

# Poly[( $\mu_5$ -*cis*-cyclohex-4-ene-1,2-dicarboxylato)-( $\mu_3$ -*cis*-cyclohex-4-ene-1,2-dicarboxylato)-dicadmium(II)]

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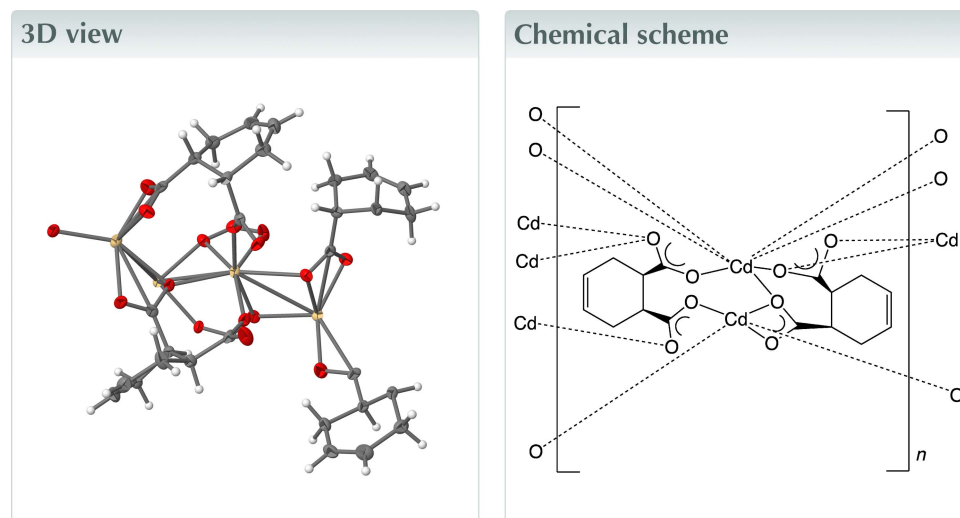
Edited by A. J. Lough, University of Toronto, Canada

Keywords: cadmium; coordination polymer; layer; crystal structure.

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Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

The title compound,  $[\text{Cd}_2(\text{C}_8\text{H}_8\text{O}_4)_2]_n$ , crystallizes in the centrosymmetric monoclinic  $P2_1/n$  space group. Via *cis*-cyclohex-4-ene-1,2-dicarboxylate ligands in two different binding modes, square pyramidally and pentagonal bipyramidally coordinated Cd atoms are connected into coordination polymer layer motifs oriented parallel to the *ab* plane. These layered motifs are aggregated into the three-dimensional supramolecular crystal structure of the title compound by means of crystal packing forces.



## Structure description

The dipodal tethering ligand propane-1,3-diylbis(piperidine-4,1-diyl)bis(pyridin-4-ylmethanone) (4-pbpp) has recently proven useful in preparing metal 1,3-thiophenedicarboxylate coordination polymers with intriguing and diverse interpenetrated topologies (Sample & LaDuca, 2016). The title compound was prepared during synthetic attempts to prepare cadmium coordination polymers containing both *cis*-cyclohex-4-ene-1,2-dicarboxylate (chedc) and 4-pbpp ligands. There have only been two reports of cadmium chedc coordination polymers with dipyrindyl-type coligands to the best of our knowledge. One possessed 1,10-phenanthroline capping coligands (Xu *et al.*, 2010), and the other 4,4'-bipyridine tethering coligands (Cui *et al.*, 2013).

The asymmetric unit of the title compound contains two crystallographically distinct Cd atoms (Cd1, Cd2) and two crystallographically distinct chedc ligands (chedc-A, chedc-B) (Fig. 1). The crystallographic distinction within the chedc ligands arises from different binding modes. The Cd1 atom displays a distorted square-pyramidal coordination environment while the Cd2 atom displays a pentagonal-bipyramidal coordination

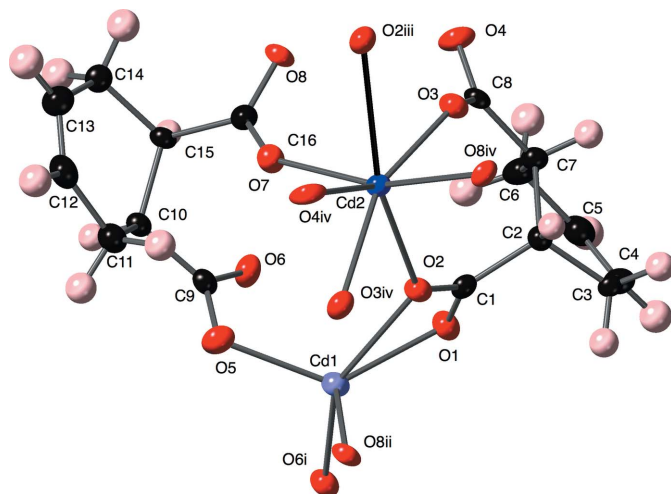
**Table 1**  
Selected geometric parameters (Å, °).

