

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

# A one-dimensional zigzag coordination polymer: catena-poly[[[triaqua-cadmium(II)]- $[\mu$ -2,2'-(5-methyl-1,3-phenylenedioxy)diacetato- $\kappa^4 O, O': O'', O''']$ ] monohydrate]

Ying Lin, Yun Wei, Xian-Wen Wei and Hong-Tao Zhang\*

College of Chemistry and Materials Science, Anhui Key Laboratory of Functional Molecular Solids, Anhui Normal University, Wuhu 241000, People's Republic of China

Correspondence e-mail: zht2006@mail.ahnu.edu.cn

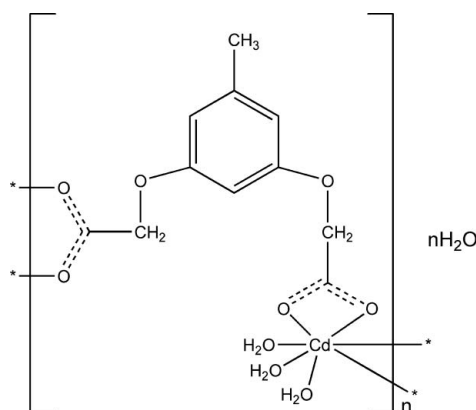
Received 21 November 2007; accepted 21 December 2007

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.040;  $wR$  factor = 0.093; data-to-parameter ratio = 13.2.

In the title one-dimensional coordination polymer,  $\{[\text{Cd}(\text{C}_{11}\text{H}_{10}\text{O}_6)(\text{H}_2\text{O})_3] \cdot \text{H}_2\text{O}\}_n$ , the 2,2'-(5-methyl-1,3-phenylenedioxy)diacetate dianions connect  $\text{Cd}^{\text{II}}$  ions in a head-to-tail fashion to generate zigzag chains. The coordination geometry of the Cd atom is distorted pentagonal bipyramidal. There are  $\text{O}-\text{H} \cdots \text{O}$  hydrogen bonds between the carboxyl O atoms, the aqua ligands and the uncoordinated water molecules.

## Related literature

For related literature on coordination polymers, see: Burrows *et al.* (2004); Hong *et al.* (2006); Janiak (2000, 2003); Kitagawa *et al.* (2004); Moulton & Zaworotko (2001); Russell *et al.* (2001).



## Experimental

### Crystal data

$[\text{Cd}(\text{C}_{11}\text{H}_{10}\text{O}_6)(\text{H}_2\text{O})_3] \cdot \text{H}_2\text{O}$   
 $M_r = 422.66$   
 Triclinic,  $P\bar{1}$   
 $a = 7.3792$  (11) Å  
 $b = 8.6946$  (12) Å  
 $c = 11.9495$  (17) Å  
 $\alpha = 85.294$  (19)°  
 $\beta = 82.52$  (2)°

$\gamma = 88.44$  (2)°  
 $V = 757.47$  (19) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.49$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 $0.24 \times 0.08 \times 0.02$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.717$ ,  $T_{\text{max}} = 0.971$

5397 measured reflections  
 2647 independent reflections  
 2121 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.037$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.093$   
 $S = 0.98$   
 2647 reflections

200 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.41$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.75$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cd—O9	2.262 (4)	Cd—O8	2.381 (4)
Cd—O7	2.297 (4)	Cd—O5 <sup>i</sup>	2.432 (4)
Cd—O1	2.303 (3)	Cd—O2	2.573 (4)
Cd—O6 <sup>i</sup>	2.331 (4)		
O9—Cd—O7	167.09 (14)	O6 <sup>i</sup> —Cd—O8	80.48 (13)
O9—Cd—O1	85.66 (14)	O9—Cd—O5 <sup>i</sup>	88.92 (13)
O9—Cd—O8	92.24 (14)	O9—Cd—O2	83.86 (14)
O7—Cd—O8	88.31 (14)	O8—Cd—O2	77.69 (12)
O1—Cd—O8	130.96 (13)	O5 <sup>i</sup> —Cd—O2	146.90 (12)

Symmetry code: (i)  $x - 1, y, z + 1$ .

