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Poly[di-μ_3-hydroxy[μ_4-5-(4-carboxyphenyl)pyridine-2-carboxylato-$\kappa^5N,O^2:O^{2'}:O^4:O^{4'}$]dicadmium]

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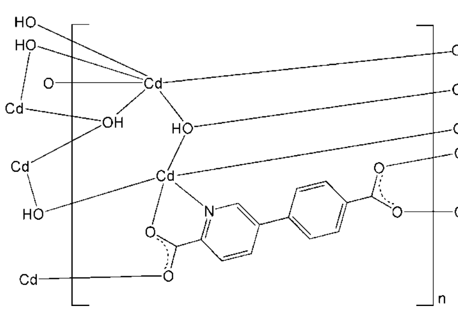
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.037; wR factor = 0.087; data-to-parameter ratio = 11.9.

The asymmetric unit of the title polymeric complex, $[Cd_2(C_{13}H_7NO_4)(OH)_2]_n$, consists of two independent Cd^{II} atoms, one 5-(4-carboxyphenyl)pyridine-2-carboxylate ligand and two hydroxy groups. One Cd^{II} atom is six-coordinated by two O atoms from two ligand molecules and by four μ_3-OH groups in a distorted trigonal–prismatic geometry. The other is five-coordinated by one N and two O atoms from two ligands and by two μ_3-OH groups, forming a distorted square-pyramidal geometry. The two independent Cd^{II} atoms are connected by the ligand molecules and the OH groups into a three-dimensional framework. O—H⋯O hydrogen bonds between the OH groups and the carboxylate O atoms are observed.

Related literature

For related structures and applications of metal complexes with *N*-heterocyclic multicarboxylate ligands, see: Li *et al.* (2008); Mahata & Natarajan (2005); Sun *et al.* (2001); Wang *et al.* (2009). For the synthesis of the ligand, see: Ben & Gordon (1951); Liu *et al.* (2005).



Experimental

Crystal data

$[Cd_2(C_{13}H_7NO_4)(OH)_2]$
M_r = 500.03
Monoclinic, $P2_1/c$
a = 15.4316 (17) Å
b = 3.8261 (4) Å
c = 21.586 (2) Å
β = 102.114 (2)°
V = 1246.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.44 mm^{-1}
T = 293 K
0.27 × 0.21 × 0.14 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.457, T_{max} = 0.644
6277 measured reflections
2448 independent reflections
2109 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.087
S = 1.04
2448 reflections
205 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.82 e Å^{-3}
$\Delta\rho_{min}$ = −1.36 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O5—H5A⋯O1^{i}	0.81 (3)	2.08 (4)	2.818 (6)	150 (6)
O6—H6A⋯O3^{ii}	0.82 (2)	2.39 (4)	2.887 (6)	120 (6)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5190).

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Poly[di-μ_3-hydroxy[μ_4-5-(4-carboxyphenyl)pyridine-2-carboxylato-$\kappa^5N,O^2:O^{2\prime}:O^4:O^{4\prime}$]dicadmium]

Fan-Jin Meng, Heng-Qing Jia, Ning-Hai Hu and Hua Zhou

S1. Comment

The rational design and construction of coordination polymers based on metal ions and N-heterocyclic multicarboxylate ligands have attracted considerable attention for their intriguing structural topologies along with potential applications (Li *et al.*, 2008; Mahata & Natarajan, 2005; Sun *et al.*, 2001; Wang *et al.*, 2009). In this paper, we report a cadmium complex with a three-dimensional framework based on 5-(4-carboxyphenyl)pyridine-2-carboxylic acid (H_2L).

The asymmetric unit of the title compound contains two crystallographically independent Cd^{II} ions with different coordination geometries (Fig. 1). The Cd1 atom is six-coordinated by two O atoms from two *L* ligands and four μ_3-OH groups in a distorted trigonal prismatic geometry. The Cd1—O bond lengths are in a range of 2.176 (4)–2.587 (4) Å. The Cd2 atom is five-coordinated by one N and two O atoms from two *L* ligands and two μ_3-OH groups in a distorted square-pyramidal geometry. The Cd2—N bond length is 2.354 (4) Å and the Cd2—O bond lengths are in a range of 2.196 (4)–2.368 (4) Å. Interestingly, the carboxylate groups and hydroxy groups connect the Cd^{II} ions into a layer parallel to (011) and adjacent layers are further linked by the *L* ligands as pillars along the *a*-axis, generating a three-dimensional framework (Fig. 2). O—H···O hydrogen bonds between the hydroxy groups and carboxylate O atoms stabilize the structure (Table 1).