Cd1—O1	2.269 (4)	Cd2—O2	2.346 (3)
Cd1—O2	2.430 (4)	Cd2—O3	2.286 (4)
Cd1—O5	2.173 (4)	Cd2—O3 <sup>iv</sup>	2.357 (4)
Cd1—O6 <sup>i</sup>	2.181 (4)	Cd2—O4 <sup>iv</sup>	2.387 (4)
Cd1—O8 <sup>ii</sup>	2.283 (4)	Cd2—O7	2.231 (4)
Cd2—O2 <sup>iii</sup>	2.555 (4)	Cd2—O8 <sup>iv</sup>	2.286 (4)
O1—Cd1—O2	55.39 (12)	O3—Cd2—O3 <sup>iv</sup>	155.99 (11)
O1—Cd1—O8 <sup>ii</sup>	118.49 (14)	O3—Cd2—O4 <sup>iv</sup>	145.60 (13)
O5—Cd1—O1	133.22 (15)	O3 <sup>iv</sup> —Cd2—O4 <sup>iv</sup>	54.92 (13)
O5—Cd1—O2	99.66 (14)	O4 <sup>iv</sup> —Cd2—O2 <sup>iii</sup>	76.42 (12)
O5—Cd1—O6 <sup>i</sup>	110.36 (16)	O7—Cd2—O2 <sup>iii</sup>	82.99 (13)
O5—Cd1—O8 <sup>ii</sup>	92.17 (15)	O7—Cd2—O2	92.78 (14)
O6 <sup>i</sup> —Cd1—O1	99.08 (14)	O7—Cd2—O3	90.21 (14)
O6 <sup>i</sup> —Cd1—O2	149.76 (13)	O7—Cd2—O3 <sup>iv</sup>	101.45 (13)
O6 <sup>i</sup> —Cd1—O8 <sup>ii</sup>	99.42 (14)	O7—Cd2—O4 <sup>iv</sup>	94.95 (14)
O8 <sup>ii</sup> —Cd1—O2	82.52 (13)	O7—Cd2—O8 <sup>iv</sup>	162.73 (14)
O2—Cd2—O2 <sup>iii</sup>	155.57 (11)	O8 <sup>iv</sup> —Cd2—O2 <sup>iii</sup>	79.75 (12)
O2—Cd2—O3 <sup>iv</sup>	73.13 (13)	O8 <sup>iv</sup> —Cd2—O2	102.80 (13)
O2—Cd2—O4 <sup>iv</sup>	128.00 (13)	O8 <sup>iv</sup> —Cd2—O3	83.70 (14)
O3 <sup>iv</sup> —Cd2—O2 <sup>iii</sup>	131.30 (12)	O8 <sup>iv</sup> —Cd2—O3 <sup>iv</sup>	90.31 (14)
O3—Cd2—O2 <sup>iii</sup>	70.49 (12)	O8 <sup>iv</sup> —Cd2—O4 <sup>iv</sup>	81.41 (14)
O3—Cd2—O2	85.52 (13)		

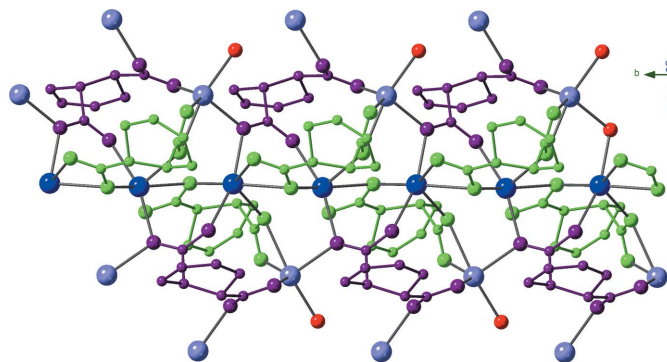
Symmetry codes: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $x, y + 1, z$ ; (iii)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (iv)  $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ .

geometry. Bond lengths and angles within the coordination environments are listed in Table 1.

The Cd atoms and chedc ligands construct  $[\text{Cd}_2(\text{chedc-A})(\text{chedc-B})]_n$  ribbon motifs (Fig. 2) that are oriented parallel to the *b*-axis direction. Within the cores of the ribbon motifs are embedded  $[\text{Cd}(\mu\text{-O})]_n$  chains with a Cd2...Cd2 internuclear distance of 3.606 (2) Å. The bridging oxygen atoms are the O3 atoms within the chedc-A ligands. The Cd1 atoms at the periphery of the ribbon motifs are anchored to the Cd1 atoms at the cores of the ribbon motifs by both chedc-A and chedc-B ligands.



