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Triaquabis(4-formylbenzoato-κ^2O,O')-cadmium(II) trihydrate

Zhao-Peng Deng, Shan Gao,* Li-Hua Huo and Hui Zhao

School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China
Correspondence e-mail: shangao67@yahoo.com

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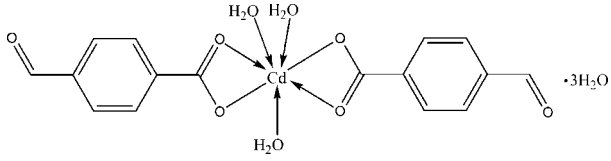
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.022; wR factor = 0.055; data-to-parameter ratio = 15.5.

The title complex, $[Cd(C_8H_5O_3)_2(H_2O)_3]\cdot 3H_2O$, is a neutral mononuclear molecule consisting of a Cd^{II} atom chelated by two 4-formylbenzoate ligands and coordinated by three water molecules in a pentagonal–bipyramidal geometry. A three-dimensional hydrogen-bonded supramolecular network is formed by intermolecular hydrogen bonds.

Related literature

For the 3.5-hydrated cadmium bis(4-formylbenzoate), see Deng *et al.* (2006).



Experimental

Crystal data

$[Cd(C_8H_5O_3)_2(H_2O)_3]\cdot 3H_2O$
M_r = 518.74
Monoclinic, $P2_1/n$
a = 7.4463 (15) Å
b = 8.8000 (18) Å
c = 30.843 (6) Å
β = 90.01 (3)°
V = 2021.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 295 (2) K
0.26 × 0.18 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.756, T_{max} = 0.847
19107 measured reflections
4607 independent reflections
4152 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.055
S = 1.10
4607 reflections
298 parameters
18 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O3*W*	2.2546 (16)	Cd1—O2*W*	2.3603 (16)
Cd1—O5	2.2995 (15)	Cd1—O2	2.4659 (15)
Cd1—O1*W*	2.3290 (15)	Cd1—O4	2.5153 (15)
Cd1—O1	2.3339 (13)		
O3*W*—Cd1—O5	92.34 (7)	O5—Cd1—O2	166.77 (5)
O3*W*—Cd1—O1*W*	175.58 (6)	O1*W*—Cd1—O2	92.84 (6)
O5—Cd1—O1*W*	87.68 (6)	O1—Cd1—O2	54.33 (5)
O3*W*—Cd1—O1	88.77 (7)	O2*W*—Cd1—O2	80.51 (6)
O5—Cd1—O1	138.84 (5)	O3*W*—Cd1—O4	93.31 (6)
O1*W*—Cd1—O1	94.13 (6)	O5—Cd1—O4	53.94 (5)
O3*W*—Cd1—O2*W*	90.13 (6)	O1*W*—Cd1—O4	90.28 (5)
O5—Cd1—O2*W*	86.35 (6)	O1—Cd1—O4	84.91 (5)
O1*W*—Cd1—O2*W*	85.45 (6)	O2*W*—Cd1—O4	140.23 (5)
O1—Cd1—O2*W*	134.81 (6)	O2—Cd1—O4	139.24 (4)
O3*W*—Cd1—O2	86.14 (7)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O4^{i}	0.838 (19)	1.902 (19)	2.739 (2)	176 (2)
O1*W*—H1*W*2···O6*W*	0.843 (9)	1.948 (11)	2.775 (2)	166 (3)
O2*W*—H2*W*1···O2^{ii}	0.850 (10)	2.082 (11)	2.929 (2)	174 (3)
O2*W*—H2*W*2···O1*W*^{iii}	0.846 (10)	2.203 (13)	3.027 (2)	165 (3)
O3*W*—H3*W*1···O6*W*^{iv}	0.84 (3)	1.90 (3)	2.720 (3)	168 (3)
O3*W*—H3*W*2···O1^{v}	0.834 (10)	1.879 (10)	2.711 (2)	176 (3)
O4*W*—H4*W*1···O5*W*^{vi}	0.849 (10)	1.965 (10)	2.812 (3)	175 (4)
O4*W*—H4*W*2···O6^{vii}	0.85 (3)	2.07 (3)	2.919 (3)	174 (3)
O5*W*—H5*W*1···O3^{viii}	0.849 (10)	2.020 (10)	2.866 (3)	174 (3)
O5*W*—H5*W*2···O5	0.847 (10)	2.00 (3)	2.844 (2)	174 (4)
O6*W*—H6*W*1···O2^{iii}	0.852 (10)	1.938 (11)	2.777 (2)	168 (3)
O6*W*—H6*W*2···O4*W*	0.850 (9)	1.946 (13)	2.775 (3)	165 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2342).

