Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[pentaaqua[μ_4-(5-carboxylato-*m*-phenylenedioxy)diacetato]cadmium(II)-sodium(I)] tetrahydrate]

Yi-Hang Wen[a] and Seik Weng Ng[b]*

[a]Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua, Zhejiang 321004, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

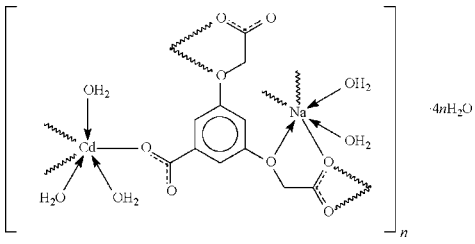
Received 8 August 2007; accepted 8 August 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.101; data-to-parameter ratio = 14.2.

In the crystal structure of the title compound, [CdNa($C_{11}H_7O_8$)(H_2O)$_5$]·4H_2O, the carboxylate trianion binds to a triaquacadmium unit through one O atom of its 5-carboxylate group. It also chelates through two O atoms of the 5-oxyacetate group to an adjacent triaquacadmium unit to form a linear chain. The diaquasodium unit is chelated by the 1-oxyacetate [–O–CH_2–C(O)O–] group of one trianion and by the 3-oxyacetate group of another trianion. Both cadmium and sodium have six-coordinate octahedral geometries in a ribbon structure. The ribbons are linked into a three-dimensional network by hydrogen bonds.

Related literature

For the crystal structures of metal derivatives of 3-carboxyphenoxyacetic acids, see Gao & Ng (2006); Gao, Huo, Deng *et al.* (2005); Zhao, Huo, Gao *et al.* (2005); Li *et al.* (2004); Zhao, Gu, Gao *et al.* (2005); Gao, Gu, Huo *et al.* (2004*a*); Gao, Gu, Huo *et al.* (2004*b*); Gao, Gu, Zhao *et al.* (2004); Gao, Huo, Cheng *et al.* (2005); Gu *et al.* (2005); Gao, Huo, Liu *et al.* (2005); Zhao, Gu, Huo *et al.* (2005). For the sole reference to 5-carboxy-1,3-diphenoxyacetic acid, see the patent for antibacterial properties by Leslie *et al.* (2004).



Experimental

Crystal data

[CdNa($C_{11}H_7O_8$)(H_2O)$_5$]·4H_2O
M_r = 564.70
Triclinic, $P\overline{1}$
a = 7.2853 (2) Å
b = 11.1525 (3) Å
c = 14.0096 (3) Å
α = 70.123 (1)°
β = 78.582 (1)°
γ = 75.987 (1)°
V = 1030.23 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.16 mm^{-1}
T = 295 (2) K
0.18 × 0.08 × 0.05 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.832, T_{max} = 0.944
12790 measured reflections
4627 independent reflections
3861 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.101
S = 1.03
4627 reflections
325 parameters
32 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*w*—H1*w*1···O6*w*	0.84 (1)	1.83 (2)	2.651 (4)	165 (5)
O1*w*—H1*w*2···O7*w*	0.85 (1)	1.92 (1)	2.750 (4)	165 (4)
O2*w*—H2*w*1···O5^{i}	0.85 (1)	1.92 (1)	2.748 (4)	168 (2)
O2*w*—H2*w*2···O2^{ii}	0.85 (1)	1.93 (1)	2.780 (3)	178 (5)
O3*w*—H3*w*1···O7*w*^{iii}	0.85 (1)	1.91 (1)	2.759 (4)	171 (3)
O3*w*—H3*w*2···O5^{iv}	0.85 (1)	1.89 (1)	2.736 (4)	173 (3)
O4*w*—H4*w*1···O8*w*^{v}	0.86 (1)	2.04 (3)	2.796 (6)	147 (4)
O4*w*—H4*w*2···O9*w*^{iii}	0.86 (1)	1.96 (2)	2.790 (7)	164 (6)
O5*w*—H5*w*1···O8*w*^{vi}	0.86 (1)	2.09 (5)	2.805 (8)	140 (7)
O5*w*—H5*w*2···O9*w*	0.86 (1)	2.35 (9)	2.798 (9)	113 (8)
O6*w*—H6*w*1···O3^{ii}	0.85 (1)	1.96 (2)	2.790 (4)	165 (4)
O6*w*—H6*w*2···O6^{vii}	0.85 (1)	1.90 (2)	2.730 (4)	165 (4)
O7*w*—H7*w*1···O2^{ii}	0.85 (1)	2.09 (2)	2.859 (4)	152 (4)
O7*w*—H7*w*2···O5^{viii}	0.85 (1)	1.99 (2)	2.780 (3)	154 (4)
O8*w*—H8*w*1···O3*w*^{ix}	0.85 (1)	2.04 (3)	2.874 (5)	165 (8)
O8*w*—H8*w*2···O1*w*	0.85 (1)	2.13 (4)	2.929 (6)	155 (8)
O9*w*—H9*w*1···O4*w*^{ix}	0.86 (1)	2.02 (4)	2.790 (7)	150 (7)
O9*w*—H9*w*2···O1^{v}	0.85 (1)	1.96 (2)	2.794 (4)	166 (7)

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2007).