**Figure 1**  
The coordination environments within the title compound, showing the square-pyramidal coordination at atom Cd1 and the pentagonal-bipyramidal coordination at atom Cd2. Displacement ellipsoids are drawn at the 50% probability level. All non-H atoms are labeled. Color code: Cd1, violet; Cd2, blue; O, red; C, black; H, pink. The symmetry codes are as listed in Table 1.

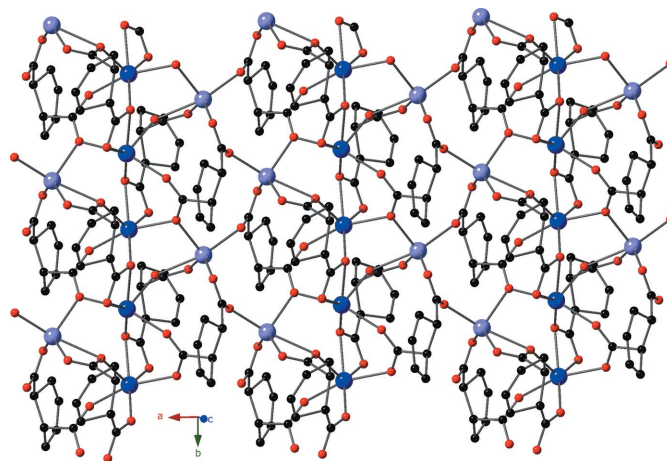


**Figure 2**  
 $[\text{Cd}_2(\text{chedc-A})(\text{chedc-B})]_n$  ribbon motif parallel to *b*-axis direction in the crystal structure of the title compound. Color code: Cd1, violet; Cd2, blue; chedc-A ligands, green; chedc-B ligands, purple.

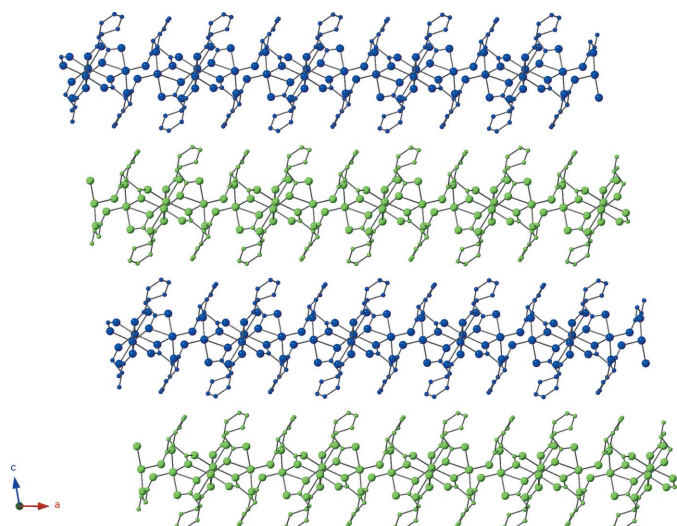
The ribbon motifs are connected into  $[\text{Cd}_2(\text{chedc-A})(\text{chedc-B})]_n$  coordination polymer layers (Fig. 3) that are arranged parallel to the *ab* plane. The inter-ribbon connection is provided by O6 atoms belonging to the chedc-B ligands. Adjacent  $[\text{Cd}_2(\text{chedc-A})(\text{chedc-B})]_n$  coordination polymer layer motifs stack in an *ABAB* pattern along the *c*-axis direction, related by crystallographic glide planes (Fig. 4). Crystal packing forces provide the impetus for the layer aggregation.

### Synthesis and crystallization

$\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$  (115 mg, 0.37 mmol), *cis*-cyclohex-4-ene-1,2-dicarboxylic acid (63 mg, 0.37 mol), propane-1,3-diylbis-(piperidine-4,1-diyl)bis(pyridin-4-ylmethanone) (153 mg, 0.37 mol) and 0.75 ml of a 1.0 M NaOH solution were placed into 10 ml of distilled  $\text{H}_2\text{O}$  in a Teflon-lined acid digestion bomb. The bomb was sealed and heated in an oven at 393 K for 48 h, and then cooled slowly to 278 K. Colorless block-shaped crystals of the title compound were isolated after washing with distilled water and acetone, and drying in air.



**Figure 3**  
 $[\text{Cd}_2(\text{chedc-A})(\text{chedc-B})]_n$  coordination polymer layer motif in the title compound, oriented parallel to the *ab* plane. Color code: Cd1, violet; Cd2, blue.



**Figure 4**  
 ABAB stacking pattern of the  $[\text{Cd}_2(\text{chedc-A})(\text{chedc-B})]_n$  coordination polymer layer motifs to construct the three-dimensional crystal structure of the title compound.

## Refinement

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

## Funding information

We thank the Honors College of Michigan State University for funding this work.