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  doi:10.1107/S1600536807052014

supplementary materials

Acta Cryst. (2007). E**63**, m2818 [**doi:10.1107/S1600536807052014**]

Triaquabis(4-formylbenzoato-κ^2O,O')cadmium(II) trihydrate

Z.-P. Deng, S. Gao, L.-H. Huo and H. Zhao

Comment

In our previous work, we have reported the structure of cadmium and 4-FBAH (Deng *et al.*, 2006) which crystallizes as a 3.5-hydrate. We have synthesized a trihydrated compound by a modified reaction of $Cd(Ac)_2$, KSCN and 4-FBAH in aqueous solution. The compound has cadmium in a pentagonal bipyramidal geometry, and a three-dimensional supramolecular network is formed by intermolecular hydrogen bonds.

Experimental

Cadmium(II) diacetate dihydrate (2.66 g, 10 mmol) was added to an aqueous solution of 4-formylbenzoic acid (3.00 g, 20 mmol) and KSCN (0.972 g 10 mmol). Sodium hydroxide (0.1 *M*) was added dropwise until the solution registered a pH of 5. Colorless single crystals separated from the filtered solution after several days. CH&N analysis. Calc. for $C_{16}H_{22}O_{12}Cd$: C 37.05, H 4.27. Found: C 37.01, H 4.24.

Refinement

Carbon-bound H atoms were placed in calculated positions, with C—H = 0.93 and $U_{iso}(H) = 1.2U_{eq}(C)$, and were included in the refinement in the riding model approximation. The H atoms of water molecules were located in difference Fourier maps and refined with the O—H and H···H distance restraints to 0.85 (1) and 1.39 (1) Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

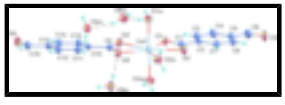


Fig. 1. Molecular structure of the title compound with 30% probability ellipsoid for the non-H atoms. Dashed lines indicate O—H···O hydrogen bonds.

Triaquabis(4-formylbenzoato-κ^2O,O')cadmium(II) trihydrate

Crystal data

$[Cd(C_8H_5O_3)_2(H_2O)_3]\cdot 3H_2O$	F_{000} = 1048
M_r = 518.74	D_x = 1.705 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 16828 reflections
a = 7.4463 (15) Å	θ = 3.1–27.4°
b = 8.8000 (18) Å	μ = 1.14 mm^{-1}
c = 30.843 (6) Å	T = 295 (2) K

β = 90.01 (3)°
V = 2021.1 (7) Å^3
Z = 4

Prism, colourless
0.26 × 0.18 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 10.000 pixels mm^{-1}
T = 295(2) K
ω scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.756, T_{max} = 0.847
19107 measured reflections

4607 independent reflections
4152 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.4°
θ_{min} = 3.1°
h = −9→9
k = −11→11
l = −39→40