The authors thank the Foundation of the Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces (grant No. 0506) and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2469).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.

Bruker (2006). *APEX2* (Version 1.2A) and *SAINT* (Version 7.23A). Bruker AXS Inc., Madison, Wisconsin, USA.

Dolomanov, O. V., Blake, A. J., Champness, N. R. & Schröder, M. (2003). *J. Appl. Cryst.* **36**, 1283–1284.

Gao, S., Gu, C.-S., Huo, L.-H., Liu, J.-W. & Zhao, J.-G. (2004*a*). *Acta Cryst.* E**60**, m1933–m1935.

Gao, S., Gu, C.-S., Huo, L.-H., Liu, J.-W. & Zhao, J.-G. (2004*b*). *Acta Cryst.* E**60**, m1936–m1938.

Gao, S., Gu, C.-S., Zhao, H., Huo, L.-H. & Zhao, J.-G. (2004). *Chin. J. Inorg. Chem.* **20**, 1437–1440.

Gao, S., Huo, L.-H., Cheng, X.-L., Zhao, H. & Zhao, J.-G. (2005). *Chin. J. Struct. Chem.* **24**, 499–502.

Gao, S., Huo, L.-H., Deng, Z.-P. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m685–m687.

Gao, S., Huo, L.-H., Liu, J.-W. & Gu, C.-S. (2005). *Acta Cryst.* E**61**, m494–m495.

Gao, S. & Ng, S. W. (2006). *Acta Cryst.* E**62**, m267–m268.

Gu, C.-S., Gao, S., Zhao, H., Huo, L.-H. & Zhao, J.-G. (2005). *Heilongjiang Daxue Ziran Kexue Xuebao*, **22**, 38–41.

Leslie, B. W., Lawson, C., Zhao, L.-H., Thomson, S., Davies, R. & Allanson, N. M. (2004). Br. Patent GB 2002-15 773 2002 0708.

Li, S.-J., Gu, C.-S., Gao, S., Zhao, H., Zhao, J.-G. & Huo, L.-H. (2004). *Chin. J. Struct. Chem.* **23**, 835–838.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Westrip, S. P. (2007). *publCIF*. In preparation.

Zhao, H., Huo, L.-H., Gao, S. & Zhao, J.-G. (2005). *Acta Cryst.* E**61**, m2686–m2688.

Zhao, J.-G., Gu, C.-S., Gao, S., Huo, L.-H. & Liu, J.-W. (2005). *Acta Cryst.* E**61**, m33–m35.

Zhao, J.-G., Gu, C.-S., Huo, L.-H., Liu, J.-W. & Gao, S. (2005). *Acta Cryst.* E**61**, m76–m78.

supplementary materials

Acta Cryst. (2007). E**63**, m2321-m2322 [**doi:10.1107/S1600536807039220**]

Poly[[pentaaqua[μ_4-(5-carboxylato-*m*-phenylenedioxy)diacetato]cadmium(II)sodium(I)] tetrahydrate]

Y.-H. Wen and S. W. Ng

Comment

There is a number of metal derivatives of 3-carboxyphenoxyacetic acid, a carboxylic acid whose deprotonated dianion is regarded as a flexible dianion. The phenoxy linkage in the dianion is also capable of bonding, and this feature is noted in some of the calcium (Gao & Ng, 2006), cadmium (Gao, Huo, Deng & Ng, 2005; Zhao, Gu, Gao, Huo & Liu, 2005), cobalt (Li *et al.*, 2004; Zhao, Gu, Huo *et al.*, 2005), copper (Gao, Gu, Huo *et al.*, 2004*a*, Gao, Gu, Huo *et al.*, 2004*b*; Gao, Gu, Zhao *et al.*, 2004), manganese (Gao, Huo, Cheng *et al.*, 2005), nickel (Gu *et al.*, 2005) and zinc (Gao, Huo, Liu *et al.*, 2005; Zhao, Gu, Huo *et al.*, 2005) derivatives. There is a similar number of divalent metal derivatives of the "two-armed" (and much more flexible) acid, benzene-1,3-dioxyacetic acid in the crystallographic literature (CSD Version 5.28, May 2007). Curiously, there is almost no crystallographic mention of the related tricarboxylic acid, 5-carboxy-1,3-diphenoxyacetic acid, the sole mention possibly being a patent claim for antibaterial properties (Leslie *et al.*, 2004) only.