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
O7—H7B <sup>ii</sup> ···O8 <sup>ii</sup>	0.85	2.08	2.875 (5)	156
O7—H7C <sup>iii</sup> ···O5 <sup>iii</sup>	0.85	2.00	2.846 (5)	174
O8—H8C <sup>iv</sup> ···O9 <sup>iv</sup>	0.85	2.51	3.263 (5)	148
O8—H8C <sup>v</sup> ···O10 <sup>v</sup>	0.85	2.38	3.008 (7)	131
O8—H8D <sup>vi</sup> ···O2 <sup>vi</sup>	0.85	2.14	2.808 (5)	136
O9—H9E <sup>vii</sup> ···O1 <sup>vii</sup>	0.85	1.92	2.752 (5)	165
O9—H9F <sup>vii</sup> ···O10 <sup>vii</sup>	0.85	2.10	2.659 (6)	123
O10—H10C <sup>v</sup> ···O6	0.85	2.08	2.731 (6)	133
O10—H10D <sup>v</sup> ···O2 <sup>v</sup>	0.85	1.95	2.793 (6)	170

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

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 2000); software used to prepare material for publication: SHELXTL.

This work was funded by the Doctoral Research Launch Foundation of Anhui Normal University and the Youth

Research Foundation of Anhui Normal University (grant No. 2006xqn64).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OB2104).

## References

- Bruker (2000). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Burrows, A. D., Donovan, A. S., Harrington, R. W. & Mahon, M. (2004). *Eur. J. Inorg. Chem.* pp. 4686–4695.
- Hong, X.-L., Bai, J., Song, Y., Li, Y.-Z. & Pan, Y. (2006). *Eur. J. Inorg. Chem.* pp. 3659–3666.
- Janiak, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3885–3896.
- Janiak, C. (2003). *Dalton Trans.* pp. 2781–2804.
- Kitagawa, S., Kitaura, R. & Noro, S. (2004). *Angew. Chem. Int. Ed.* **43**, 2334–2375.
- Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.
- Russell, V., Craig, D., Scudder, M. & Dance, I. (2001). *CrystEngComm*, **3**, 96–106.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (2000). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

**supplementary materials**

*Acta Cryst.* (2008). E64, m280-m281 [ doi:10.1107/S1600536807068031 ]

**A one-dimensional zigzag coordination polymer: catena-poly[[[triaquacadmium(II)]- $[\mu$ -2,2'-(5-methyl-1,3-phenylenedioxy)diacetato- $\kappa^4$ O,O':O'',O''']] monohydrate]**

**Y. Lin, Y. Wei, X.-W. Wei and H.-T. Zhang**

**Comment**

Supramolecular self-assembly of coordination polymers have been one of the areas of rapid growth in chemistry recently, owing to their intriguing molecular topologies and useful properties, such as molecular recognition, electronic, optical, magnetic and catalytic properties (Janiak, 2003; Kitagawa *et al.*, 2004). Generally, the structure of such a molecular architecture is governed by coordination interaction and other non-covalent interactions such as hydrogen bonding and  $\pi$ - $\pi$  stacking as well as the conformations of ligands depending on their rigidity and flexibility (Russell *et al.*, 2001; Moulton & Zaworotko, 2001; Burrows *et al.*, 2004). To date, there is a great research interest focused on the coordination interaction, hydrogen bonding and  $\pi$ - $\pi$  stacking as well as the rigidity of ligands, whereas there is scant attention to the influence of the flexibility of ligands on the structure of coordination polymer. In order to further understand the role of the flexibility of ligands in the self-assembly of coordination polymers, we have designed and synthesized a ligand bearing the flexible group, 2,2'-(5-methyl-1,3-phenylenedioxy)diacetic acid (abbreviated to H<sub>2</sub>5-mpdoa), and employed it with Cd<sup>II</sup> ion to assemble the title coordination polymer, (I), [Cd(5-mpdoa)(H<sub>2</sub>O)<sub>3</sub>]<sub>n</sub>·nH<sub>2</sub>O.