S2. Experimental

The H_2L ligand was prepared by a similar method described by Ben & Gordon (1951) and Liu *et al.* (2005). A precursor ligand, 2-methyl-5-p-tolylpyridine, was prepared through the Suzuki reaction between 4-methylphenylboronic acid (2.039 g, 15 mmol) and 5-bromo-2-methylpyridine (1.730 g, 10 mmol). The H_2L ligand was obtained by the oxidation of potassium permanganate. The title compound was synthesized under hydrothermal conditions. A mixture of $Cd(CH_3CO_2)_2.2H_2O$ (0.053 g, 0.2mmol) and H_2L (0.024 g, 0.1 mmol) in methanol (2 ml) and distilled water (5 ml) was stirred for 20 min in air, and the pH value was adjusted to about 8.5 with 0.1M CH_3COOH and 0.1M NaOH solutions. Then the mixture was sealed in a 23 ml Teflon-lined stainless steel autoclave, which was heated to 433 K for 72 h. After cooling to room temperature, colorless block crystals of the title compound suitable for X-ray diffraction were obtained.

S3. Refinement

C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C). H atoms of hydroxy groups were located in a difference Fourier map and their positions were refined with bond-length restraints of 0.82 (1) Å, and with U_{iso}(H) = 1.5U_{eq}(O). The highest residual electron density was found at 0.96 Å from Cd1 atom and the deepest hole at 0.70 Å from Cd1 atom.

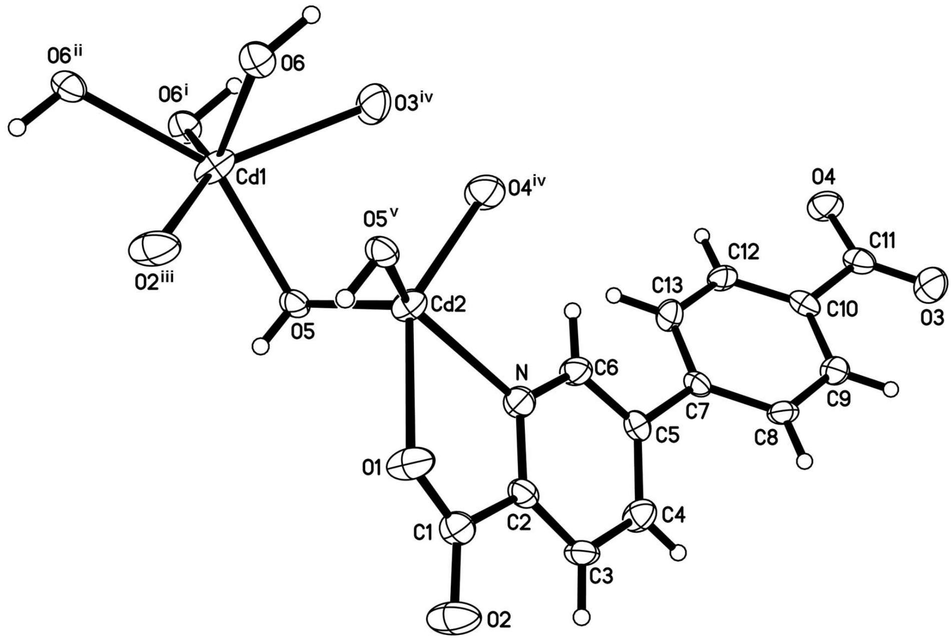

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) x, -1+y, z; (ii) 1-x, -1/2+y, 1/2-z; (iii) 1-x, 2-y, 1-z; (iv) 2-x, 1-y, 1-z; (v) x, 1+y, z.]

