

Caesium propanoate monohydrate

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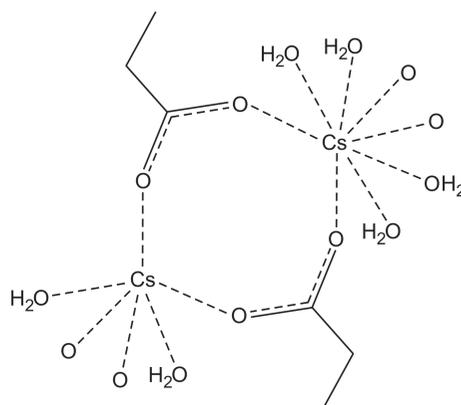
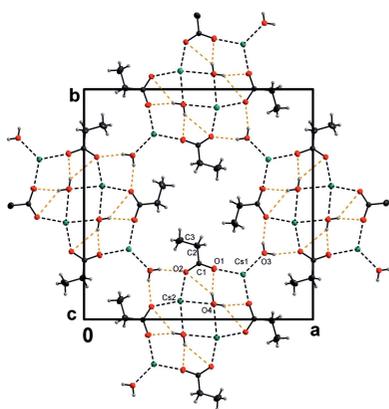
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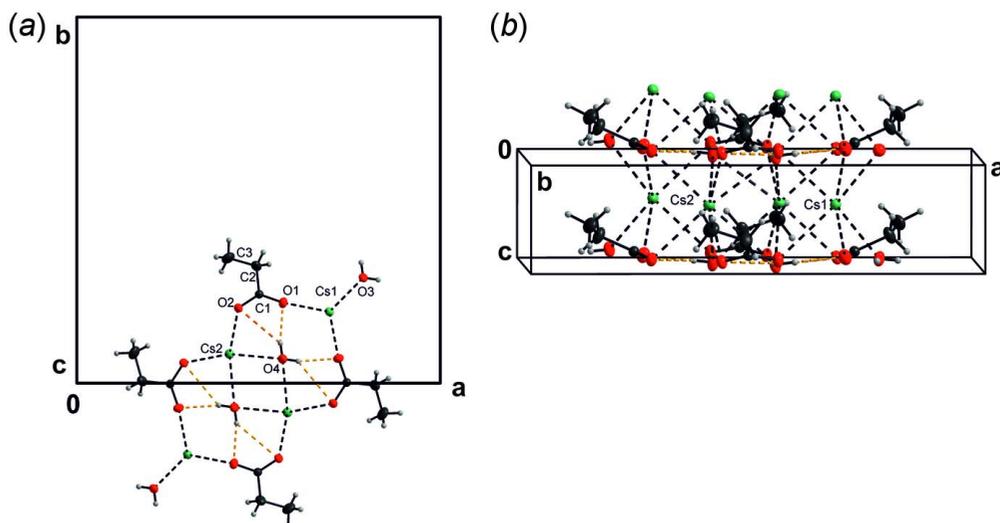
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Caesium propanoate monohydrate, $\text{Cs}^+\cdot\text{C}_3\text{H}_5\text{O}_2^-\cdot\text{H}_2\text{O}$, is composed of two symmetry-independent Cs^+ cations, which are situated on the special position $4e$ of space group $P\bar{4}2_1m$, one symmetry-independent propanoate molecule in a general position and a pair of water molecules also situated on special position $4e$. Two pairs of these symmetry-independent cations, four propanoate molecules and two pairs of symmetry-independent water molecules form a repeat unit. These units form columns that are directed along the c axis and possess symmetry $mm2$. There are four such columns passing through each unit cell. Each column is interconnected to its neighbours by four bifurcated three-centred $\text{O}_w\text{—H}\cdots\text{O}_p$ (w = water, p = propanoate) hydrogen bonds of moderate strength. There are also four intramolecular $\text{O}_w\text{—H}\cdots\text{O}_p$ hydrogen bonds of moderate strength within each column. One Cs^+ cation is coordinated by six oxygen atoms (two water and four carboxylate) in a trigonal–prismatic geometry, while the other Cs^+ cation is coordinated by four water and four carboxylate O atoms in a tetragonal–prismatic arrangement.