As shown in Fig. 1, the coordination geometry of the Cd<sup>II</sup> atom is a distorted pentagonal bipyramid. The equatorial positions are occupied by four carboxyl O atoms (O1, O2, O5<sup>i</sup>, O6<sup>i</sup>, symmetry code (i)  $x - 1, y, z + 1$ ) from two symmetry related 5-mpdoa ligands and the aqua O8 atom. The aqua O7 and O9 atoms are located at the axial vertices of the pentagonal bipyramid. Both two carboxylate groups of the 5-mpdoa ligands, O1/C1/O2 and O5<sup>i</sup>/C11<sup>i</sup>/O6<sup>i</sup>, chelate the Cd<sup>II</sup> atom in the same mode. The O5/C11/O6 carboxylate is almost coplanar with the benzene ring C3—C8, whereas the O1/C1/O2 carboxylate has a slightly twisted from the benzene ring with the dihedral angle of 10.7 (7)°. Due to the flexibility of the molecule induced by the  $\sigma$ -rotation of the C—O bond (selected torsion angles are listed in Table 1), the 5-mpdoa ligand adopts a W-shape conformation.

The 5-mpdoa ligands connect the neighbouring Cd<sup>II</sup> atoms in a head-to-tail mode to construct an infinite zigzag chain which runs along the [T01] direction. Such a supramolecular geometry could be regarded as a result of the cooperation of coordination interaction, the symmetry and the flexibility of ligand molecule as well as the hydrogen bonds. All zigzag chains are packing together through an amount of hydrogen bonding interactions between the carboxyl O atoms, the aqua ligands and the lattice water molecules (Fig. 2, Table 2). The shortest center-center distance between two adjacent benzene rings of the different chains is 4.997 (15) Å, indicating no interchain  $\pi$ - $\pi$  interaction of 5-mpdoa (Janiak *et al.*, 2000).

**Experimental**

The H<sub>2</sub>5-mpdoa ligand, 2,2'-(5-methyl-1,3-phenylenedioxy)diacetic acid, was synthesized from 5-methylbenzene-1,3-diol and 2-chloroacetic acid according to a literature method reported by Hong *et al.* (2006). Cd(CH<sub>3</sub>COO)<sub>2</sub>·2(H<sub>2</sub>O) (26.8 mg, 0.10 mmol) and H<sub>2</sub>5-mpdoa (24.0 mg, 0.10 mmol) were dissolved in 10 ml water. The resulting yellow solution was filtered

## supplementary materials

and the filtrate was left at room temperature. Yellow column-like crystals were obtained (25.5 mg, yield *ca* 60%) after several weeks by slow evaporation of the solvent.

### Refinement

All non-hydrogen atoms were refined anisotropically. H atoms bonded to C atoms were introduced at calculated positions and refined using a riding model with C—H distances of 0.93–0.97 Å. All hydrogen atoms of the water molecules were located in difference maps at an intermediate stage of the refinement and were then treated as riding, with O—H=0.85 (3) Å. In all cases, the H-atom  $U_{\text{iso}}(\text{H})$  is 1.2 times  $U_{\text{eq}}$  of the parent atom.

### Figures

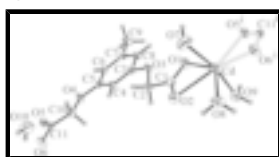


Fig. 1. A drawing of the asymmetric unit of (I) (solid line portion) with displacement ellipsoids at the 30% probability level. [symmetry code: (i)  $x - 1, y, z + 1$ ].