In the crystal structure of pentaaqua(5-carboxy-1,3-phenoxydiacetato)cadmiumsodium tetrahydrate, the carboxylate trianion binds to a triaquacadmium unit through one oxygen atom of its 5-carboxyl group. It also chelates through two oxygen atoms of the 5-oxyacetate group to an adjacent triaquacadmium unit to form a linear chain. Meanwhile, the diaquasodium unit is chelated by the 1-oxyacetate [–O–CH2–C(O)O–] group of one trianion and as well as by the 3-oxyacetate group of another trianion. Both cadmium and sodium sites exist six-coordinate octahedral geometries in the ribbon structure. The ribbons are linked into a three-dimensional network by extensive hydrogen bonds.

The lattice water molecules occupy the space within the ribbon; however, their contribution to the total volume is small as their exclusion is not seen in any significant voids in the unit cell.

Experimental

Sodium hydroxide was added to an aqueous soluiton consisting of 3 molar equivalents of chloroacetic acid and one equivalent of 3,5-dihydroxybenzoic acid until the solution was basic (pH approximately 11). The solution was heated for 3 h. The cool solution was neutralized with concentrated hydrochloric acid to a pH of about 3. The light-yellow solid that was precipitated was collected and dried.

5-Carboxy-1,3-diphenoxyacetic acid (0.282 g, 1 mol) and cadmium acetate dihydrate (0.266 g, 1 mol) were mixed in 20 ml e thanol-water (1:1, *v*/*v*) solution. The pH value was adjusted to 7 by sodium carbonate solution. The filtered solution was set aside for the growth of crystals after a week.

Refinement

The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.85±0.01 Å and H.·H 1.39 + 00.01 Å); their displacement parameters were freely refined. The carbon-bound H-atoms were generated

geometrically (C–H 0.93 to 0.97 Å); they were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).

Figures

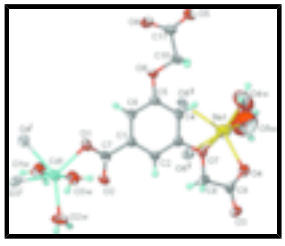


Fig. 1. Thermal ellipsoid plot depicting the coordination geometries of cadmium and sodium; displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radius. The lattice water molecules are not shown. [Translational/symmery code (i) 1 + x, y − 1, z; (ii) 1 − x, 1 − y, 2 − z.]

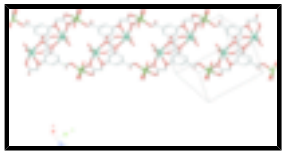


Fig. 2. *OLEX* (Dolomanov *et al.*, 2003) depiction of the ribbon motif, shown projected against the unit cell. The lattice water molecules are not shown.

Poly[[pentaaqua[μ4-(5-carboxylato-*m*-\ phenylenedioxy)diacetato]cadmium(II)sodium(I)] tetrahydrate]

Crystal data

$[CdNa(C_{11}H_7O_8)(H_2O)_5]\cdot 4H_2O$	$Z = 2$
$M_r = 564.70$	$F_{000} = 572$
Triclinic, $P\overline{1}$	$D_x = 1.820$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 7.2853$ (2) Å	Cell parameters from 3652 reflections
$b = 11.1525$ (3) Å	θ = 2.7–26.2º
$c = 14.0096$ (3) Å	μ = 1.16 mm^{-1}
α = 70.123 (1)º	$T = 295$ (2) K
β = 78.582 (1)º	Block, colourless
γ = 75.987 (1)º	0.18 × 0.08 × 0.05 mm
$V = 1030.23$ (5) Å^3	