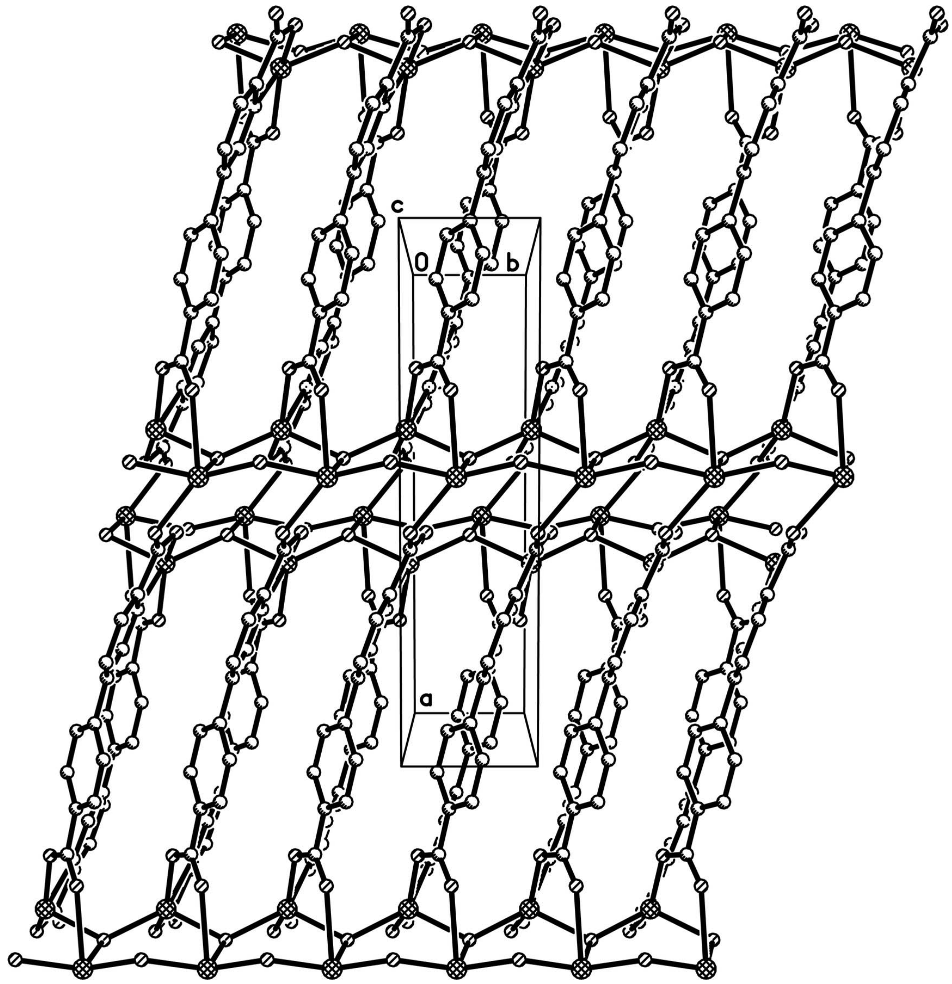

Figure 2

The packing diagram of the title compound, showing the three-dimensional framework.

Poly[di-μ_3-hydroxy[μ_4-5-(4-carboxyphenyl)pyridine-2-carboxylato- $\kappa^5N,O^2:O^{2'}:O^4:O^{4'}$]dicadmium]

Crystal data

$[Cd_2(C_{13}H_7NO_4)(OH)_2]$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 15.4316 (17) Å
b = 3.8261 (4) Å
c = 21.586 (2) Å
β = 102.114 (2)°
V = 1246.1 (2) Å^3
Z = 4
F(000) = 952
D_x = 2.665 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2448 reflections
θ = 2.1–26.0°
μ = 3.44 mm^{-1}
T = 293 K
Block, colourless
0.27 × 0.21 × 0.14 mm

Data collection

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.457, T_{max} = 0.644

6277 measured reflections
2448 independent reflections
2109 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.1°$
$h = -19 \rightarrow 14$
$k = -3 \rightarrow 4$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.087$
$S = 1.04$
2448 reflections
205 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 3.8222P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.82$ e Å^{-3}
$\Delta\rho_{min} = -1.36$ e Å^{-3}