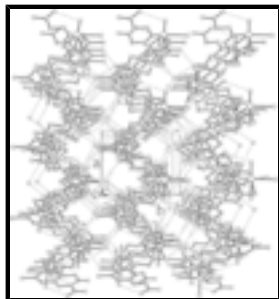


Fig. 2. A packing diagram of (I) viewed down the  $c$  axis. Dotted lines show O—H...O hydrogen bonds. All hydrogen atoms have been omitted for clarity.

### **catena-poly[[[triacuacadmium(II)]- $[\mu$ -2,2'-(5-methyl-1,3-phenylenedioxy)diacetato- $\kappa^4$ O,O':O'',O''']] mono-hydrate]**

#### Crystal data

$[\text{Cd}(\text{C}_{11}\text{H}_{10}\text{O}_6)(\text{H}_2\text{O})_3] \cdot \text{H}_2\text{O}$

$M_r = 422.66$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.3792$  (11) Å

$b = 8.6946$  (12) Å

$c = 11.9495$  (17) Å

$\alpha = 85.294$  (19)°

$\beta = 82.52$  (2)°

$\gamma = 88.44$  (2)°

$V = 757.47$  (19) Å<sup>3</sup>

$Z = 2$

$F_{000} = 424$

$D_x = 1.853$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 1908 reflections

$\theta = 2.4$ – $25.5$ °

$\mu = 1.49$  mm<sup>-1</sup>

$T = 298$  (2) K

Column, yellow

$0.24 \times 0.08 \times 0.02$  mm

*Data collection*

Bruker SMART CCD area-detector diffractometer	2647 independent reflections
Radiation source: fine-focus sealed tube	2121 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.037$
$T = 274(2)$ K	$\theta_{\text{max}} = 25.0^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\text{min}} = 1.7^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{\text{min}} = 0.717$ , $T_{\text{max}} = 0.971$	$k = -10 \rightarrow 10$
5397 measured reflections	$l = -14 \rightarrow 14$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H-atom parameters constrained
$wR(F^2) = 0.093$	$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2]$
$S = 0.98$	where $P = (F_o^2 + 2F_c^2)/3$
2647 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
200 parameters	$\Delta\rho_{\text{max}} = 0.41 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.75 \text{ e } \text{\AA}^{-3}$
	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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	-0.0333 (7)	0.3276 (6)	0.8172 (4)	0.0364 (12)
C2	0.0773 (7)	0.3784 (6)	0.7048 (4)	0.0357 (12)
H2A	0.2052	0.3511	0.7070	0.043*
H2B	0.0346	0.3267	0.6445	0.043*
C3	0.1556 (6)	0.6127 (6)	0.5904 (4)	0.0304 (11)