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.055
S = 1.10
4607 reflections
298 parameters
18 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
$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 0.9488P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.263224 (17)	0.725332 (16)	0.517000 (4)	0.03039 (5)
O1W	−0.03102 (19)	0.78382 (17)	0.49757 (5)	0.0388 (3)
H1W1	−0.073 (3)	0.705 (2)	0.4862 (7)	0.058*
H1W2	−0.081 (3)	0.802 (3)	0.5216 (5)	0.058*
O2W	0.2803 (2)	0.97992 (18)	0.54073 (6)	0.0499 (4)
H2W1	0.3798 (18)	1.027 (3)	0.5416 (9)	0.075*
H2W2	0.196 (2)	1.040 (3)	0.5338 (9)	0.075*
O3W	0.5507 (2)	0.68768 (19)	0.53728 (7)	0.0564 (4)
H3W1	0.612 (4)	0.755 (2)	0.5493 (10)	0.085*
H3W2	0.592 (4)	0.6008 (14)	0.5416 (10)	0.085*
O4W	−0.2789 (3)	0.8267 (3)	0.65703 (7)	0.0744 (5)

H4W1	−0.3929 (14)	0.830 (5)	0.6563 (12)	0.112*
H4W2	−0.240 (4)	0.888 (4)	0.6762 (10)	0.112*
O5W	0.3438 (3)	0.8194 (2)	0.65344 (6)	0.0657 (5)
H5W1	0.302 (5)	0.787 (4)	0.6774 (5)	0.099*
H5W2	0.285 (4)	0.781 (4)	0.6326 (6)	0.099*
O6W	−0.2097 (3)	0.8899 (2)	0.57049 (6)	0.0552 (4)
H6W1	−0.253 (4)	0.9780 (18)	0.5661 (8)	0.083*
H6W2	−0.210 (4)	0.872 (3)	0.5976 (4)	0.083*
O1	0.32583 (18)	0.59974 (16)	0.45209 (4)	0.0354 (3)
O2	0.3881 (2)	0.84348 (16)	0.45107 (4)	0.0396 (3)
O3	0.7110 (3)	0.7666 (2)	0.23713 (5)	0.0665 (5)
O4	0.1637 (2)	0.46839 (17)	0.54343 (4)	0.0418 (3)
O5	0.1573 (2)	0.66985 (18)	0.58521 (4)	0.0449 (3)
O6	−0.1723 (2)	0.0469 (2)	0.72296 (5)	0.0607 (5)
C1	0.3860 (2)	0.7147 (2)	0.43293 (5)	0.0292 (3)
C2	0.4561 (2)	0.7004 (2)	0.38740 (5)	0.0278 (3)
C3	0.4630 (3)	0.5598 (2)	0.36709 (6)	0.0333 (4)
H3	0.4240	0.4732	0.3816	0.040*
C4	0.5283 (3)	0.5489 (2)	0.32510 (6)	0.0373 (4)
H4	0.5334	0.4547	0.3115	0.045*
C5	0.5860 (2)	0.6777 (2)	0.30336 (6)	0.0336 (4)
C6	0.5786 (3)	0.8186 (2)	0.32360 (6)	0.0367 (4)
H6	0.6163	0.9052	0.3089	0.044*
C7	0.5153 (3)	0.8297 (2)	0.36550 (6)	0.0347 (4)
H7	0.5120	0.9238	0.3792	0.042*
C8	0.6590 (3)	0.6623 (3)	0.25904 (6)	0.0446 (5)
H8	0.6653	0.5651	0.2473	0.053*
C9	0.1296 (2)	0.5302 (2)	0.57915 (6)	0.0330 (4)
C10	0.0552 (2)	0.4376 (2)	0.61615 (5)	0.0306 (4)
C11	−0.0033 (3)	0.5105 (2)	0.65354 (6)	0.0384 (4)
H11	0.0016	0.6159	0.6554	0.046*
C12	−0.0688 (3)	0.4261 (3)	0.68795 (6)	0.0408 (4)
H12	−0.1073	0.4749	0.7130	0.049*
C13	−0.0772 (3)	0.2695 (2)	0.68519 (6)	0.0364 (4)
C14	−0.0189 (3)	0.1959 (2)	0.64772 (6)	0.0381 (4)
H14	−0.0243	0.0906	0.6458	0.046*
C15	0.0469 (3)	0.2805 (2)	0.61348 (6)	0.0358 (4)
H15	0.0859	0.2316	0.5885	0.043*
C16	−0.1499 (3)	0.1825 (3)	0.72217 (7)	0.0475 (5)
H16	−0.1811	0.2368	0.7469	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03483 (8)	0.03249 (8)	0.02384 (7)	0.00035 (5)	0.00560 (5)	0.00137 (5)
O1W	0.0394 (7)	0.0410 (8)	0.0359 (7)	−0.0008 (6)	0.0019 (6)	−0.0026 (6)
O2W	0.0543 (9)	0.0393 (9)	0.0561 (9)	0.0009 (7)	−0.0032 (8)	−0.0114 (7)
O3W	0.0466 (9)	0.0358 (9)	0.0867 (13)	0.0053 (7)	−0.0167 (9)	−0.0019 (9)