1. Chemical context

No structure of a simple hydrated alkali propanoate has been determined until now. ('Simple' means a structure where the constituting cation belongs just to one chemical species.) This is in contrast to alkali formates and acetates where water-free alkali salts and complexes with parent acids as well as hydrates are known. These structures show different structural motifs: Some of them are layered, such as lithium acetate dihydrate, $\text{LiC}_2\text{H}_3\text{O}_2\cdot 2\text{H}_2\text{O}$ [refcode LIACET06 (Kearley *et al.*, 1996) in the Cambridge Structural Database, version 5.41, update of November 2019 (Groom *et al.*, 2016)], some are columnar including sodium dihydrogen triacetate, $\text{NaC}_2\text{H}_3\text{O}_2\cdot 2\text{C}_2\text{H}_4\text{O}_2$ (NADHAC; Perotti & Tazzoli, 1981) while the cations and anions surround each other in the structure of *catena*-[bis(μ_4 -acetato)tetrakis(μ_3 -acetato)bis(μ_2 -acetato)octaaquaocalithium] (UVELAJ; Martínez Casado *et al.*, 2011).




Figure 1

View (*DIAMOND*; Brandenburg, 2005) of the title motif along (a) the *c* axis and (b) the *b* axis. Displacement ellipsoids are shown at the 30% probability level: the cations and the O and C atoms are shown in green, red and grey, respectively. H atoms are shown as small light-grey spheres. The covalent bonds are represented by solid lines, Cs—O bonds by dashed black lines and hydrogen bonds by yellow dashed lines.

In the series of carboxylic acids with an increasing number of carbon atoms, it is propionic acid where the hydrophobic properties start to be prominent. Formates and acetates are definitely distinct from propanoates and other carboxylates related to the acids $C_nH_{2n+1}CO_2$ where $n > 2$. This is due to the longer and more voluminous organic chains in the latter compounds, which need space [cf. Duruz & Ubbelohde (1972) and Dumbleton & Lomer, 1965]. Cohesion is provided by van der Waals forces. Occasionally, positional disorder of these groups may take place. Dicalcium barium hexakis(propionate) (Stadnicka & Glazer, 1980) can serve as an example.

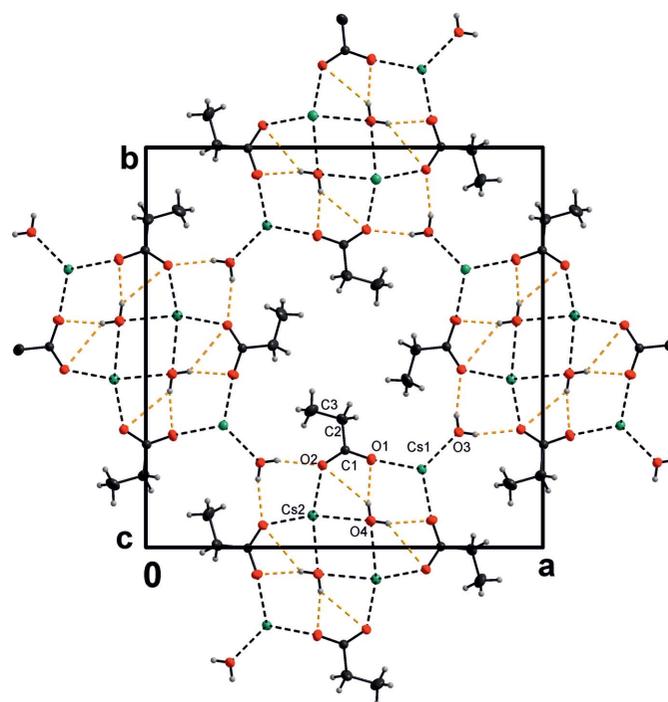
The structural differences between alkali formates and acetates on one hand and simple alkali propanoates such as $Li(C_3H_5O_2)$ (Martínez Casado *et al.*, 2009) and $M(C_3H_5O_2)_2$; $M = Na, K, Rb, Cs$ (Fábry & Samolová, 2020) on the other reflect the chemical differences between these two groups of compounds. The latter structures are characterized by stacking of layers that are composed of a metal–oxygen bilayer surrounded by hydrophobic layers comprising the ethyl groups. The cohesion forces between the hydrophobic layers hold these structures together. The structure of the chemically related compound $Tl(C_3H_5O_2)$ (refcode WEWKAM; Martínez Casado *et al.*, 2010) is also a layered structure with three symmetry-independent cations.