## supplementary materials

---

C4	0.2445 (6)	0.5368 (5)	0.5016 (4)	0.0289 (11)
H4	0.2422	0.4298	0.5022	0.035*
C5	0.3370 (6)	0.6246 (6)	0.4120 (4)	0.0301 (11)
C6	0.3419 (6)	0.7843 (6)	0.4103 (4)	0.0339 (12)
H6	0.4059	0.8411	0.3491	0.041*
C7	0.2513 (7)	0.8586 (6)	0.4997 (5)	0.0350 (12)
C8	0.1596 (7)	0.7715 (6)	0.5901 (4)	0.0358 (12)
H8	0.0999	0.8201	0.6514	0.043*
C9	0.2558 (8)	1.0326 (6)	0.5005 (5)	0.0515 (15)
H9A	0.1448	1.0770	0.4773	0.061*
H9B	0.3583	1.0715	0.4492	0.061*
H9C	0.2671	1.0595	0.5756	0.061*
C10	0.4195 (7)	0.4039 (5)	0.3083 (4)	0.0348 (12)
H10A	0.2934	0.3767	0.3065	0.042*
H10B	0.4627	0.3468	0.3732	0.042*
C11	0.5344 (6)	0.3625 (7)	0.2014 (4)	0.0363 (13)
Cd	-0.24893 (5)	0.25748 (4)	1.02124 (3)	0.03576 (16)
O1	-0.1211 (5)	0.4250 (4)	0.8748 (3)	0.0411 (9)
O2	-0.0333 (5)	0.1860 (4)	0.8455 (3)	0.0499 (10)
O3	0.0573 (5)	0.5399 (4)	0.6840 (3)	0.0387 (9)
O4	0.4307 (5)	0.5637 (4)	0.3184 (3)	0.0383 (9)
O5	0.6157 (5)	0.4624 (4)	0.1334 (3)	0.0455 (9)
O6	0.5458 (5)	0.2198 (4)	0.1862 (3)	0.0500 (10)
O7	-0.4729 (5)	0.2338 (5)	0.9073 (3)	0.0635 (12)
H7B	-0.5520	0.1705	0.9401	0.076*
H7C	-0.5233	0.3214	0.8950	0.076*
O8	-0.2346 (5)	-0.0167 (4)	1.0480 (3)	0.0570 (11)
H8C	-0.1671	-0.0518	0.9923	0.069*
H8D	-0.1896	-0.0430	1.1088	0.069*
O9	0.0139 (5)	0.2816 (4)	1.0963 (3)	0.0580 (11)
H9E	0.0262	0.3754	1.1086	0.069*
H9F	0.0093	0.2255	1.1580	0.069*
O10	0.2207 (6)	0.0730 (5)	0.1980 (4)	0.0801 (15)
H10C	0.3344	0.0701	0.1748	0.096*
H10D	0.1737	-0.0127	0.1891	0.096*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.028 (3)	0.047 (3)	0.034 (3)	-0.010 (2)	-0.003 (2)	-0.001 (3)
C2	0.040 (3)	0.035 (3)	0.031 (3)	-0.001 (2)	0.000 (2)	-0.002 (2)
C3	0.030 (3)	0.036 (3)	0.024 (3)	-0.004 (2)	-0.001 (2)	0.002 (2)
C4	0.029 (3)	0.027 (3)	0.031 (3)	-0.002 (2)	-0.003 (2)	-0.003 (2)
C5	0.027 (3)	0.039 (3)	0.025 (3)	-0.001 (2)	-0.002 (2)	-0.003 (2)
C6	0.030 (3)	0.037 (3)	0.031 (3)	-0.005 (2)	0.004 (2)	0.000 (2)
C7	0.034 (3)	0.030 (3)	0.043 (3)	-0.003 (2)	-0.010 (2)	-0.003 (2)
C8	0.043 (3)	0.032 (3)	0.032 (3)	0.008 (2)	-0.001 (2)	-0.008 (2)
C9	0.050 (4)	0.035 (3)	0.067 (4)	-0.002 (3)	0.003 (3)	-0.006 (3)

C10	0.034 (3)	0.036 (3)	0.032 (3)	-0.005 (2)	0.004 (2)	-0.001 (2)
C11	0.027 (3)	0.057 (4)	0.026 (3)	0.004 (3)	-0.002 (2)	-0.007 (3)
Cd	0.0367 (2)	0.0382 (2)	0.0297 (2)	-0.00158 (16)	0.00579 (15)	-0.00233 (16)
O1	0.043 (2)	0.046 (2)	0.030 (2)	-0.0051 (18)	0.0085 (17)	0.0003 (17)
O2	0.059 (3)	0.038 (2)	0.050 (3)	-0.0106 (19)	-0.003 (2)	0.0085 (19)
O3	0.047 (2)	0.0324 (19)	0.031 (2)	0.0022 (16)	0.0131 (16)	-0.0004 (16)
O4	0.051 (2)	0.031 (2)	0.029 (2)	-0.0055 (16)	0.0096 (17)	-0.0030 (16)
O5	0.045 (2)	0.053 (2)	0.033 (2)	0.0000 (19)	0.0115 (17)	-0.0003 (18)
O6	0.058 (3)	0.040 (2)	0.050 (3)	-0.0003 (19)	0.0103 (19)	-0.0144 (19)
O7	0.060 (3)	0.059 (3)	0.072 (3)	-0.022 (2)	-0.023 (2)	0.023 (2)
O8	0.047 (2)	0.046 (2)	0.072 (3)	0.0030 (19)	0.006 (2)	0.005 (2)
O9	0.070 (3)	0.048 (2)	0.062 (3)	-0.001 (2)	-0.023 (2)	-0.013 (2)
O10	0.078 (3)	0.047 (3)	0.124 (4)	-0.006 (2)	-0.044 (3)	-0.008 (3)