O4W	0.0944 (15)	0.0565 (12)	0.0721 (13)	0.0091 (11)	0.0054 (12)	−0.0022 (10)
O5W	0.0982 (15)	0.0554 (11)	0.0436 (9)	−0.0277 (10)	0.0078 (10)	−0.0036 (8)
O6W	0.0691 (10)	0.0429 (9)	0.0538 (9)	0.0151 (8)	−0.0035 (9)	−0.0092 (8)
O1	0.0432 (7)	0.0343 (7)	0.0287 (6)	−0.0009 (6)	0.0101 (5)	0.0035 (5)
O2	0.0582 (8)	0.0304 (7)	0.0301 (6)	0.0026 (6)	0.0105 (6)	−0.0026 (5)
O3	0.0960 (14)	0.0697 (12)	0.0339 (8)	−0.0040 (10)	0.0233 (9)	0.0072 (8)
O4	0.0528 (8)	0.0460 (8)	0.0264 (6)	−0.0096 (7)	0.0108 (6)	−0.0003 (6)
O5	0.0649 (9)	0.0385 (8)	0.0314 (7)	−0.0077 (7)	0.0072 (7)	0.0036 (6)
O6	0.0742 (11)	0.0645 (12)	0.0435 (9)	−0.0132 (9)	0.0052 (8)	0.0197 (8)
C1	0.0314 (8)	0.0321 (9)	0.0243 (8)	0.0039 (7)	0.0034 (7)	0.0012 (7)
C2	0.0281 (8)	0.0310 (10)	0.0243 (8)	0.0028 (7)	0.0018 (6)	0.0016 (6)
C3	0.0419 (10)	0.0291 (9)	0.0289 (8)	−0.0018 (8)	0.0050 (7)	0.0007 (7)
C4	0.0477 (11)	0.0336 (10)	0.0304 (9)	0.0022 (8)	0.0057 (8)	−0.0051 (7)
C5	0.0346 (9)	0.0418 (10)	0.0246 (8)	0.0027 (8)	0.0040 (7)	0.0006 (7)
C6	0.0458 (10)	0.0346 (10)	0.0298 (9)	−0.0024 (8)	0.0080 (8)	0.0059 (7)
C7	0.0450 (10)	0.0284 (9)	0.0307 (9)	0.0005 (8)	0.0064 (8)	−0.0002 (7)
C8	0.0493 (11)	0.0558 (13)	0.0286 (9)	0.0017 (10)	0.0070 (8)	−0.0047 (9)
C9	0.0309 (8)	0.0404 (11)	0.0276 (8)	−0.0026 (7)	0.0014 (7)	0.0055 (7)
C10	0.0276 (8)	0.0400 (10)	0.0242 (8)	−0.0013 (7)	0.0020 (7)	0.0037 (7)
C11	0.0414 (10)	0.0388 (11)	0.0350 (9)	0.0000 (8)	0.0089 (8)	−0.0007 (8)
C12	0.0425 (10)	0.0508 (13)	0.0290 (9)	0.0010 (9)	0.0096 (8)	−0.0021 (8)
C13	0.0314 (9)	0.0510 (12)	0.0269 (9)	−0.0014 (8)	0.0028 (7)	0.0068 (8)
C14	0.0454 (11)	0.0373 (11)	0.0317 (9)	−0.0031 (8)	0.0037 (8)	0.0049 (8)
C15	0.0419 (10)	0.0397 (10)	0.0258 (8)	−0.0012 (8)	0.0064 (8)	0.0011 (7)
C16	0.0470 (12)	0.0648 (16)	0.0307 (10)	−0.0043 (11)	0.0060 (9)	0.0115 (10)