Special details

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. 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 > 2sigma(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	0.54015 (3)	0.60259 (12)	0.317372 (18)	0.02773 (14)
Cd2	0.63702 (3)	1.00568 (11)	0.464037 (18)	0.02162 (14)
C1	0.6046 (4)	1.0297 (15)	0.6045 (3)	0.0230 (12)
C2	0.6959 (3)	0.8660 (15)	0.6131 (3)	0.0197 (11)
C3	0.7430 (3)	0.7675 (16)	0.6720 (3)	0.0226 (12)
H3	0.7181	0.7837	0.7075	0.027*
C4	0.8292 (4)	0.6427 (16)	0.6769 (3)	0.0251 (13)
H4	0.8629	0.5804	0.7163	0.030*
C5	0.8646 (3)	0.6115 (14)	0.6239 (3)	0.0185 (11)
C6	0.8105 (3)	0.7034 (16)	0.5659 (3)	0.0231 (12)
H6	0.8327	0.6758	0.5293	0.028*
C7	0.9584 (3)	0.5045 (14)	0.6255 (3)	0.0185 (11)
C8	1.0268 (3)	0.6001 (15)	0.6757 (2)	0.0216 (12)
H8	1.0139	0.7186	0.7103	0.026*
C9	1.1138 (3)	0.5190 (15)	0.6742 (3)	0.0216 (12)
H9	1.1589	0.5883	0.7076	0.026*
C10	1.1350 (3)	0.3358 (15)	0.6238 (3)	0.0216 (12)
C11	1.2310 (4)	0.2519 (16)	0.6218 (3)	0.0241 (12)
C12	1.0658 (3)	0.2371 (15)	0.5748 (2)	0.0224 (12)
H12	1.0782	0.1098	0.5410	0.027*

C13	0.9795 (4)	0.3229 (16)	0.5751 (3)	0.0238 (13)
H13	0.9347	0.2583	0.5412	0.029*
N1	0.7283 (3)	0.8293 (13)	0.5604 (2)	0.0224 (10)
O1	0.5713 (3)	1.1503 (12)	0.55044 (18)	0.0330 (10)
O2	0.5712 (3)	1.0362 (13)	0.6518 (2)	0.0408 (12)
O3	1.2893 (3)	0.3539 (12)	0.66625 (19)	0.0342 (10)
O4	1.2417 (3)	0.0784 (12)	0.57409 (19)	0.0324 (10)
O5	0.5786 (2)	0.5013 (10)	0.42462 (18)	0.0197 (8)
H5A	0.5284 (17)	0.528 (16)	0.430 (3)	0.030*
O6	0.5682 (2)	1.1069 (11)	0.27639 (19)	0.0238 (8)
H6A	0.6206 (13)	1.093 (18)	0.275 (3)	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0398 (3)	0.0251 (3)	0.0162 (2)	0.00757 (19)	0.00127 (18)	−0.00045 (18)
Cd2	0.0247 (2)	0.0217 (2)	0.0182 (2)	0.00551 (16)	0.00379 (16)	−0.00076 (16)
C1	0.020 (3)	0.025 (3)	0.025 (3)	0.006 (2)	0.006 (2)	−0.001 (2)
C2	0.017 (3)	0.021 (3)	0.023 (3)	−0.001 (2)	0.008 (2)	−0.002 (2)
C3	0.021 (3)	0.031 (3)	0.018 (3)	0.003 (2)	0.009 (2)	0.003 (2)
C4	0.025 (3)	0.029 (3)	0.020 (3)	0.005 (2)	0.002 (2)	0.000 (3)
C5	0.016 (3)	0.016 (3)	0.024 (3)	−0.001 (2)	0.005 (2)	0.000 (2)
C6	0.019 (3)	0.033 (3)	0.018 (3)	0.004 (2)	0.005 (2)	0.000 (3)
C7	0.014 (2)	0.022 (3)	0.021 (3)	−0.001 (2)	0.007 (2)	0.000 (2)
C8	0.022 (3)	0.030 (3)	0.015 (2)	0.001 (2)	0.007 (2)	0.000 (2)
C9	0.018 (3)	0.027 (3)	0.019 (3)	0.003 (2)	0.001 (2)	0.004 (2)
C10	0.020 (3)	0.021 (3)	0.026 (3)	0.001 (2)	0.010 (2)	0.007 (2)
C11	0.023 (3)	0.027 (3)	0.024 (3)	0.003 (2)	0.008 (2)	0.008 (3)
C12	0.023 (3)	0.029 (3)	0.018 (3)	0.001 (2)	0.008 (2)	−0.006 (3)
C13	0.020 (3)	0.028 (3)	0.022 (3)	−0.001 (2)	−0.001 (2)	0.001 (2)
N1	0.018 (2)	0.028 (3)	0.022 (2)	0.0040 (19)	0.0048 (19)	−0.002 (2)
O1	0.027 (2)	0.053 (3)	0.020 (2)	0.022 (2)	0.0073 (17)	0.008 (2)
O2	0.035 (2)	0.064 (3)	0.027 (2)	0.025 (2)	0.015 (2)	0.010 (2)
O3	0.022 (2)	0.049 (3)	0.031 (2)	0.006 (2)	0.0018 (18)	−0.003 (2)
O4	0.028 (2)	0.046 (3)	0.026 (2)	0.006 (2)	0.0105 (18)	−0.004 (2)
O5	0.0139 (17)	0.025 (2)	0.0215 (19)	0.0029 (15)	0.0058 (15)	0.0022 (16)
O6	0.0217 (19)	0.023 (2)	0.028 (2)	0.0027 (17)	0.0088 (17)	−0.0046 (18)