*Geometric parameters (Å, °)*

C1—O1	1.249 (6)	C10—O4	1.409 (5)
C1—O2	1.250 (6)	C10—C11	1.503 (7)
C1—C2	1.517 (7)	C10—H10A	0.9700
C1—Cd	2.766 (5)	C10—H10B	0.9700
C2—O3	1.413 (6)	C11—O5	1.249 (6)
C2—H2A	0.9700	C11—O6	1.268 (6)
C2—H2B	0.9700	C11—Cd <sup>i</sup>	2.715 (5)
C3—O3	1.370 (6)	Cd—O9	2.262 (4)
C3—C4	1.379 (7)	Cd—O7	2.297 (4)
C3—C8	1.382 (7)	Cd—O1	2.303 (3)
C4—C5	1.378 (7)	Cd—O6 <sup>ii</sup>	2.331 (4)
C4—H4	0.9300	Cd—O8	2.381 (4)
C5—O4	1.374 (5)	Cd—O5 <sup>ii</sup>	2.432 (4)
C5—C6	1.388 (7)	Cd—O2	2.573 (4)
C6—C7	1.382 (7)	O7—H7B	0.8489
C6—H6	0.9300	O7—H7C	0.8491
C7—C8	1.379 (7)	O8—H8C	0.8499
C7—C9	1.515 (7)	O8—H8D	0.8492
C8—H8	0.9300	O9—H9E	0.8495
C9—H9A	0.9600	O9—H9F	0.8482
C9—H9B	0.9600	O10—H10C	0.8492
C9—H9C	0.9600	O10—H10D	0.8499
O1—C1—O2	123.5 (5)	O7—Cd—O1	84.25 (13)
O1—C1—C2	120.1 (5)	O9—Cd—O6 <sup>ii</sup>	100.20 (15)
O2—C1—C2	116.4 (5)	O7—Cd—O6 <sup>ii</sup>	92.61 (15)
O1—C1—Cd	55.6 (3)	O1—Cd—O6 <sup>ii</sup>	148.09 (13)
O2—C1—Cd	68.0 (3)	O9—Cd—O8	92.24 (14)
C2—C1—Cd	175.5 (4)	O7—Cd—O8	88.31 (14)
O3—C2—C1	109.0 (4)	O1—Cd—O8	130.96 (13)
O3—C2—H2A	109.9	O6 <sup>ii</sup> —Cd—O8	80.48 (13)
C1—C2—H2A	109.9	O9—Cd—O5 <sup>ii</sup>	88.92 (13)