Geometric parameters (Å, °)

Cd1—O3W	2.2546 (16)	C1—C2	1.503 (2)
Cd1—O5	2.2995 (15)	C2—C3	1.388 (3)
Cd1—O1W	2.3290 (15)	C2—C7	1.394 (3)
Cd1—O1	2.3339 (13)	C3—C4	1.387 (2)
Cd1—O2W	2.3603 (16)	C3—H3	0.9300
Cd1—O2	2.4659 (15)	C4—C5	1.386 (3)
Cd1—O4	2.5153 (15)	C4—H4	0.9300
Cd1—C1	2.7514 (18)	C5—C6	1.389 (3)
Cd1—C9	2.7591 (19)	C5—C8	1.477 (3)
O1W—H1W1	0.838 (19)	C6—C7	1.379 (3)
O1W—H1W2	0.843 (9)	C6—H6	0.9300
O2W—H2W1	0.850 (10)	C7—H7	0.9300
O2W—H2W2	0.846 (10)	C8—H8	0.9300
O3W—H3W1	0.84 (3)	C9—C10	1.508 (2)
O3W—H3W2	0.834 (10)	C10—C15	1.386 (3)
O4W—H4W1	0.849 (10)	C10—C11	1.390 (3)
O4W—H4W2	0.85 (3)	C11—C12	1.384 (3)
O5W—H5W1	0.849 (10)	C11—H11	0.9300
O5W—H5W2	0.847 (10)	C12—C13	1.382 (3)
O6W—H6W1	0.852 (10)	C12—H12	0.9300
O6W—H6W2	0.850 (9)	C13—C14	1.394 (3)