## References

- Bruker (2015). *APEX2*, *COSMO*, *SAINT* and *SADABS*. Bruker AXS, Inc., Madison, Wisconsin, USA.  
 Cui, Z., Qi, J., Xu, X., Liu, L. & Wang, Y. (2013). *J. Solid State Chem.* **205**, 142–148.

**Table 2**

Experimental details.

<b>Crystal data</b>	
Chemical formula	$[\text{Cd}_2(\text{C}_8\text{H}_8\text{CdO}_4)_2]$
$M_r$	561.09
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	173
$a, b, c$ (Å)	9.8377 (11), 7.0700 (8), 24.268 (3)
$\beta$ (°)	100.120 (1)
$V$ (Å <sup>3</sup> )	1661.6 (3)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	2.60
Crystal size (mm)	0.25 × 0.16 × 0.15
<b>Data collection</b>	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2015)
$T_{\min}$ , $T_{\max}$	0.613, 0.745
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	12875, 3038, 2500
$R_{\text{int}}$	0.047
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.602
<b>Refinement</b>	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , $S$	0.037, 0.091, 1.07
No. of reflections	3038
No. of parameters	235
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	1.47, -0.84

Computer programs: *COSMO*, *APEX2* and *SAINT* (Bruker, 2015), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.  
 Sample, A. D. & LaDuca, R. L. (2016). *Inorg. Chim. Acta*, **443**, 198–206.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Sheldrick, G. M. (2015). *Acta Cryst.* **A71**, 3–8.  
 Xu, X., Liu, X., Zhang, X. & Sun, T. (2010). *Solid State Sci.* **12**, 355–360.

## full crystallographic data

*IUCrData* (2018). 3, x180924 [https://doi.org/10.1107/S2414314618009240]

**Poly[( $\mu_5$ -*cis*-cyclohex-4-ene-1,2-dicarboxylato)( $\mu_3$ -*cis*-cyclohex-4-ene-1,2-dicarboxylato)dicadmium(II)]**

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Poly[( $\mu_5$ -*cis*-cyclohex-4-ene-1,2-dicarboxylato)( $\mu_3$ -*cis*-cyclohex-4-ene-1,2-dicarboxylato)dicadmium(II)]

*Crystal data*

[Cd<sub>2</sub>(C<sub>8</sub>H<sub>8</sub>CdO<sub>4</sub>)<sub>2</sub>]

$M_r = 561.09$

Monoclinic,  $P2_1/n$

$a = 9.8377$  (11) Å

$b = 7.0700$  (8) Å

$c = 24.268$  (3) Å

$\beta = 100.120$  (1)°

$V = 1661.6$  (3) Å<sup>3</sup>

$Z = 4$

$F(000) = 1088$

$D_x = 2.243$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 5975 reflections

$\theta = 2.4$ – $25.3$ °

$\mu = 2.60$  mm<sup>-1</sup>

$T = 173$  K

Block, colourless

$0.25 \times 0.16 \times 0.15$  mm

*Data collection*

Bruker APEXII CCD  
diffractometer

Radiation source: sealed tube

Graphite monochromator

Detector resolution: 8.4 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2015)

$T_{\min} = 0.613$ ,  $T_{\max} = 0.745$

12875 measured reflections

3038 independent reflections

2500 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

$\theta_{\max} = 25.3$ °,  $\theta_{\min} = 1.7$ °

$h = -11 \rightarrow 11$

$k = -8 \rightarrow 8$

$l = -29 \rightarrow 29$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.091$

$S = 1.07$

3038 reflections

235 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 3.7886P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.47$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.83$  e Å<sup>-3</sup>

*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 and phi 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 structures are solved by the direct method using the SHELXS-97 program and refined by least squares method on F<sup>2</sup>, SHELXL-97, 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.** Hydrogen atoms bound to C were placed in calculated positions with a riding model with  $U_{\text{iso}} = 1.2U_{\text{eq}}$ .