Mirnaya *et al.* (1991) pointed out the tendency for various alkanooates to form hydrates. Such a case is reported in this study – see the *Synthesis and crystallization* section. It is of interest how strikingly different the title structure $Cs(C_3H_5O_2) \cdot H_2O$ is from $Cs(C_3H_5O_2)$ (Fábry & Samolová, 2020), despite the chemical similarity.

2. Structural commentary

The title structure confirms the tendency for various alkanooates to form hydrates, as noted by Mirnaya *et al.* (1991). Caesium propanoate monohydrate is composed of two

symmetry-independent Cs^+ cations, which are situated on the special position $4e$, *i.e.* on a symmetry plane, one symmetry-independent propanoate molecule in a general position and a pair of water molecules also situated on special position $4e$ of space group $P\bar{4}2_1m$. Two pairs of these symmetry-independent cations, four propanoate molecules and two pairs of symmetry-independent water molecules form a repeat unit.


Figure 2

Packing of the title molecules in the unit cell (*DIAMOND*; Brandenburg, 2005). Displacement ellipsoids are shown at the 30% probability level: the cations and the O and C atoms are shown in green, red and grey, respectively. H atoms are shown as small light-grey spheres. The covalent bonds are represented by solid lines, Cs—O bonds by dashed black lines and hydrogen bonds by yellow dashed lines.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H1o3 ⁱ ···O2 ⁱ	0.820 (9)	1.988 (7)	2.783 (2)	163.3 (19)
O4—H1o4 ⁱⁱ ···O1 ⁱⁱ	0.820 (7)	1.941 (6)	2.748 (2)	168.0 (5)
O4—H1o4 ⁱⁱⁱ ···O2 ⁱⁱⁱ	0.820 (7)	2.646 (5)	3.293 (2)	137.0 (5)
O3—H1o3 ⁱⁱⁱ ···O2 ^{iv}	0.820 (9)	1.988 (7)	2.783 (2)	163.3 (19)
O4—H1o4 ⁱⁱⁱ ···O1 ^v	0.820 (7)	1.941 (6)	2.748 (2)	168.0 (5)
O4—H1o4 ⁱⁱⁱ ···O2 ^v	0.820 (7)	2.646 (5)	3.293 (2)	137.0 (5)

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

These units form columns along the c -axis direction (Fig. 1a). The length of the repeat unit along the c axis corresponds to this unit-axis length. Each column has $mm2$ symmetry (Fig. 1b). There are four such columns passing through each unit cell (Fig. 2). The columns are interconnected by bifurcated three-centered $O_w-H\cdots O_p$ (w = water, p = propanoate) hydrogen bonds (Jeffrey, 1995), whose lengths and angles are quite different, but which are still of moderate strength (Gilli & Gilli, 2009); the donor is O4 and the donated hydrogen is H1o4 (Table 1). Each column thus donates four three-centered bifurcated hydrogen bonds (Jeffrey, 1995) to its neighbours (Fig. 2). There are also intramolecular two-centered $O_w-H\cdots O_p$ hydrogen bonds of moderate strength within each column in the structure; the donor is O3 and the donated atom is H1o3.