Data collection

Bruker APEXII area-detector diffractometer	4627 independent reflections
Radiation source: fine-focus sealed tube	3861 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 295$(2) K	$\theta_{max} = 27.4$º
φ and ω scans	$\theta_{min} = 1.6$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9\rightarrow 9$
$T_{min} = 0.832$, $T_{max} = 0.944$	$k = -14\rightarrow 14$
12790 measured reflections	$l = -18\rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.3078P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
4627 reflections	$\Delta\rho_{max} = 0.76$ e Å^{-3}
325 parameters	$\Delta\rho_{min} = -0.55$ e Å^{-3}
32 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	1.28299 (4)	0.23883 (2)	0.62583 (2)	0.0322 (1)
Na1	0.2853 (3)	0.8385 (2)	0.8649 (1)	0.0524 (4)
O1	1.1165 (4)	0.2998 (2)	0.75921 (18)	0.0397 (6)
O2	0.9974 (4)	0.4538 (2)	0.62858 (16)	0.0334 (5)
O3	0.5501 (4)	1.0908 (2)	0.58968 (18)	0.0408 (6)
O4	0.3957 (4)	1.0247 (2)	0.74276 (19)	0.0385 (6)
O5	0.6126 (4)	0.4270 (2)	1.31888 (17)	0.0352 (5)
O6	0.7003 (5)	0.2613 (2)	1.25572 (19)	0.0490 (7)
O7	0.6542 (4)	0.8090 (2)	0.79807 (17)	0.0355 (6)
O8	0.7473 (4)	0.4093 (2)	1.06632 (16)	0.0320 (5)
O1w	1.0518 (4)	0.1510 (3)	0.6042 (2)	0.0460 (7)
O2w	1.3042 (4)	0.3643 (3)	0.46121 (18)	0.0437 (7)
O3w	1.5094 (4)	0.3321 (2)	0.6562 (2)	0.0400 (6)
O4w	0.3611 (7)	0.8572 (5)	1.0106 (3)	0.0911 (13)
O5w	−0.0312 (9)	0.8991 (6)	0.8870 (6)	0.136 (2)
O6w	1.1643 (4)	−0.0793 (3)	0.5740 (2)	0.0481 (7)
O7w	0.7948 (4)	0.3467 (3)	0.49288 (19)	0.0388 (6)
O8w	0.7747 (7)	0.1473 (6)	0.7873 (3)	0.1127 (17)
O9w	−0.2894 (7)	0.8524 (4)	1.0663 (3)	0.0920 (13)
C1	0.9022 (4)	0.4805 (3)	0.7950 (2)	0.0244 (6)
C2	0.8351 (5)	0.6139 (3)	0.7571 (2)	0.0248 (6)
C3	0.7358 (5)	0.6791 (3)	0.8258 (2)	0.0256 (7)
C4	0.7065 (5)	0.6153 (3)	0.9298 (2)	0.0263 (7)
C5	0.7738 (5)	0.4826 (3)	0.9658 (2)	0.0243 (6)
C6	0.8721 (5)	0.4156 (3)	0.8980 (2)	0.0256 (6)
C7	1.0108 (5)	0.4069 (3)	0.7223 (2)	0.0268 (7)
C8	0.6719 (5)	0.8809 (3)	0.6921 (3)	0.0330 (8)
C9	0.5281 (5)	1.0077 (3)	0.6758 (2)	0.0288 (7)

C10	0.6691 (5)	0.4765 (3)	1.1399 (2)	0.0263 (7)
C11	0.6619 (5)	0.3788 (3)	1.2460 (2)	0.0291 (7)
H1w1	1.101 (5)	0.085 (3)	0.586 (3)	0.069*
H1w2	0.985 (5)	0.207 (2)	0.561 (3)	0.069*
H2w1	1.4081 (18)	0.379 (4)	0.4243 (19)	0.066*
H2w2	1.212 (2)	0.421 (3)	0.4350 (19)	0.066*
H3w1	1.604 (4)	0.340 (3)	0.609 (2)	0.060*
H3w2	1.463 (4)	0.405 (2)	0.666 (3)	0.060*
H4w1	0.291 (5)	0.838 (8)	1.0682 (15)	0.137*
H4w2	0.477 (2)	0.844 (8)	1.022 (3)	0.137*
H5w1	−0.045 (12)	0.966 (6)	0.834 (4)	0.204*
H5w2	−0.043 (12)	0.926 (9)	0.939 (4)	0.204*
H6w1	1.238 (5)	−0.070 (5)	0.5176 (17)	0.072*
H6w2	1.226 (5)	−0.132 (4)	0.622 (2)	0.072*
H7w1	0.841 (6)	0.415 (3)	0.475 (3)	0.058*
H7w2	0.743 (6)	0.345 (4)	0.444 (2)	0.058*
H8w1	0.680 (7)	0.195 (8)	0.757 (5)	0.169*
H8w2	0.877 (6)	0.151 (9)	0.746 (5)	0.169*
H9w1	−0.410 (2)	0.862 (8)	1.070 (5)	0.138*
H9w2	−0.256 (10)	0.807 (7)	1.125 (3)	0.138*
H2	0.8565	0.6580	0.6876	0.030*
H4	0.6423	0.6610	0.9750	0.032*
H6	0.9175	0.3267	0.9222	0.031*
H8a	0.6486	0.8309	0.6525	0.040*
H8b	0.8001	0.8986	0.6695	0.040*
H10a	0.5416	0.5242	1.1268	0.032*
H10b	0.7474	0.5379	1.1348	0.032*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03883 (16)	0.02743 (14)	0.02517 (14)	0.00241 (10)	−0.00134 (10)	−0.00911 (10)
Na1	0.0671 (11)	0.0479 (9)	0.0390 (8)	−0.0109 (8)	0.0015 (8)	−0.0138 (7)
O1	0.0479 (15)	0.0292 (12)	0.0302 (12)	0.0144 (11)	0.0000 (11)	−0.0119 (10)
O2	0.0450 (14)	0.0313 (12)	0.0192 (11)	−0.0005 (10)	0.0011 (10)	−0.0095 (9)
O3	0.0540 (16)	0.0247 (12)	0.0284 (12)	0.0046 (11)	0.0006 (11)	−0.0003 (10)
O4	0.0446 (15)	0.0265 (12)	0.0347 (13)	0.0042 (10)	0.0004 (11)	−0.0076 (10)
O5	0.0476 (15)	0.0379 (13)	0.0206 (11)	−0.0089 (11)	−0.0005 (10)	−0.0110 (10)
O6	0.090 (2)	0.0276 (13)	0.0242 (12)	−0.0078 (13)	−0.0079 (13)	−0.0036 (10)
O7	0.0548 (16)	0.0202 (11)	0.0235 (11)	0.0070 (10)	−0.0038 (11)	−0.0072 (9)
O8	0.0479 (15)	0.0248 (11)	0.0153 (10)	0.0017 (10)	0.0019 (10)	−0.0050 (8)
O1w	0.0441 (16)	0.0383 (14)	0.0569 (17)	−0.0003 (12)	−0.0147 (14)	−0.0169 (13)
O2w	0.0364 (14)	0.0544 (17)	0.0240 (12)	0.0018 (13)	−0.0015 (11)	0.0001 (11)
O3w	0.0438 (15)	0.0390 (14)	0.0390 (14)	−0.0078 (12)	0.0015 (12)	−0.0181 (12)
O4w	0.106 (3)	0.115 (3)	0.072 (3)	−0.032 (3)	0.002 (2)	−0.054 (3)
O5w	0.089 (4)	0.140 (5)	0.146 (5)	−0.001 (4)	−0.004 (4)	−0.023 (4)
O6w	0.0618 (19)	0.0391 (15)	0.0342 (14)	0.0004 (13)	−0.0062 (13)	−0.0063 (12)
O7w	0.0451 (16)	0.0401 (14)	0.0340 (13)	−0.0101 (12)	−0.0102 (12)	−0.0107 (11)