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)*

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.39348 (4)	0.94716 (6)	0.74436 (2)	0.02049 (14)
Cd2	0.76663 (4)	0.61706 (5)	0.76431 (2)	0.01681 (13)
O1	0.3949 (4)	0.8233 (6)	0.65823 (15)	0.0237 (9)
O2	0.5952 (4)	0.8119 (5)	0.71409 (14)	0.0194 (8)
O3	0.7149 (4)	0.4133 (5)	0.69043 (16)	0.0224 (9)
O4	0.5747 (4)	0.1907 (5)	0.65224 (16)	0.0300 (10)
O5	0.4160 (4)	0.8240 (6)	0.82752 (17)	0.0317 (10)
O6	0.2972 (4)	0.6105 (5)	0.77425 (16)	0.0244 (9)
O7	0.6164 (4)	0.4686 (5)	0.80826 (16)	0.0233 (9)
O8	0.5445 (4)	0.1854 (5)	0.77511 (16)	0.0230 (8)
C1	0.5190 (6)	0.7816 (8)	0.6655 (2)	0.0199 (12)
C2	0.5848 (5)	0.7039 (8)	0.6184 (2)	0.0180 (11)
H2	0.6872	0.7182	0.6291	0.022*
C3	0.5376 (6)	0.8158 (8)	0.5642 (2)	0.0213 (12)
H3A	0.5285	0.9507	0.5738	0.026*
H3B	0.6100	0.8068	0.5407	0.026*
C4	0.4048 (6)	0.7508 (8)	0.5308 (2)	0.0270 (13)
H4	0.3630	0.8274	0.5004	0.032*
C5	0.3402 (6)	0.5921 (8)	0.5409 (2)	0.0280 (14)
H5	0.2540	0.5634	0.5180	0.034*
C6	0.3978 (6)	0.4568 (8)	0.5867 (3)	0.0275 (14)
H6A	0.3835	0.3253	0.5728	0.033*
H6B	0.3483	0.4724	0.6185	0.033*
C7	0.5525 (6)	0.4926 (7)	0.6064 (2)	0.0204 (12)
H7	0.5974	0.4602	0.5737	0.025*
C8	0.6151 (6)	0.3584 (7)	0.6527 (2)	0.0203 (12)
C9	0.3695 (6)	0.6591 (8)	0.8208 (2)	0.0219 (12)
C10	0.4064 (6)	0.5202 (7)	0.8687 (2)	0.0191 (12)
H10	0.3235	0.5082	0.8871	0.023*
C11	0.5243 (6)	0.5972 (8)	0.9129 (2)	0.0240 (13)

H11A	0.5956	0.6531	0.8938	0.029*
H11B	0.4879	0.6994	0.9341	0.029*
C12	0.5896 (6)	0.4506 (9)	0.9528 (2)	0.0270 (13)
H12	0.6480	0.4913	0.9861	0.032*
C13	0.5711 (6)	0.2671 (9)	0.9448 (2)	0.0302 (14)
H13	0.6184	0.1837	0.9724	0.036*
C14	0.4806 (6)	0.1819 (8)	0.8949 (2)	0.0265 (13)
H14A	0.3970	0.1294	0.9068	0.032*
H14B	0.5305	0.0757	0.8809	0.032*
C15	0.4357 (5)	0.3224 (7)	0.8468 (2)	0.0178 (11)
H15	0.3470	0.2743	0.8247	0.021*
C16	0.5398 (5)	0.3300 (8)	0.8071 (2)	0.0180 (11)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cd1	0.0174 (2)	0.0198 (2)	0.0242 (2)	0.00097 (16)	0.00357 (17)	-0.00307 (16)
Cd2	0.0151 (2)	0.0146 (2)	0.0210 (2)	-0.00088 (14)	0.00367 (16)	0.00038 (15)
O1	0.018 (2)	0.030 (2)	0.022 (2)	0.0032 (17)	0.0035 (16)	-0.0028 (17)
O2	0.0166 (19)	0.021 (2)	0.0191 (19)	0.0036 (16)	-0.0009 (15)	-0.0020 (16)
O3	0.023 (2)	0.022 (2)	0.022 (2)	0.0041 (16)	0.0017 (17)	-0.0045 (16)
O4	0.043 (3)	0.012 (2)	0.031 (2)	-0.0039 (18)	-0.0055 (19)	-0.0007 (18)
O5	0.046 (3)	0.019 (2)	0.029 (2)	-0.0047 (19)	0.003 (2)	-0.0005 (18)
O6	0.022 (2)	0.029 (2)	0.021 (2)	-0.0074 (17)	0.0020 (17)	0.0037 (17)
O7	0.024 (2)	0.021 (2)	0.027 (2)	-0.0083 (17)	0.0091 (17)	-0.0044 (17)
O8	0.026 (2)	0.018 (2)	0.028 (2)	0.0025 (17)	0.0099 (17)	-0.0079 (17)
C1	0.023 (3)	0.015 (3)	0.021 (3)	-0.003 (2)	0.004 (2)	0.003 (2)
C2	0.015 (3)	0.021 (3)	0.018 (3)	0.002 (2)	0.002 (2)	0.000 (2)
C3	0.027 (3)	0.015 (3)	0.023 (3)	0.004 (2)	0.008 (2)	0.004 (2)
C4	0.033 (3)	0.024 (3)	0.021 (3)	0.008 (3)	-0.004 (3)	0.001 (2)
C5	0.023 (3)	0.032 (4)	0.027 (3)	0.003 (3)	-0.001 (3)	-0.007 (3)
C6	0.028 (3)	0.020 (3)	0.029 (3)	-0.003 (2)	-0.010 (3)	-0.001 (3)
C7	0.025 (3)	0.015 (3)	0.020 (3)	-0.001 (2)	0.002 (2)	-0.003 (2)
C8	0.023 (3)	0.018 (3)	0.021 (3)	0.008 (2)	0.006 (2)	-0.003 (2)
C9	0.020 (3)	0.022 (3)	0.028 (3)	0.001 (2)	0.015 (2)	-0.001 (2)
C10	0.019 (3)	0.017 (3)	0.023 (3)	-0.002 (2)	0.008 (2)	-0.003 (2)
C11	0.022 (3)	0.026 (3)	0.022 (3)	-0.003 (2)	0.001 (2)	-0.006 (2)
C12	0.022 (3)	0.038 (4)	0.020 (3)	0.001 (3)	0.001 (2)	-0.006 (3)
C13	0.031 (3)	0.032 (4)	0.027 (3)	0.008 (3)	0.000 (3)	0.005 (3)
C14	0.032 (3)	0.022 (3)	0.028 (3)	-0.002 (3)	0.011 (3)	0.001 (3)
C15	0.016 (3)	0.015 (3)	0.024 (3)	0.000 (2)	0.006 (2)	-0.004 (2)
C16	0.012 (3)	0.020 (3)	0.020 (3)	0.000 (2)	-0.001 (2)	0.001 (2)