Cs1 is coordinated by six oxygen atoms (two of them are water O atoms and four are carboxylate O atoms) in a trigonal–prismatic geometry, while Cs2 is in a less regular tetragonal–prismatic coordination environment (by four water and four carboxylate oxygen atoms) (Fig. 2). The bond-valence sums (Brese & O’Keeffe, 1991) of Cs1 and Cs2 are 0.902 (3) and 0.997 (2) v.u., respectively. The fact that the cation with a smaller number of ligands that exhibits a regular coordination environment has a smaller bond-valence sum than that with the larger number of surrounding cations seems to be a peculiarity of the present structure, for example compared to β -K₂SO₄ compounds with two symmetry-independent cations (Fábry & Pérez-Mato, 1994). One has eleven ligands while the other has nine. The former has a more irregular coordination compared to the latter and its bond-valence sum is also lower than that of the latter cation. This example is a specific case that has been considered by Brown (1992): The larger coordination number usually results in the formation of a larger cavity around the cation. Stabilization of the cation causes the cation to shift towards some ligand. Such a shift contributes to irregularity of the coordination polyhedron with large numbers of ligands. Despite this stabilization, the bonding of a cation with a high coordination number tends to be lower than that of a cation with a low coordination number.

In contrast to the alkali propanoates, $M(C_nH_{2n+1}COO)$, the methylene–methylene, methyl–methyl carbon atoms are not in close contact in the title structure. The closest contact C2···C3^{vi}, *i.e.* a methylene–methyl contact is 3.961 (4) Å; symmetry code: (vi) $-y + 1, x, -z + 1$. This is related to the

Table 2
Experimental details.

Crystal data	
Chemical formula	Cs ⁺ ·C ₃ H ₅ O ₂ [−] ·H ₂ O
M_r	224
Crystal system, space group	Tetragonal, $P\bar{4}_2/m$
Temperature (K)	230
a, c (Å)	17.7764 (3), 4.2223 (1)
V (Å ³)	1334.25 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm ^{−1})	5.47
Crystal size (mm)	0.46 × 0.04 × 0.03
Data collection	
Diffractometer	Bruker D8 VENTURE Kappa Duo PHOTON 100 CMOS
Absorption correction	Multi-scan (SADABS; Bruker, 2017)
T_{\min}, T_{\max}	0.190, 0.866
No. of measured, independent and observed [$I > 3\sigma(I)$] reflections	12844, 2019, 1872
R_{int}	0.021
$(\sin \theta/\lambda)_{\text{max}}$ (Å ^{−1})	0.703
Refinement	
$R[F > 3\sigma(F)], wR(F), S$	0.014, 0.037, 1.10
No. of reflections	2019
No. of parameters	78
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ^{−3})	0.24, −0.33
Absolute structure	Flack (1983), 831 Friedel pairs
Absolute structure parameter	0.03 (3)

Computer programs: *Instrument Service* and *SAINT* (Bruker, 2017), *SUPERFLIP* (Palatinus & Chapuis, 2007) and *JANA2006* (Petříček *et al.*, 2014), *DIAMOND* (Brandenburg, 2005); extinction correction according to Becker & Coppens (1974).

fact that no disorder of the ethyl groups is observed in the studied structure. At the same time, there are elongated voids in the c -axis direction that run parallel through the $4d$ positions and which are surrounded by the ethyl groups. The radius of the void is 1.381 Å while its height nearly corresponds to the c axis. The voids were calculated and depicted (see the supporting information) using *Mercury* 4.0 (Macrae *et al.*, 2020).

3. Synthesis and crystallization

The crystals formed spontaneously in a droplet from dissolved deliquescent crystals of Cs(C₃H₅O₂) that otherwise have been grown from an aqueous solution of Cs₂CO₃ with a little excess of propionic acid (Fábry & Samolová, 2020).