O8w	0.077 (3)	0.159 (5)	0.068 (3)	−0.014 (3)	−0.008 (2)	0.003 (3)
O9w	0.113 (4)	0.074 (3)	0.079 (3)	0.016 (3)	−0.044 (3)	−0.017 (2)
C1	0.0245 (15)	0.0221 (14)	0.0240 (15)	0.0008 (12)	−0.0011 (12)	−0.0086 (12)
C2	0.0301 (16)	0.0234 (15)	0.0171 (14)	−0.0008 (12)	−0.0015 (12)	−0.0053 (11)
C3	0.0304 (17)	0.0195 (14)	0.0240 (15)	0.0015 (12)	−0.0045 (13)	−0.0066 (12)
C4	0.0317 (17)	0.0235 (15)	0.0219 (14)	0.0032 (13)	−0.0036 (13)	−0.0107 (12)
C5	0.0280 (16)	0.0241 (15)	0.0169 (14)	−0.0002 (12)	−0.0035 (12)	−0.0046 (11)
C6	0.0285 (16)	0.0216 (14)	0.0212 (14)	0.0035 (12)	−0.0036 (12)	−0.0051 (11)
C7	0.0298 (17)	0.0250 (15)	0.0242 (15)	−0.0041 (13)	0.0014 (13)	−0.0095 (12)
C8	0.041 (2)	0.0202 (15)	0.0286 (16)	0.0027 (14)	−0.0032 (15)	−0.0027 (13)
C9	0.0374 (19)	0.0195 (14)	0.0272 (16)	−0.0010 (13)	−0.0061 (14)	−0.0061 (12)
C10	0.0293 (16)	0.0279 (16)	0.0208 (14)	−0.0017 (13)	−0.0018 (12)	−0.0096 (12)
C11	0.0343 (18)	0.0325 (17)	0.0187 (14)	−0.0076 (14)	−0.0026 (13)	−0.0052 (13)

Geometric parameters (Å, °)