## supplementary materials

---

O3—C2—H2B	109.9	O7—Cd—O5 <sup>ii</sup>	99.79 (15)
C1—C2—H2B	109.9	O1—Cd—O5 <sup>ii</sup>	93.99 (12)
H2A—C2—H2B	108.3	O6 <sup>ii</sup> —Cd—O5 <sup>ii</sup>	55.16 (12)
O3—C3—C4	123.9 (4)	O8—Cd—O5 <sup>ii</sup>	135.00 (13)
O3—C3—C8	114.8 (4)	O9—Cd—O2	83.86 (14)
C4—C3—C8	121.3 (5)	O7—Cd—O2	83.67 (14)
C3—C4—C5	117.8 (4)	O1—Cd—O2	53.34 (12)
C3—C4—H4	121.1	O6 <sup>ii</sup> —Cd—O2	157.94 (13)
C5—C4—H4	121.1	O8—Cd—O2	77.69 (12)
O4—C5—C4	123.7 (4)	O5 <sup>ii</sup> —Cd—O2	146.90 (12)
O4—C5—C6	114.6 (4)	O9—Cd—C11 <sup>ii</sup>	94.48 (14)
C4—C5—C6	121.7 (5)	O7—Cd—C11 <sup>ii</sup>	97.62 (15)
C5—C6—C7	119.8 (5)	O1—Cd—C11 <sup>ii</sup>	121.12 (15)
C5—C6—H6	120.1	O6 <sup>ii</sup> —Cd—C11 <sup>ii</sup>	27.78 (14)
C7—C6—H6	120.1	O8—Cd—C11 <sup>ii</sup>	107.90 (16)
C8—C7—C6	118.9 (4)	O5 <sup>ii</sup> —Cd—C11 <sup>ii</sup>	27.38 (14)
C8—C7—C9	120.1 (5)	O2—Cd—C11 <sup>ii</sup>	174.26 (15)
C6—C7—C9	120.9 (5)	O9—Cd—C1	84.11 (15)
C7—C8—C3	120.5 (5)	O7—Cd—C1	83.27 (14)
C7—C8—H8	119.7	O1—Cd—C1	26.58 (14)
C3—C8—H8	119.7	O6 <sup>ii</sup> —Cd—C1	173.43 (14)
C7—C9—H9A	109.5	O8—Cd—C1	104.43 (15)
C7—C9—H9B	109.5	O5 <sup>ii</sup> —Cd—C1	120.41 (15)
H9A—C9—H9B	109.5	O2—Cd—C1	26.77 (13)
C7—C9—H9C	109.5	C11 <sup>ii</sup> —Cd—C1	147.67 (18)
H9A—C9—H9C	109.5	C1—O1—Cd	97.9 (3)
H9B—C9—H9C	109.5	C1—O2—Cd	85.3 (3)
O4—C10—C11	109.4 (4)	C3—O3—C2	119.1 (4)
O4—C10—H10A	109.8	C5—O4—C10	118.4 (4)
C11—C10—H10A	109.8	C11—O5—Cd <sup>i</sup>	89.0 (3)
O4—C10—H10B	109.8	C11—O6—Cd <sup>i</sup>	93.2 (3)
C11—C10—H10B	109.8	Cd—O7—H7B	109.4
H10A—C10—H10B	108.3	Cd—O7—H7C	109.2
O5—C11—O6	122.5 (5)	H7B—O7—H7C	109.7
O5—C11—C10	121.9 (5)	Cd—O8—H8C	109.3
O6—C11—C10	115.6 (5)	Cd—O8—H8D	109.2
O5—C11—Cd <sup>i</sup>	63.6 (3)	H8C—O8—H8D	109.6
O6—C11—Cd <sup>i</sup>	59.0 (3)	Cd—O9—H9E	109.2
C10—C11—Cd <sup>i</sup>	173.6 (4)	Cd—O9—H9F	109.1
O9—Cd—O7	167.09 (14)	H9E—O9—H9F	109.7
O9—Cd—O1	85.66 (14)	H10C—O10—H10D	109.6
O1—C1—C2—O3	-0.6 (7)	O2—C1—O1—Cd	0.1 (6)
O2—C1—C2—O3	177.9 (4)	C2—C1—O1—Cd	178.5 (4)
O3—C3—C4—C5	179.3 (4)	O9—Cd—O1—C1	85.5 (3)