4. Structure determination and refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The non-hydrogen atoms were determined by a charge-flipping method (Palatinus & Chapuis, 2007). The positions of the methylene hydrogen atoms were calculated and refined under the following constraints: C—H = 0.97 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The methyl hydrogen atoms were found in the difference electron-density maps and

refined under the constraints $C-H = 0.96 \text{ \AA}$ and $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$. The water hydrogen atoms were also found in the difference electron density maps. The $O-H$ distances were restrained to $0.820(1) \text{ \AA}$ with $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(O)$. When the water H atoms were refined, the $O-H_{\text{water}}$ distances converged to values of $\sim 0.78 \text{ \AA}$. The structure was treated as an inversion twin. The Flack (1983) parameter is 0.03 (3).

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Computing details

Data collection: *Instrument Service* (Bruker, 2017); cell refinement: *SAINTE* (Bruker, 2017); data reduction: *SAINTE* (Bruker, 2017); program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *JANA2006* (Petříček *et al.*, 2014); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *JANA2006* (Petříček *et al.*, 2014).

Caesium propanoate monohydrate

Crystal data

$\text{Cs}^+\cdot\text{C}_3\text{H}_5\text{O}_2^-\cdot\text{H}_2\text{O}$

$M_r = 224$

Tetragonal, $P\bar{4}2_1m$

Hall symbol: P -4 2ab

$a = 17.7764$ (3) Å

$c = 4.2223$ (1) Å

$V = 1334.25$ (4) Å³

$Z = 8$

$F(000) = 832$

There have been used diffractions with $I/\sigma(I) > 20$ for the unit cell determination.

$D_x = 2.230$ Mg m⁻³

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

Cell parameters from 9815 reflections

$\theta = 2.3\text{--}30.0^\circ$

$\mu = 5.47$ mm⁻¹

$T = 230$ K

Needle, colourless

$0.46 \times 0.04 \times 0.03$ mm

Data collection

Bruker D8 VENTURE Kappa Duo PHOTON
100 CMOS
diffractometer

Radiation source: $I\mu\text{S}$ micro-focus sealed tube

Quazar Mo multilayer optic monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2017)

$T_{\min} = 0.190$, $T_{\max} = 0.866$

12844 measured reflections

2019 independent reflections

1872 reflections with $I > 3\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 30.0^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -24 \rightarrow 24$

$k = -19 \rightarrow 24$

$l = -5 \rightarrow 4$

Refinement

Refinement on F^2

$R[F > 3\sigma(F)] = 0.014$

$wR(F) = 0.037$

$S = 1.10$

2019 reflections

78 parameters

4 restraints

22 constraints

Primary atom site location: charge flipping

H atoms treated by a mixture of independent and constrained refinement

Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(I) + 0.0004I^2)$

$(\Delta/\sigma)_{\max} = 0.042$

$\Delta\rho_{\max} = 0.24$ e Å⁻³

$\Delta\rho_{\min} = -0.33$ e Å⁻³

Extinction correction: B-C type 1 Lorentzian isotropic (Becker & Coppens, 1974)

Extinction coefficient: 330 (110)

Absolute structure: Flack (1983), 831 Friedel
pairs
Absolute structure parameter: 0.03 (3)