Cd1—O1	2.234 (2)	O4w—H4w1	0.86 (1)
Cd1—O3^{i}	2.322 (2)	O4w—H4w2	0.86 (1)
Cd1—O4^{i}	2.446 (2)	O5w—H5w1	0.86 (1)
Cd1—O1w	2.256 (3)	O5w—H5w2	0.86 (1)
Cd1—O2w	2.251 (2)	O6w—H6w1	0.85 (1)
Cd1—O3w	2.323 (3)	O6w—H6w2	0.85 (1)
Na1—O4	2.395 (3)	O7w—H7w1	0.85 (1)
Na1—O6^{ii}	2.292 (3)	O7w—H7w2	0.85 (1)
Na1—O7	2.645 (3)	O8w—H8w1	0.85 (1)
Na1—O8^{ii}	2.653 (3)	O8w—H8w2	0.85 (1)
Na1—O4w	2.304 (4)	O9w—H9w1	0.86 (1)
Na1—O5w	2.230 (7)	O9w—H9w2	0.85 (1)
O1—C7	1.257 (4)	C1—C6	1.376 (4)
O2—C7	1.251 (4)	C1—C2	1.396 (4)
O3—C9	1.256 (4)	C1—C7	1.508 (4)
O4—C9	1.233 (4)	C2—C3	1.388 (4)
O5—C11	1.263 (4)	C3—C4	1.385 (4)
O6—C11	1.237 (4)	C4—C5	1.387 (4)
O7—C3	1.376 (4)	C5—C6	1.389 (4)
O7—C8	1.424 (4)	C8—C9	1.519 (4)
O8—C5	1.369 (4)	C10—C11	1.515 (4)
O8—C10	1.426 (4)	C2—H2	0.93
O1w—H1w1	0.84 (1)	C4—H4	0.93
O1w—H1w2	0.85 (1)	C6—H6	0.93
O2w—H2w1	0.85 (1)	C8—H8a	0.97
O2w—H2w2	0.85 (1)	C8—H8b	0.97
O3w—H3w1	0.85 (1)	C10—H10a	0.97
O3w—H3w2	0.85 (1)	C10—H10b	0.97
O1—Cd1—O3^{i}	139.6 (1)	O8—C5—C4	124.2 (3)
O1—Cd1—O4^{i}	89.5 (1)	O8—C5—C6	115.9 (3)
O1—Cd1—O1w	94.8 (1)	C4—C5—C6	120.0 (3)
O1—Cd1—O2w	126.1 (1)	C1—C6—C5	120.1 (3)

O1—Cd1—O3w	81.9 (1)	O2—C7—O1	122.2 (3)
O3^{i}—Cd1—O4^{i}	54.5 (1)	O2—C7—C1	120.2 (3)
O3^{i}—Cd1—O1w	100.0 (1)	O1—C7—C1	117.5 (3)
O3^{i}—Cd1—O2w	91.0 (1)	O7—C8—C9	109.0 (3)
O3^{i}—Cd1—O3w	82.7 (1)	O4—C9—O3	122.9 (3)
O4^{i}—Cd1—O1w	86.4 (1)	O4—C9—C8	121.3 (3)
O4^{i}—Cd1—O2w	144.4 (1)	O3—C9—C8	115.8 (3)
O4^{i}—Cd1—O3w	93.5 (1)	O8—C10—C11	109.1 (2)
O1w—Cd1—O2w	91.7 (1)	O6—C11—O5	125.1 (3)
O1w—Cd1—O3w	176.7 (1)	O6—C11—C10	119.6 (3)
O2w—Cd1—O3w	90.3 (1)	O5—C11—C10	115.3 (3)
O4—Na1—O6^{ii}	93.7 (1)	Cd1—O1w—H1w1	110 (2)
O4—Na1—O7	63.4 (1)	Cd1—O1w—H1w2	109 (2)
O4—Na1—O8^{ii}	154.1 (1)	H1w1—O1w—H1w2	112 (2)
O4—Na1—O4w	98.7 (2)	Cd1—O2w—H2w1	124 (1)
O4—Na1—O5w	104.7 (2)	Cd1—O2w—H2w2	123 (1)
O6^{ii}—Na1—O7	79.3 (1)	H2w1—O2w—H2w2	110 (2)
O6^{ii}—Na1—O8^{ii}	63.3 (1)	Cd1—O3w—H3w1	113 (2)
O6^{ii}—Na1—O4w	155.4 (2)	Cd1—O3w—H3w2	113 (2)
O6^{ii}—Na1—O5w	96.8 (2)	H3w1—O3w—H3w2	110 (2)
O7—Na1—O8^{ii}	98.9 (1)	Na1—O4w—H4w1	122 (2)
O7—Na1—O4w	87.3 (2)	Na1—O4w—H4w2	122 (2)
O7—Na1—O5w	166.9 (2)	H4w1—O4w—H4w2	108 (2)
O8^{ii}—Na1—O4w	99.1 (2)	Na1—O5w—H5w1	100 (6)
O8^{ii}—Na1—O5w	90.4 (2)	Na1—O5w—H5w2	99 (6)
O4w—Na1—O5w	100.4 (2)	H5w1—O5w—H5w2	108 (2)
C7—O1—Cd1	106.1 (2)	H6w1—O6w—H6w2	109 (2)
C9—O3—Cd1^{iii}	93.9 (2)	H7w1—O7w—H7w2	110 (2)
C9—O4—Na1	118.4 (2)	H8w1—O8w—H8w2	110 (2)
C9—O4—Cd1^{iii}	88.7 (2)	H9w1—O9w—H9w2	109 (2)
Na1—O4—Cd1^{iii}	142.2 (1)	C3—C2—H2	120.9
C11—O6—Na1^{ii}	128.3 (2)	C1—C2—H2	120.9
C3—O7—C8	118.0 (2)	C3—C4—H4	120.3
C3—O7—Na1	109.8 (2)	C5—C4—H4	120.3
C8—O7—Na1	106.7 (2)	C1—C6—H6	119.9
C5—O8—C10	117.5 (2)	C5—C6—H6	119.9
C5—O8—Na1^{ii}	126.2 (2)	O7—C8—H8a	109.9
C10—O8—Na1^{ii}	113.1 (2)	C9—C8—H8a	109.9
C6—C1—C2	120.9 (3)	O7—C8—H8b	109.9
C6—C1—C7	119.6 (3)	C9—C8—H8b	109.9
C2—C1—C7	119.5 (3)	H8a—C8—H8b	108.3
C3—C2—C1	118.2 (3)	O8—C10—H10a	109.9
O7—C3—C4	114.4 (3)	C11—C10—H10a	109.9
O7—C3—C2	124.1 (3)	O8—C10—H10b	109.9

