)
O5—Cd2—O10^{iii}	96.64 (8)	O4—C9—O5	120.5 (3)
O5—Cd2—O10^{ii}	142.74 (8)	O4—C9—C8	122.9 (3)
O7^{i}—Cd2—O4	151.33 (8)	O5—C9—C8	116.6 (3)
O7^{i}—Cd2—O9^{i}	93.14 (8)	O6—C10—Cd1	55.65 (16)
O7^{i}—Cd2—O9^{ii}	129.27 (7)	O6—C10—O7	122.3 (3)
O7^{i}—Cd2—O10^{ii}	88.12 (8)	O6—C10—C11	117.2 (3)
O7^{i}—Cd2—O10^{iii}	79.41 (8)	O7—C10—Cd1	67.22 (17)
O9^{ii}—Cd2—O4	70.79 (7)	O7—C10—C11	120.4 (3)
O9^{i}—Cd2—O4	114.63 (7)	C11—C10—Cd1	168.7 (2)
O9^{i}—Cd2—O9^{ii}	69.96 (8)	O8—C11—C10	107.5 (2)
O9^{i}—Cd2—O10^{iii}	171.93 (7)	O8—C11—H11C	110.2
O9^{i}—Cd2—O10^{ii}	103.18 (8)	O8—C11—H11D	110.2
O10^{ii}—Cd2—O4	92.11 (7)	C10—C11—H11C	110.2
O10^{iii}—Cd2—O4	72.43 (7)	C10—C11—H11D	110.2
O10^{ii}—Cd2—O9^{ii}	53.09 (7)	H11C—C11—H11D	108.5
O10^{iii}—Cd2—O9^{ii}	117.19 (7)	O8—C12—C13	121.1 (3)
O10^{ii}—Cd2—O10^{iii}	79.83 (8)	O8—C12—C17	117.7 (3)
C1—O1—Cd1	121.9 (2)	C13—C12—C17	121.2 (3)
C2—O3—Cd1	110.90 (18)	C12—C13—H13	120.2
C3—O3—Cd1	117.78 (18)	C12—C13—C14	119.6 (3)

C3—O3—C2	118.6 (2)	C14—C13—H13	120.2
Cd1—O4—Cd2	140.68 (10)	C13—C14—H14	119.9
C9—O4—Cd1	132.37 (19)	C15—C14—C13	120.1 (3)
C9—O4—Cd2	84.27 (17)	C15—C14—H14	119.9
C9—O5—Cd2	102.8 (2)	C14—C15—H15	120.0
C10—O6—Cd1	97.50 (19)	C16—C15—C14	120.0 (3)
Cd2^{i}—O7—Cd1	145.62 (10)	C16—C15—H15	120.0
C10—O7—Cd1	85.18 (17)	C15—C16—H16	119.2
C10—O7—Cd2^{i}	128.9 (2)	C15—C16—C17	121.5 (3)
C12—O8—C11	118.3 (2)	C17—C16—H16	119.2
Cd2^{i}—O9—Cd2^{iv}	110.04 (8)	C12—C17—C18	123.0 (3)
C18—O9—Cd2^{iv}	89.97 (18)	C16—C17—C12	117.5 (3)
C18—O9—Cd2^{i}	122.20 (19)	C16—C17—C18	119.4 (3)
Cd2^{iv}—O10—Cd2^{iii}	100.17 (8)	O9—C18—O10	119.3 (3)
C18—O10—Cd2^{iii}	133.07 (19)	O9—C18—C17	121.7 (3)
C18—O10—Cd2^{iv}	97.67 (19)	O10—C18—C17	119.0 (3)
Cd1—O11—H11A	109.7		

Cd1—O1—C1—O2	−161.2 (2)	O8—C12—C13—C14	−177.7 (3)
Cd1—O1—C1—C2	17.5 (4)	O8—C12—C17—C16	174.8 (3)
Cd1—O3—C2—C1	−35.1 (3)	O8—C12—C17—C18	−7.4 (4)
Cd1—O3—C3—C4	−134.4 (3)	C2—O3—C3—C4	3.9 (4)
Cd1—O3—C3—C8	47.0 (3)	C2—O3—C3—C8	−174.8 (3)
Cd1—O4—C9—O5	167.2 (2)	C3—O3—C2—C1	−176.0 (3)
Cd1—O4—C9—C8	−14.0 (5)	C3—C4—C5—C6	−0.5 (5)
Cd1—O6—C10—O7	8.9 (3)	C3—C8—C9—O4	−31.0 (5)
Cd1—O6—C10—C11	−169.8 (2)	C3—C8—C9—O5	147.8 (3)
Cd1—O7—C10—O6	−8.0 (3)	C4—C3—C8—C7	4.2 (5)
Cd1—O7—C10—C11	170.7 (3)	C4—C3—C8—C9	−172.0 (3)
Cd1—C10—C11—O8	124.5 (10)	C4—C5—C6—C7	2.6 (5)
Cd2—O4—C9—O5	3.3 (3)	C5—C6—C7—C8	−1.3 (5)
Cd2—O4—C9—C8	−177.9 (3)	C6—C7—C8—C3	−2.1 (5)
Cd2—O5—C9—O4	−4.0 (3)	C6—C7—C8—C9	174.2 (3)
Cd2—O5—C9—C8	177.1 (2)	C7—C8—C9—O4	152.9 (3)
Cd2^{i}—O7—C10—Cd1	174.7 (2)	C7—C8—C9—O5	−28.3 (4)
Cd2^{i}—O7—C10—O6	166.7 (2)	C8—C3—C4—C5	−2.9 (5)
Cd2^{i}—O7—C10—C11	−14.6 (4)	C11—O8—C12—C13	−30.0 (4)
Cd2^{i}—O9—C18—O10	−115.1 (3)	C11—O8—C12—C17	152.0 (3)
Cd2^{iv}—O9—C18—O10	−1.2 (3)	C12—O8—C11—C10	−163.6 (3)
Cd2^{iv}—O9—C18—C17	−179.4 (2)	C12—C13—C14—C15	2.2 (5)
Cd2^{i}—O9—C18—C17	66.8 (3)	C12—C17—C18—O9	−6.1 (5)
Cd2^{iv}—O10—C18—O9	1.3 (3)	C12—C17—C18—O10	175.8 (3)
Cd2^{iii}—O10—C18—O9	−110.4 (3)	C13—C12—C17—C16	−3.2 (4)
Cd2^{iii}—O10—C18—C17	67.8 (4)	C13—C12—C17—C18	174.6 (3)
Cd2^{iv}—O10—C18—C17	179.5 (2)	C13—C14—C15—C16	−1.6 (5)
O1—C1—C2—O3	14.8 (4)	C14—C15—C16—C17	−1.5 (5)
O2—C1—C2—O3	−166.4 (3)	C15—C16—C17—C12	3.9 (5)
O3—C3—C4—C5	178.5 (3)	C15—C16—C17—C18	−174.0 (3)

O3—C3—C8—C7	−177.2 (3)	C16—C17—C18—O9	171.7 (3)
O3—C3—C8—C9	6.7 (4)	C16—C17—C18—O10	−6.4 (4)
O6—C10—C11—O8	173.0 (3)	C17—C12—C13—C14	0.2 (5)
O7—C10—C11—O8	−5.7 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H11*A*···O9^{ii}	0.88	2.03	2.873 (3)	162
O11—H11*B*···O1^{ii}	0.88	1.91	2.782 (3)	178
O12—H12*A*···O2^{v}	0.90	1.94	2.788 (3)	158
O12—H12*B*···O2^{ii}	0.90	1.86	2.756 (3)	174

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