O1—C1	1.255 (2)	C13—C16	1.477 (3)
O2—C1	1.264 (2)	C14—C15	1.382 (3)
O3—C8	1.204 (3)	C14—H14	0.9300
O4—C9	1.255 (2)	C15—H15	0.9300
O5—C9	1.260 (3)	C16—H16	0.9300
O6—C16	1.205 (3)		
O3W—Cd1—O5	92.34 (7)	O1—C1—C2	119.79 (16)
O3W—Cd1—O1W	175.58 (6)	O2—C1—C2	118.97 (16)
O5—Cd1—O1W	87.68 (6)	O1—C1—Cd1	57.62 (9)
O3W—Cd1—O1	88.77 (7)	O2—C1—Cd1	63.65 (9)
O5—Cd1—O1	138.84 (5)	C2—C1—Cd1	177.00 (13)
O1W—Cd1—O1	94.13 (6)	C3—C2—C7	119.79 (16)
O3W—Cd1—O2W	90.13 (6)	C3—C2—C1	120.59 (16)
O5—Cd1—O2W	86.35 (6)	C7—C2—C1	119.62 (16)
O1W—Cd1—O2W	85.45 (6)	C4—C3—C2	119.76 (18)
O1—Cd1—O2W	134.81 (6)	C4—C3—H3	120.1
O3W—Cd1—O2	86.14 (7)	C2—C3—H3	120.1
O5—Cd1—O2	166.77 (5)	C5—C4—C3	120.25 (18)
O1W—Cd1—O2	92.84 (6)	C5—C4—H4	119.9
O1—Cd1—O2	54.33 (5)	C3—C4—H4	119.9
O2W—Cd1—O2	80.51 (6)	C4—C5—C6	120.03 (17)
O3W—Cd1—O4	93.31 (6)	C4—C5—C8	119.09 (19)
O5—Cd1—O4	53.94 (5)	C6—C5—C8	120.86 (19)
O1W—Cd1—O4	90.28 (5)	C7—C6—C5	119.89 (18)
O1—Cd1—O4	84.91 (5)	C7—C6—H6	120.1
O2W—Cd1—O4	140.23 (5)	C5—C6—H6	120.1
O2—Cd1—O4	139.24 (4)	C6—C7—C2	120.27 (18)
O3W—Cd1—C1	86.60 (7)	C6—C7—H7	119.9
O5—Cd1—C1	165.75 (6)	C2—C7—H7	119.9
O1W—Cd1—C1	94.47 (6)	O3—C8—C5	124.6 (2)
O1—Cd1—C1	27.00 (5)	O3—C8—H8	117.7
O2W—Cd1—C1	107.86 (6)	C5—C8—H8	117.7
O2—Cd1—C1	27.35 (5)	O4—C9—O5	121.35 (17)
O4—Cd1—C1	111.89 (5)	O4—C9—C10	120.29 (18)
O3W—Cd1—C9	93.34 (7)	O5—C9—C10	118.36 (17)
O5—Cd1—C9	26.93 (6)	O4—C9—Cd1	65.60 (10)
O1W—Cd1—C9	88.67 (6)	O5—C9—Cd1	55.75 (10)
O1—Cd1—C9	111.92 (6)	C10—C9—Cd1	174.11 (14)
O2W—Cd1—C9	113.24 (6)	C15—C10—C11	119.71 (17)
O2—Cd1—C9	166.24 (5)	C15—C10—C9	120.70 (17)
O4—Cd1—C9	27.02 (5)	C11—C10—C9	119.58 (18)
C1—Cd1—C9	138.90 (6)	C12—C11—C10	119.9 (2)
Cd1—O1W—H1W1	105.9 (19)	C12—C11—H11	120.0
Cd1—O1W—H1W2	103.2 (18)	C10—C11—H11	120.0
H1W1—O1W—H1W2	111.3 (15)	C13—C12—C11	120.25 (19)
Cd1—O2W—H2W1	121.4 (19)	C13—C12—H12	119.9
Cd1—O2W—H2W2	118.3 (19)	C11—C12—H12	119.9
H2W1—O2W—H2W2	110.3 (16)	C12—C13—C14	119.98 (18)
Cd1—O3W—H3W1	122 (2)	C12—C13—C16	119.09 (19)