*Geometric parameters (Å, °)*

Cd1—O1	2.269 (4)	C3—H3A	0.9900
Cd1—O2	2.430 (4)	C3—H3B	0.9900
Cd1—O5	2.173 (4)	C3—C4	1.483 (8)

Cd1—O6 <sup>i</sup>	2.181 (4)	C4—H4	0.9500
Cd1—O8 <sup>ii</sup>	2.283 (4)	C4—C5	1.332 (8)
Cd2—O2 <sup>iii</sup>	2.555 (4)	C5—H5	0.9500
Cd2—O2	2.346 (3)	C5—C6	1.500 (8)
Cd2—O3	2.286 (4)	C6—H6A	0.9900
Cd2—O3 <sup>iv</sup>	2.357 (4)	C6—H6B	0.9900
Cd2—O4 <sup>iv</sup>	2.387 (4)	C6—C7	1.534 (8)
Cd2—O7	2.231 (4)	C7—H7	1.0000
Cd2—O8 <sup>iv</sup>	2.286 (4)	C7—C8	1.515 (7)
O1—C1	1.239 (6)	C8—Cd2 <sup>iii</sup>	2.739 (5)
O2—Cd2 <sup>iv</sup>	2.554 (4)	C9—C10	1.517 (8)
O2—C1	1.300 (6)	C10—H10	1.0000
O3—Cd2 <sup>iii</sup>	2.357 (4)	C10—C11	1.534 (7)
O3—C8	1.280 (7)	C10—C15	1.542 (7)
O4—Cd2 <sup>iii</sup>	2.387 (4)	C11—H11A	0.9900
O4—C8	1.250 (7)	C11—H11B	0.9900
O5—C9	1.253 (7)	C11—C12	1.486 (8)
O6—Cd1 <sup>v</sup>	2.181 (4)	C12—H12	0.9500
O6—C9	1.271 (7)	C12—C13	1.320 (8)
O7—C16	1.233 (6)	C13—H13	0.9500
O8—Cd1 <sup>vi</sup>	2.283 (4)	C13—C14	1.497 (8)
O8—Cd2 <sup>iii</sup>	2.286 (4)	C14—H14A	0.9900
O8—C16	1.290 (6)	C14—H14B	0.9900
C1—C2	1.512 (7)	C14—C15	1.538 (8)
C2—H2	1.0000	C15—H15	1.0000
C2—C3	1.535 (7)	C15—C16	1.524 (7)
C2—C7	1.545 (7)		
O1—Cd1—O2	55.39 (12)	C4—C3—C2	114.4 (5)
O1—Cd1—O8 <sup>ii</sup>	118.49 (14)	C4—C3—H3A	108.7
O5—Cd1—O1	133.22 (15)	C4—C3—H3B	108.7
O5—Cd1—O2	99.66 (14)	C3—C4—H4	117.8
O5—Cd1—O6 <sup>i</sup>	110.36 (16)	C5—C4—C3	124.3 (5)
O5—Cd1—O8 <sup>ii</sup>	92.17 (15)	C5—C4—H4	117.8
O6 <sup>i</sup> —Cd1—O1	99.08 (14)	C4—C5—H5	118.6
O6 <sup>i</sup> —Cd1—O2	149.76 (13)	C4—C5—C6	122.8 (5)
O6 <sup>i</sup> —Cd1—O8 <sup>ii</sup>	99.42 (14)	C6—C5—H5	118.6
O8 <sup>ii</sup> —Cd1—O2	82.52 (13)	C5—C6—H6A	109.5
O2—Cd2—O2 <sup>iii</sup>	155.57 (11)	C5—C6—H6B	109.5
O2—Cd2—O3 <sup>iv</sup>	73.13 (13)	C5—C6—C7	110.6 (5)
O2—Cd2—O4 <sup>iv</sup>	128.00 (13)	H6A—C6—H6B	108.1
O3 <sup>iv</sup> —Cd2—O2 <sup>iii</sup>	131.30 (12)	C7—C6—H6A	109.5
O3—Cd2—O2 <sup>iii</sup>	70.49 (12)	C7—C6—H6B	109.5
O3—Cd2—O2	85.52 (13)	C2—C7—H7	105.4
O3—Cd2—O3 <sup>iv</sup>	155.99 (11)	C6—C7—C2	112.2 (4)
O3—Cd2—O4 <sup>iv</sup>	145.60 (13)	C6—C7—H7	105.4
O3 <sup>iv</sup> —Cd2—O4 <sup>iv</sup>	54.92 (13)	C8—C7—C2	115.0 (4)
O4 <sup>iv</sup> —Cd2—O2 <sup>iii</sup>	76.42 (12)	C8—C7—C6	112.3 (5)