C4—C3—C2	121.5 (3)	C11—C10—H10b	109.9
C3—C4—C5	119.3 (3)	H10a—C10—H10b	108.3
O2w—Cd1—O1—C7	12.3 (3)	C2—C3—C4—C5	−1.6 (5)
O1w—Cd1—O1—C7	−83.4 (2)	C10—O8—C5—C4	−9.0 (5)
O3^{i}—Cd1—O1—C7	165.2 (2)	Na1^{ii}—O8—C5—C4	149.0 (3)
O3w—Cd1—O1—C7	96.7 (2)	C10—O8—C5—C6	172.2 (3)
O4^{i}—Cd1—O1—C7	−169.8 (2)	Na1^{ii}—O8—C5—C6	−29.8 (4)
O5w—Na1—O4—C9	−140.2 (3)	C3—C4—C5—O8	−177.7 (3)
O6^{ii}—Na1—O4—C9	−42.1 (3)	C3—C4—C5—C6	1.0 (5)
O4w—Na1—O4—C9	116.5 (3)	C2—C1—C6—C5	0.0 (5)
O7—Na1—O4—C9	34.0 (2)	C7—C1—C6—C5	179.4 (3)
O8^{ii}—Na1—O4—C9	−16.4 (4)	O8—C5—C6—C1	178.7 (3)
O5w—Na1—O4—Cd1^{iii}	−9.4 (3)	C4—C5—C6—C1	−0.2 (5)
O6^{ii}—Na1—O4—Cd1^{iii}	88.7 (2)	Cd1—O1—C7—O2	7.0 (4)
O4w—Na1—O4—Cd1^{iii}	−112.7 (2)	Cd1—O1—C7—C1	−171.4 (2)
O7—Na1—O4—Cd1^{iii}	164.8 (2)	C6—C1—C7—O2	161.1 (3)
O8^{ii}—Na1—O4—Cd1^{iii}	114.5 (3)	C2—C1—C7—O2	−19.4 (5)
O5w—Na1—O7—C3	−141.6 (9)	C6—C1—C7—O1	−20.4 (5)
O6^{ii}—Na1—O7—C3	−67.5 (2)	C2—C1—C7—O1	159.0 (3)
O4w—Na1—O7—C3	91.7 (2)	C3—O7—C8—C9	164.0 (3)
O4—Na1—O7—C3	−167.1 (2)	Na1—O7—C8—C9	39.9 (3)
O8^{ii}—Na1—O7—C3	−7.0 (2)	Na1—O4—C9—O3	152.2 (3)
O5w—Na1—O7—C8	−12.6 (9)	Cd1^{iii}—O4—C9—O3	−0.1 (4)
O6^{ii}—Na1—O7—C8	61.5 (2)	Na1—O4—C9—C8	−25.5 (4)
O4w—Na1—O7—C8	−139.3 (2)	Cd1^{iii}—O4—C9—C8	−177.8 (3)
O4—Na1—O7—C8	−38.1 (2)	Cd1^{iii}—O3—C9—O4	0.1 (4)
O8^{ii}—Na1—O7—C8	122.0 (2)	Cd1^{iii}—O3—C9—C8	178.0 (3)
C6—C1—C2—C3	−0.5 (5)	O7—C8—C9—O4	−14.3 (5)
C7—C1—C2—C3	−180.0 (3)	O7—C8—C9—O3	167.8 (3)
C8—O7—C3—C4	−177.9 (3)	C5—O8—C10—C11	−176.8 (3)
Na1—O7—C3—C4	−55.4 (3)	Na1^{ii}—O8—C10—C11	22.3 (3)
C8—O7—C3—C2	0.3 (5)	Na1^{ii}—O6—C11—O5	162.4 (3)
Na1—O7—C3—C2	122.8 (3)	Na1^{ii}—O6—C11—C10	−16.3 (5)
C1—C2—C3—O7	−176.7 (3)	O8—C10—C11—O6	−7.7 (5)
C1—C2—C3—C4	1.4 (5)	O8—C10—C11—O5	173.4 (3)
O7—C3—C4—C5	176.6 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···O6w	0.84 (1)	1.83 (2)	2.651 (4)	165 (5)
O1w—H1w2···O7w	0.85 (1)	1.92 (1)	2.750 (4)	165 (4)
O2w—H2w1···O5^{iv}	0.85 (1)	1.92 (1)	2.748 (4)	168 (2)
O2w—H2w2···O2^{v}	0.85 (1)	1.93 (1)	2.780 (3)	178 (5)