Cd1—O3W—H3W2	122 (2)	C14—C13—C16	120.9 (2)
H3W1—O3W—H3W2	112.6 (16)	C15—C14—C13	119.62 (19)
H4W1—O4W—H4W2	109.6 (16)	C15—C14—H14	120.2
H5W1—O5W—H5W2	109.9 (17)	C13—C14—H14	120.2
H6W1—O6W—H6W2	108.9 (15)	C14—C15—C10	120.50 (18)
C1—O1—Cd1	95.38 (11)	C14—C15—H15	119.8
C1—O2—Cd1	89.00 (11)	C10—C15—H15	119.8
C9—O4—Cd1	87.38 (12)	O6—C16—C13	125.4 (2)
C9—O5—Cd1	97.32 (12)	O6—C16—H16	117.3
O1—C1—O2	121.24 (16)	C13—C16—H16	117.3
O3W—Cd1—O1—C1	−84.92 (12)	O1—C1—C2—C7	177.06 (17)
O5—Cd1—O1—C1	−177.07 (10)	O2—C1—C2—C7	−2.5 (3)
O1W—Cd1—O1—C1	91.74 (11)	C7—C2—C3—C4	−0.2 (3)
O2W—Cd1—O1—C1	4.05 (14)	C1—C2—C3—C4	−179.92 (16)
O2—Cd1—O1—C1	1.21 (10)	C2—C3—C4—C5	−0.2 (3)
O4—Cd1—O1—C1	−178.35 (11)	C3—C4—C5—C6	0.0 (3)
C9—Cd1—O1—C1	−178.03 (10)	C3—C4—C5—C8	178.53 (18)
O3W—Cd1—O2—C1	90.06 (11)	C4—C5—C6—C7	0.6 (3)
O5—Cd1—O2—C1	173.8 (2)	C8—C5—C6—C7	−177.93 (18)
O1W—Cd1—O2—C1	−94.25 (11)	C5—C6—C7—C2	−1.0 (3)
O1—Cd1—O2—C1	−1.20 (10)	C3—C2—C7—C6	0.7 (3)
O2W—Cd1—O2—C1	−179.15 (12)	C1—C2—C7—C6	−179.50 (17)
O4—Cd1—O2—C1	−0.52 (14)	C4—C5—C8—O3	179.2 (2)
C9—Cd1—O2—C1	1.8 (3)	C6—C5—C8—O3	−2.3 (3)
O3W—Cd1—O4—C9	90.88 (12)	Cd1—O4—C9—O5	−0.67 (18)
O5—Cd1—O4—C9	0.39 (11)	Cd1—O4—C9—C10	179.81 (15)
O1W—Cd1—O4—C9	−86.53 (11)	Cd1—O5—C9—O4	0.7 (2)
O1—Cd1—O4—C9	179.34 (11)	Cd1—O5—C9—C10	−179.73 (13)
O2W—Cd1—O4—C9	−3.32 (15)	O3W—Cd1—C9—O4	−90.72 (12)
O2—Cd1—O4—C9	178.80 (10)	O5—Cd1—C9—O4	−179.31 (19)
C1—Cd1—O4—C9	178.54 (11)	O1W—Cd1—C9—O4	93.21 (11)
O3W—Cd1—O5—C9	−92.78 (13)	O1—Cd1—C9—O4	−0.70 (12)
O1W—Cd1—O5—C9	91.65 (12)	O2W—Cd1—C9—O4	177.69 (10)
O1—Cd1—O5—C9	−1.97 (16)	O2—Cd1—C9—O4	−3.3 (3)
O2W—Cd1—O5—C9	177.24 (13)	C1—Cd1—C9—O4	−2.07 (15)
O2—Cd1—O5—C9	−175.85 (19)	O3W—Cd1—C9—O5	88.59 (13)
O4—Cd1—O5—C9	−0.39 (11)	O1W—Cd1—C9—O5	−87.48 (13)
C1—Cd1—O5—C9	−7.4 (3)	O1—Cd1—C9—O5	178.61 (11)
Cd1—O1—C1—O2	−2.24 (19)	O2W—Cd1—C9—O5	−3.00 (14)
Cd1—O1—C1—C2	178.23 (14)	O2—Cd1—C9—O5	176.00 (18)
Cd1—O2—C1—O1	2.12 (18)	O4—Cd1—C9—O5	179.31 (19)
Cd1—O2—C1—C2	−178.35 (14)	C1—Cd1—C9—O5	177.24 (11)
O3W—Cd1—C1—O1	93.97 (11)	O4—C9—C10—C15	9.1 (3)
O5—Cd1—C1—O1	7.9 (3)	O5—C9—C10—C15	−170.46 (18)
O1W—Cd1—C1—O1	−90.33 (11)	O4—C9—C10—C11	−171.85 (17)
O2W—Cd1—C1—O1	−176.98 (10)	O5—C9—C10—C11	8.6 (3)
O2—Cd1—C1—O1	−177.86 (18)	C15—C10—C11—C12	0.2 (3)
O4—Cd1—C1—O1	1.77 (12)	C9—C10—C11—C12	−178.86 (17)
C9—Cd1—C1—O1	2.78 (15)	C10—C11—C12—C13	−0.3 (3)