Geometric parameters (Å, º)

Cd1—O6^{i}	2.174 (4)	C6—H6	0.9300
Cd1—O6	2.203 (4)	C7—C13	1.384 (8)
Cd1—O5	2.299 (4)	C7—C8	1.393 (7)
Cd1—O6^{ii}	2.339 (4)	C8—C9	1.385 (7)
Cd1—O2^{iii}	2.405 (4)	C8—H8	0.9300
Cd1—O3^{iv}	2.586 (4)	C9—C10	1.391 (8)
Cd2—O5^{v}	2.193 (4)	C9—H9	0.9300
Cd2—O4^{iv}	2.221 (4)	C10—C12	1.388 (7)

Cd2—O5	2.222 (4)	C10—C11	1.525 (7)
Cd2—N1	2.354 (4)	C11—O3	1.233 (7)
Cd2—O1	2.368 (4)	C11—O4	1.264 (7)
C1—O2	1.237 (7)	C12—C13	1.373 (7)
C1—O1	1.261 (7)	C12—H12	0.9300
C1—C2	1.517 (7)	C13—H13	0.9300
C2—N1	1.342 (7)	O2—Cd1^{iii}	2.405 (4)
C2—C3	1.377 (7)	O3—Cd1^{iv}	2.586 (4)
C3—C4	1.396 (7)	O4—Cd2^{iv}	2.221 (4)
C3—H3	0.9300	O5—Cd2^{i}	2.193 (4)
C4—C5	1.372 (8)	O5—H5A	0.814 (10)
C4—H4	0.9300	O6—Cd1^{v}	2.174 (4)
C5—C6	1.396 (7)	O6—Cd1^{vi}	2.339 (4)
C5—C7	1.498 (7)	O6—H6A	0.817 (10)
C6—N1	1.339 (7)		