O7—Cd2—O2 <sup>iii</sup>	82.99 (13)	C8—C7—H7	105.4
O7—Cd2—O2	92.78 (14)	O3—C8—Cd2 <sup>iii</sup>	59.3 (3)
O7—Cd2—O3	90.21 (14)	O3—C8—C7	120.1 (5)
O7—Cd2—O3 <sup>iv</sup>	101.45 (13)	O4—C8—Cd2 <sup>iii</sup>	60.6 (3)
O7—Cd2—O4 <sup>iv</sup>	94.95 (14)	O4—C8—O3	119.8 (5)
O7—Cd2—O8 <sup>iv</sup>	162.73 (14)	O4—C8—C7	120.0 (5)
O8 <sup>iv</sup> —Cd2—O2 <sup>iii</sup>	79.75 (12)	C7—C8—Cd2 <sup>iii</sup>	178.8 (4)
O8 <sup>iv</sup> —Cd2—O2	102.80 (13)	O5—C9—O6	120.1 (5)
O8 <sup>iv</sup> —Cd2—O3	83.70 (14)	O5—C9—C10	118.0 (5)
O8 <sup>iv</sup> —Cd2—O3 <sup>iv</sup>	90.31 (14)	O6—C9—C10	121.9 (5)
O8 <sup>iv</sup> —Cd2—O4 <sup>iv</sup>	81.41 (14)	C9—C10—H10	107.1
C1—O1—Cd1	97.3 (3)	C9—C10—C11	110.9 (5)
Cd1—O2—Cd2 <sup>iv</sup>	92.24 (12)	C9—C10—C15	110.9 (4)
Cd2—O2—Cd1	128.66 (15)	C11—C10—H10	107.1
Cd2—O2—Cd2 <sup>iv</sup>	94.67 (12)	C11—C10—C15	113.5 (4)
C1—O2—Cd1	88.2 (3)	C15—C10—H10	107.1
C1—O2—Cd2 <sup>iv</sup>	121.8 (3)	C10—C11—H11A	108.9
C1—O2—Cd2	128.5 (3)	C10—C11—H11B	108.9
Cd2—O3—Cd2 <sup>iii</sup>	101.89 (14)	H11A—C11—H11B	107.7
C8—O3—Cd2 <sup>iii</sup>	92.9 (3)	C12—C11—C10	113.3 (5)
C8—O3—Cd2	142.2 (3)	C12—C11—H11A	108.9
C8—O4—Cd2 <sup>iii</sup>	92.3 (3)	C12—C11—H11B	108.9
C9—O5—Cd1	106.0 (4)	C11—C12—H12	118.1
C9—O6—Cd1 <sup>v</sup>	130.8 (3)	C13—C12—C11	123.8 (5)
C16—O7—Cd2	144.7 (4)	C13—C12—H12	118.1
Cd1 <sup>vi</sup> —O8—Cd2 <sup>iii</sup>	103.74 (14)	C12—C13—H13	117.9
C16—O8—Cd1 <sup>vi</sup>	133.8 (3)	C12—C13—C14	124.2 (5)
C16—O8—Cd2 <sup>iii</sup>	122.5 (3)	C14—C13—H13	117.9
O1—C1—Cd1	55.8 (3)	C13—C14—H14A	108.8
O1—C1—O2	119.1 (5)	C13—C14—H14B	108.8
O1—C1—C2	121.5 (5)	C13—C14—C15	113.9 (5)
O2—C1—Cd1	63.3 (3)	H14A—C14—H14B	107.7
O2—C1—C2	119.4 (5)	C15—C14—H14A	108.8
C2—C1—Cd1	175.1 (4)	C15—C14—H14B	108.8
C1—C2—H2	108.1	C10—C15—H15	107.1
C1—C2—C3	110.8 (4)	C14—C15—C10	111.7 (4)
C1—C2—C7	113.1 (4)	C14—C15—H15	107.1
C3—C2—H2	108.1	C16—C15—C10	111.9 (4)
C3—C2—C7	108.4 (4)	C16—C15—C14	111.6 (4)
C7—C2—H2	108.1	C16—C15—H15	107.1
C2—C3—H3A	108.7	O7—C16—O8	123.8 (5)
C2—C3—H3B	108.7	O7—C16—C15	119.3 (5)
H3A—C3—H3B	107.6	O8—C16—C15	116.8 (5)
Cd1—O1—C1—O2	2.4 (5)	O6—C9—C10—C11	164.5 (5)
Cd1—O1—C1—C2	-175.1 (4)	O6—C9—C10—C15	37.4 (7)
Cd1—O2—C1—O1	-2.2 (5)	C1—C2—C3—C4	-85.0 (6)
Cd1—O2—C1—C2	175.3 (4)	C1—C2—C7—C6	63.1 (6)