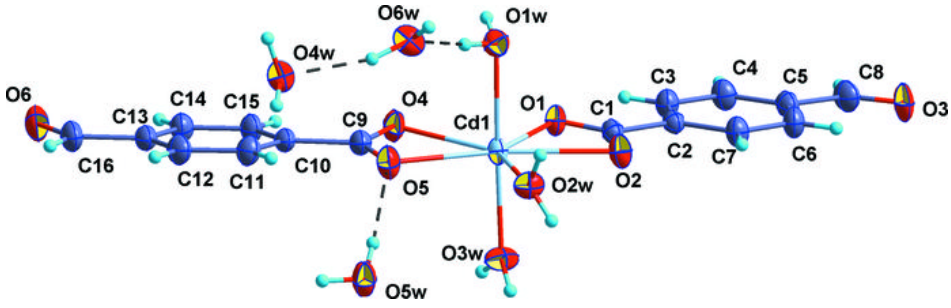
O3W—Cd1—C1—O2	−88.17 (11)	C11—C12—C13—C14	0.3 (3)
O5—Cd1—C1—O2	−174.28 (19)	C11—C12—C13—C16	−179.21 (19)
O1W—Cd1—C1—O2	87.53 (11)	C12—C13—C14—C15	−0.1 (3)
O1—Cd1—C1—O2	177.86 (18)	C16—C13—C14—C15	179.38 (18)
O2W—Cd1—C1—O2	0.88 (12)	C13—C14—C15—C10	0.0 (3)
O4—Cd1—C1—O2	179.63 (10)	C11—C10—C15—C14	−0.1 (3)
C9—Cd1—C1—O2	−179.36 (10)	C9—C10—C15—C14	179.02 (17)
O1—C1—C2—C3	−3.2 (3)	C12—C13—C16—O6	176.2 (2)
O2—C1—C2—C3	177.28 (17)	C14—C13—C16—O6	−3.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O4^{i}	0.838 (19)	1.902 (19)	2.739 (2)	176 (2)
O1W—H1W2···O6W	0.843 (9)	1.948 (11)	2.775 (2)	166 (3)
O2W—H2W1···O2^{ii}	0.850 (10)	2.082 (11)	2.929 (2)	174 (3)
O2W—H2W2···O1W^{iii}	0.846 (10)	2.203 (13)	3.027 (2)	165 (3)
O3W—H3W1···O6W^{iv}	0.84 (3)	1.90 (3)	2.720 (3)	168 (3)
O3W—H3W2···O1^{v}	0.834 (10)	1.879 (10)	2.711 (2)	176 (3)
O4W—H4W1···O5W^{vi}	0.849 (10)	1.965 (10)	2.812 (3)	175 (4)
O4W—H4W2···O6^{vii}	0.85 (3)	2.07 (3)	2.919 (3)	174 (3)
O5W—H5W1···O3^{viii}	0.849 (10)	2.020 (10)	2.866 (3)	174 (3)
O5W—H5W2···O5	0.847 (10)	2.00 (3)	2.844 (2)	174 (4)
O6W—H6W1···O2^{iii}	0.852 (10)	1.938 (11)	2.777 (2)	168 (3)
O6W—H6W2···O4W	0.850 (9)	1.946 (13)	2.775 (3)	165 (3)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+2, −*z*+1; (iii) −*x*, −*y*+2, −*z*+1; (iv) *x*+1, *y*, *z*; (v) −*x*+1, −*y*+1, −*z*+1; (vi) *x*−1, *y*, *z*; (vii) *x*, *y*+1, *z*; (viii) *x*−1/2, −*y*+3/2, *z*+1/2.

Fig. 1


O6w
O1w
O4w
O6
C14
C15
C13
C9
O4
Cd1
O1
C1
C3
C4
C5
C8
O3
C16
C12
C11
C10
O5
O2w
O2
C2
C7
C6
O3w
O5w