O6^{i}—Cd1—O6	121.88 (18)	C5—C6—H6	118.4
O6^{i}—Cd1—O5	103.38 (14)	C13—C7—C8	118.5 (5)
O6—Cd1—O5	121.41 (14)	C13—C7—C5	120.3 (5)
O6^{i}—Cd1—O6^{ii}	79.70 (13)	C8—C7—C5	121.1 (5)
O6—Cd1—O6^{ii}	79.12 (13)	C9—C8—C7	120.2 (5)
O5—Cd1—O6^{ii}	149.21 (13)	C9—C8—H8	119.9
O6^{i}—Cd1—O2^{iii}	145.94 (16)	C7—C8—H8	119.9
O6—Cd1—O2^{iii}	79.60 (15)	C8—C9—C10	121.3 (5)
O5—Cd1—O2^{iii}	82.34 (13)	C8—C9—H9	119.4
O6^{ii}—Cd1—O2^{iii}	79.22 (14)	C10—C9—H9	119.4
O6^{i}—Cd1—O3^{iv}	80.11 (14)	C12—C10—C9	117.6 (5)
O6—Cd1—O3^{iv}	73.66 (14)	C12—C10—C11	121.2 (5)
O5—Cd1—O3^{iv}	80.39 (13)	C9—C10—C11	121.2 (5)
O6^{ii}—Cd1—O3^{iv}	129.78 (13)	O3—C11—O4	127.0 (5)
O2^{iii}—Cd1—O3^{iv}	133.69 (16)	O3—C11—C10	117.7 (5)
O5^{v}—Cd2—O4^{iv}	106.95 (15)	O4—C11—C10	115.3 (5)
O5^{v}—Cd2—O5	120.10 (16)	C13—C12—C10	121.5 (5)
O4^{iv}—Cd2—O5	92.19 (15)	C13—C12—H12	119.2
O5^{v}—Cd2—N1	135.39 (16)	C10—C12—H12	119.2
O4^{iv}—Cd2—N1	83.77 (15)	C12—C13—C7	120.8 (5)
O5—Cd2—N1	102.06 (15)	C12—C13—H13	119.6
O5^{v}—Cd2—O1	83.94 (14)	C7—C13—H13	119.6
O4^{iv}—Cd2—O1	149.23 (14)	C6—N1—C2	118.5 (5)
O5—Cd2—O1	107.35 (16)	C6—N1—Cd2	124.1 (4)
N1—Cd2—O1	69.28 (14)	C2—N1—Cd2	117.3 (3)
O2—C1—O1	126.7 (5)	C1—O1—Cd2	119.1 (3)
O2—C1—C2	116.5 (5)	C1—O2—Cd1^{iii}	133.3 (4)
O1—C1—C2	116.8 (5)	C11—O3—Cd1^{iv}	133.0 (4)
N1—C2—C3	122.3 (5)	C11—O4—Cd2^{iv}	129.9 (4)
N1—C2—C1	116.2 (5)	Cd2^{i}—O5—Cd2	120.10 (16)
C3—C2—C1	121.5 (5)	Cd2^{i}—O5—Cd1	122.32 (17)
C2—C3—C4	118.3 (5)	Cd2—O5—Cd1	103.73 (15)

C2—C3—H3	120.9	Cd2^{i}—O5—H5A	112 (5)
C4—C3—H3	120.9	Cd2—O5—H5A	99 (5)
C5—C4—C3	120.4 (5)	Cd1—O5—H5A	94 (4)
C5—C4—H4	119.8	Cd1^{v}—O6—Cd1	121.87 (18)
C3—C4—H4	119.8	Cd1^{v}—O6—Cd1^{vi}	101.02 (15)
C4—C5—C6	117.2 (5)	Cd1—O6—Cd1^{vi}	100.16 (15)
C4—C5—C7	123.8 (5)	Cd1^{v}—O6—H6A	111 (5)
C6—C5—C7	118.8 (5)	Cd1—O6—H6A	104 (5)
N1—C6—C5	123.1 (5)	Cd1^{vi}—O6—H6A	120 (5)
N1—C6—H6	118.4		