Cd1—O5—C9—O6	-14.5 (6)	C1—C2—C7—C8	-67.0 (6)
Cd1—O5—C9—C10	163.5 (4)	C2—C3—C4—C5	-10.2 (8)
Cd1 <sup>v</sup> —O6—C9—O5	-136.2 (4)	C2—C7—C8—O3	-17.8 (7)
Cd1 <sup>v</sup> —O6—C9—C10	45.9 (7)	C2—C7—C8—O4	166.3 (5)
Cd1 <sup>vi</sup> —O8—C16—O7	-161.3 (4)	C3—C2—C7—C6	-60.2 (6)
Cd1 <sup>vi</sup> —O8—C16—C15	20.7 (7)	C3—C2—C7—C8	169.8 (5)
Cd2 <sup>iv</sup> —O2—C1—Cd1	-91.5 (3)	C3—C4—C5—C6	-1.9 (9)
Cd2—O2—C1—Cd1	140.6 (4)	C4—C5—C6—C7	-17.5 (8)
Cd2—O2—C1—O1	138.4 (4)	C5—C6—C7—C2	48.7 (6)
Cd2 <sup>iv</sup> —O2—C1—O1	-93.7 (5)	C5—C6—C7—C8	-179.9 (5)
Cd2 <sup>iv</sup> —O2—C1—C2	83.8 (5)	C6—C7—C8—O3	-147.8 (5)
Cd2—O2—C1—C2	-44.1 (6)	C6—C7—C8—O4	36.3 (7)
Cd2—O3—C8—Cd2 <sup>iii</sup>	-113.7 (5)	C7—C2—C3—C4	39.7 (6)
Cd2 <sup>iii</sup> —O3—C8—O4	-2.9 (5)	C9—C10—C11—C12	-164.9 (5)
Cd2—O3—C8—O4	-116.6 (6)	C9—C10—C15—C14	177.1 (4)
Cd2—O3—C8—C7	67.4 (8)	C9—C10—C15—C16	51.2 (6)
Cd2 <sup>iii</sup> —O3—C8—C7	-178.9 (4)	C10—C11—C12—C13	14.2 (8)
Cd2 <sup>iii</sup> —O4—C8—O3	2.9 (5)	C10—C15—C16—O7	19.9 (7)
Cd2 <sup>iii</sup> —O4—C8—C7	178.9 (4)	C10—C15—C16—O8	-162.0 (4)
Cd2—O7—C16—O8	13.4 (10)	C11—C10—C15—C14	51.5 (6)
Cd2—O7—C16—C15	-168.7 (4)	C11—C10—C15—C16	-74.4 (6)
Cd2 <sup>iii</sup> —O8—C16—O7	19.6 (7)	C11—C12—C13—C14	-1.0 (10)
Cd2 <sup>iii</sup> —O8—C16—C15	-158.4 (3)	C12—C13—C14—C15	13.3 (8)
O1—C1—C2—C3	44.2 (7)	C13—C14—C15—C10	-37.7 (7)
O1—C1—C2—C7	-77.8 (6)	C13—C14—C15—C16	88.4 (6)
O2—C1—C2—C3	-133.3 (5)	C14—C15—C16—O7	-106.0 (6)
O2—C1—C2—C7	104.8 (6)	C14—C15—C16—O8	72.1 (6)
O5—C9—C10—C11	-13.4 (7)	C15—C10—C11—C12	-39.4 (7)
O5—C9—C10—C15	-140.4 (5)		

Symmetry codes: (i)  $-x+1/2, y+1/2, -z+3/2$ ; (ii)  $x, y+1, z$ ; (iii)  $-x+3/2, y-1/2, -z+3/2$ ; (iv)  $-x+3/2, y+1/2, -z+3/2$ ; (v)  $-x+1/2, y-1/2, -z+3/2$ ; (vi)  $x, y-1, z$ .