O3w—H3w1···O7w^{vi}	0.85 (1)	1.91 (1)	2.759 (4)	171 (3)
O3w—H3w2···O5^{vii}	0.85 (1)	1.89 (1)	2.736 (4)	173 (3)
O4w—H4w1···O8w^{ii}	0.86 (1)	2.04 (3)	2.796 (6)	147 (4)
O4w—H4w2···O9w^{vi}	0.86 (1)	1.96 (2)	2.790 (7)	164 (6)
O5w—H5w1···O8w^{iii}	0.86 (1)	2.09 (5)	2.805 (8)	140 (7)
O5w—H5w2···O9w	0.86 (1)	2.35 (9)	2.798 (9)	113 (8)
O6w—H6w1···O3^{v}	0.85 (1)	1.96 (2)	2.790 (4)	165 (4)
O6w—H6w2···O6^{viii}	0.85 (1)	1.90 (2)	2.730 (4)	165 (4)
O7w—H7w1···O2^{v}	0.85 (1)	2.09 (2)	2.859 (4)	152 (4)
O7w—H7w2···O5^{ix}	0.85 (1)	1.99 (2)	2.780 (3)	154 (4)
O8w—H8w1···O3w^{x}	0.85 (1)	2.04 (3)	2.874 (5)	165 (8)
O8w—H8w2···O1w	0.85 (1)	2.13 (4)	2.929 (6)	155 (8)
O9w—H9w1···O4w^{x}	0.86 (1)	2.02 (4)	2.790 (7)	150 (7)
O9w—H9w2···O1^{ii}	0.85 (1)	1.96 (2)	2.794 (4)	166 (7)

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

Fig. 1

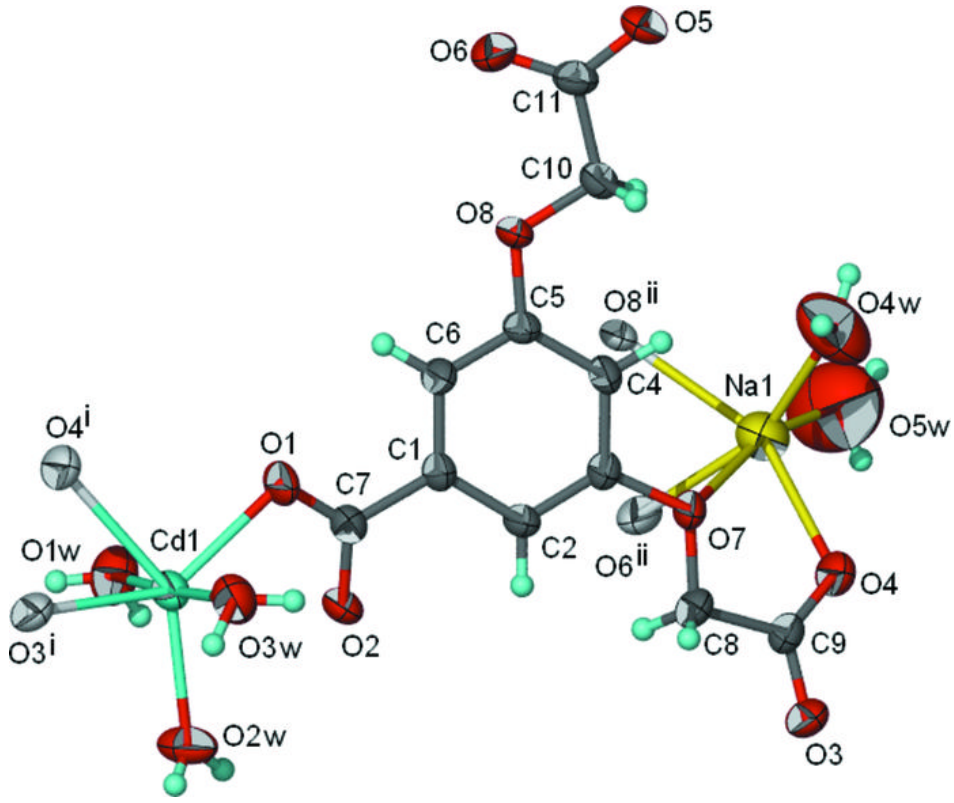

O5
O6
C11
C10
O8
C5
O8ii
O4w
C6
C4
Na1
O5w
O4i
O1
C1
C7
O1w
Cd1
C2
O6ii
O7
O4
O3i
O3w
O2
C8
C9
O2w
O3

Fig. 2