C8—C3—C4—C5	-0.3 (7)	O7—Cd—O1—C1	-86.4 (3)
C3—C4—C5—O4	-179.9 (4)	O6 <sup>ii</sup> —Cd—O1—C1	-172.1 (3)
C3—C4—C5—C6	0.1 (7)	O8—Cd—O1—C1	-3.7 (4)
O4—C5—C6—C7	179.5 (4)	O5 <sup>ii</sup> —Cd—O1—C1	174.1 (3)
C4—C5—C6—C7	-0.5 (7)	O2—Cd—O1—C1	-0.1 (3)
C5—C6—C7—C8	0.9 (7)	C11 <sup>ii</sup> —Cd—O1—C1	178.1 (3)
C5—C6—C7—C9	179.4 (5)	O1—C1—O2—Cd	-0.1 (5)
C6—C7—C8—C3	-1.1 (7)	C2—C1—O2—Cd	-178.5 (4)
C9—C7—C8—C3	-179.6 (5)	O9—Cd—O2—C1	-89.1 (3)
O3—C3—C8—C7	-178.9 (4)	O7—Cd—O2—C1	87.6 (3)
C4—C3—C8—C7	0.8 (7)	O1—Cd—O2—C1	0.1 (3)
O4—C10—C11—O5	-3.2 (7)	O6 <sup>ii</sup> —Cd—O2—C1	168.9 (3)
O4—C10—C11—O6	175.4 (4)	O8—Cd—O2—C1	177.3 (3)
O1—C1—Cd—O9	-92.1 (3)	O5 <sup>ii</sup> —Cd—O2—C1	-10.6 (4)
O2—C1—Cd—O9	88.0 (3)	C4—C3—O3—C2	14.2 (7)
O1—C1—Cd—O7	90.6 (3)	C8—C3—O3—C2	-166.1 (4)
O2—C1—Cd—O7	-89.3 (3)	C1—C2—O3—C3	175.6 (4)
O2—C1—Cd—O1	-179.9 (5)	C4—C5—O4—C10	5.6 (7)
O1—C1—Cd—O8	177.1 (3)	C6—C5—O4—C10	-174.4 (4)
O2—C1—Cd—O8	-2.8 (3)	C11—C10—O4—C5	-179.0 (4)
O1—C1—Cd—O5 <sup>ii</sup>	-6.8 (4)	O6—C11—O5—Cd <sup>i</sup>	-2.4 (5)
O2—C1—Cd—O5 <sup>ii</sup>	173.3 (3)	C10—C11—O5—Cd <sup>i</sup>	176.1 (4)
O1—C1—Cd—O2	179.9 (5)	O5—C11—O6—Cd <sup>i</sup>	2.5 (5)
O1—C1—Cd—C11 <sup>ii</sup>	-3.0 (5)	C10—C11—O6—Cd <sup>i</sup>	-176.1 (4)
O2—C1—Cd—C11 <sup>ii</sup>	177.1 (3)		

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

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O7—H7B $\cdots$ O8 <sup>iii</sup>	0.85	2.08	2.875 (5)	156
O7—H7C $\cdots$ O5 <sup>iv</sup>	0.85	2.00	2.846 (5)	174
O8—H8C $\cdots$ O9 <sup>v</sup>	0.85	2.51	3.263 (5)	148
O8—H8C $\cdots$ O10 <sup>vi</sup>	0.85	2.38	3.008 (7)	131
O8—H8D $\cdots$ O2 <sup>v</sup>	0.85	2.14	2.808 (5)	136
O9—H9E $\cdots$ O1 <sup>vii</sup>	0.85	1.92	2.752 (5)	165
O9—H9F $\cdots$ O10 <sup>viii</sup>	0.85	2.10	2.659 (6)	123
O10—H10C $\cdots$ O6	0.85	2.08	2.731 (6)	133
O10—H10D $\cdots$ O2 <sup>vi</sup>	0.85	1.95	2.793 (6)	170

Symmetry codes: (iii)  $-x-1, -y, -z+2$ ; (iv)  $-x, -y+1, -z+1$ ; (v)  $-x, -y, -z+2$ ; (vi)  $-x, -y, -z+1$ ; (vii)  $-x, -y+1, -z+2$ ; (viii)  $x, y, z+1$ .



Fig. 2