O2—C1—C2—N1	173.9 (6)	O1—Cd2—N1—C2	5.9 (4)
O1—C1—C2—N1	−7.3 (8)	O2—C1—O1—Cd2	−168.3 (5)
O2—C1—C2—C3	−7.3 (8)	C2—C1—O1—Cd2	13.0 (7)
O1—C1—C2—C3	171.5 (6)	O5^{v}—Cd2—O1—C1	−154.0 (5)
N1—C2—C3—C4	3.5 (9)	O4^{iv}—Cd2—O1—C1	−40.8 (6)
C1—C2—C3—C4	−175.3 (5)	O5—Cd2—O1—C1	86.3 (5)
C2—C3—C4—C5	−1.7 (9)	N1—Cd2—O1—C1	−10.4 (4)
C3—C4—C5—C6	−1.1 (9)	O1—C1—O2—Cd1^{iii}	−22.3 (10)
C3—C4—C5—C7	175.5 (5)	C2—C1—O2—Cd1^{iii}	156.4 (4)
C4—C5—C6—N1	2.3 (9)	O4—C11—O3—Cd1^{iv}	13.6 (10)
C7—C5—C6—N1	−174.4 (5)	C10—C11—O3—Cd1^{iv}	−167.4 (4)
C4—C5—C7—C13	149.3 (6)	O3—C11—O4—Cd2^{iv}	−17.1 (9)
C6—C5—C7—C13	−34.2 (8)	C10—C11—O4—Cd2^{iv}	163.9 (4)
C4—C5—C7—C8	−34.0 (8)	O5^{v}—Cd2—O5—Cd2^{i}	−179.992 (1)
C6—C5—C7—C8	142.5 (6)	O4^{iv}—Cd2—O5—Cd2^{i}	69.0 (2)
C13—C7—C8—C9	1.1 (8)	N1—Cd2—O5—Cd2^{i}	−15.1 (2)
C5—C7—C8—C9	−175.6 (5)	O1—Cd2—O5—Cd2^{i}	−86.94 (19)
C7—C8—C9—C10	−1.3 (9)	O5^{v}—Cd2—O5—Cd1	39.0 (3)
C8—C9—C10—C12	0.0 (8)	O4^{iv}—Cd2—O5—Cd1	−72.10 (16)
C8—C9—C10—C11	179.0 (5)	N1—Cd2—O5—Cd1	−156.20 (15)
C12—C10—C11—O3	178.5 (6)	O1—Cd2—O5—Cd1	132.00 (14)
C9—C10—C11—O3	−0.4 (8)	O6^{i}—Cd1—O5—Cd2^{i}	3.5 (2)
C12—C10—C11—O4	−2.4 (8)	O6—Cd1—O5—Cd2^{i}	−137.88 (18)
C9—C10—C11—O4	178.7 (5)	O6^{ii}—Cd1—O5—Cd2^{i}	95.8 (3)
C9—C10—C12—C13	1.4 (9)	O2^{iii}—Cd1—O5—Cd2^{i}	149.3 (2)
C11—C10—C12—C13	−177.6 (5)	O3^{iv}—Cd1—O5—Cd2^{i}	−73.8 (2)
C10—C12—C13—C7	−1.6 (9)	O6^{i}—Cd1—O5—Cd2	143.42 (15)
C8—C7—C13—C12	0.3 (9)	O6—Cd1—O5—Cd2	2.1 (2)
C5—C7—C13—C12	177.1 (5)	O6^{ii}—Cd1—O5—Cd2	−124.3 (2)
C5—C6—N1—C2	−0.7 (9)	O2^{iii}—Cd1—O5—Cd2	−70.76 (17)
C5—C6—N1—Cd2	177.7 (4)	O3^{iv}—Cd1—O5—Cd2	66.10 (15)
C3—C2—N1—C6	−2.3 (9)	O6^{i}—Cd1—O6—Cd1^{v}	180.0
C1—C2—N1—C6	176.5 (5)	O5—Cd1—O6—Cd1^{v}	−45.7 (2)
C3—C2—N1—Cd2	179.2 (4)	O6^{ii}—Cd1—O6—Cd1^{v}	109.5 (2)
C1—C2—N1—Cd2	−2.0 (6)	O2^{iii}—Cd1—O6—Cd1^{v}	28.6 (2)
O5^{v}—Cd2—N1—C6	−115.5 (5)	O3^{iv}—Cd1—O6—Cd1^{v}	−113.2 (2)
O4^{iv}—Cd2—N1—C6	−7.7 (5)	O6^{i}—Cd1—O6—Cd1^{vi}	70.1 (2)

O5—Cd2—N1—C6	83.3 (5)	O5—Cd1—O6—Cd1^{vi}	−155.55 (12)
O1—Cd2—N1—C6	−172.6 (5)	O6^{ii}—Cd1—O6—Cd1^{vi}	−0.37 (9)
O5^{v}—Cd2—N1—C2	62.9 (5)	O2^{iii}—Cd1—O6—Cd1^{vi}	−81.26 (15)
O4^{iv}—Cd2—N1—C2	170.8 (4)	O3^{iv}—Cd1—O6—Cd1^{vi}	136.96 (17)
O5—Cd2—N1—C2	−98.3 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O1^{iii}	0.81 (3)	2.08 (4)	2.818 (6)	150 (6)
O6—H6*A*···O3^{iv}	0.82 (2)	2.39 (4)	2.887 (6)	120 (6)

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