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cs1	0.695062 (6)	0.195062 (6)	0.48412 (6)	0.03299 (4)
Cs2	0.420270 (6)	0.079730 (6)	0.51015 (5)	0.03461 (4)
O1	0.56778 (8)	0.21997 (9)	0.9877 (8)	0.0493 (5)
O2	0.44454 (7)	0.20549 (7)	1.0090 (6)	0.0395 (4)
O3	0.78820 (8)	0.28820 (8)	0.9682 (10)	0.0442 (7)
O4	0.56624 (9)	0.06624 (9)	0.0554 (10)	0.0534 (9)
C1	0.50192 (12)	0.24285 (12)	0.9444 (5)	0.0310 (6)
C2	0.49413 (16)	0.32018 (16)	0.7976 (7)	0.0549 (9)
C3	0.41676 (19)	0.34209 (18)	0.6915 (8)	0.0631 (11)
H1c2	0.513302	0.35775	0.943391	0.0658*
H2c2	0.528887	0.324875	0.621629	0.0658*
H1c3	0.383944	0.344695	0.871774	0.0947*
H2c3	0.418684	0.390343	0.589772	0.0947*
H3c3	0.398058	0.305262	0.545034	0.0947*
H1o3	0.7817 (4)	0.3335 (4)	0.994 (9)	0.0662*
H1o4	0.5599 (3)	0.1117 (3)	0.035 (8)	0.0801*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1	0.03383 (7)	0.03383 (7)	0.03130 (9)	−0.00310 (6)	−0.00090 (7)	−0.00090 (7)
Cs2	0.03802 (7)	0.03802 (7)	0.02778 (8)	−0.00027 (6)	0.00236 (8)	−0.00236 (8)
O1	0.0321 (7)	0.0484 (8)	0.0675 (11)	0.0054 (6)	0.0002 (13)	0.0072 (13)
O2	0.0324 (6)	0.0340 (7)	0.0520 (9)	−0.0018 (5)	0.0050 (10)	0.0042 (11)
O3	0.0348 (6)	0.0348 (6)	0.0629 (18)	−0.0038 (8)	−0.0063 (12)	−0.0063 (12)
O4	0.0372 (7)	0.0372 (7)	0.086 (2)	−0.0007 (9)	0.0092 (11)	0.0092 (11)
C1	0.0314 (9)	0.0300 (9)	0.0316 (12)	0.0010 (8)	0.0005 (9)	0.0018 (9)
C2	0.0470 (15)	0.0427 (15)	0.0749 (18)	−0.0065 (12)	−0.0065 (14)	0.0230 (14)
C3	0.070 (2)	0.0518 (18)	0.067 (2)	0.0210 (16)	−0.0106 (17)	0.0148 (15)

Geometric parameters (\AA , $^\circ$)

O1—C1	1.253 (3)	Cs1—O3	3.108 (3)
O2—C1	1.247 (3)	Cs2—O2	3.102 (2)
C1—C2	1.514 (4)	Cs2—O2 ^{iv}	3.108 (2)
C2—C3	1.498 (4)	Cs2—O2 ^v	3.102 (2)
C2—H1c2	0.97	Cs2—O3 ^{vi}	3.886 (3)
C2—H2c2	0.97	Cs2—O3 ^{vii}	3.984 (3)
C3—H1c3	0.96	Cs2—O4	3.237 (3)
C3—H2c3	0.96	Cs2—O4 ^{viii}	3.477 (3)
C3—H3c3	0.96	Cs2—O4 ^{ix}	3.237 (3)

Cs1—O1 ⁱ	3.116 (2)	Cs2—O4 ^x	3.477 (3)
Cs1—O1	3.136 (2)	O3—H1o3	0.820 (9)
Cs1—O1 ⁱⁱ	3.116 (2)	O3—H1o3 ⁱⁱⁱ	0.820 (9)
Cs1—O1 ⁱⁱⁱ	3.136 (2)	O4—H1o4	0.820 (7)
Cs1—O3 ⁱ	3.198 (3)	O4—H1o4 ⁱⁱⁱ	0.820 (7)
O1 ⁱ —Cs1—O1	84.96 (7)	O2 ^v —Cs2—O4 ^x	59.75 (5)
O1 ⁱ —Cs1—O1 ⁱⁱ	75.75 (6)	O3 ^{vi} —Cs2—O3 ^{vii}	64.87 (8)
O1 ⁱ —Cs1—O1 ⁱⁱⁱ	131.38 (5)	O3 ^{vi} —Cs2—O4	102.75 (7)
O1 ⁱ —Cs1—O3 ⁱ	81.03 (6)	O3 ^{vi} —Cs2—O4 ^{viii}	146.78 (4)
O1 ⁱ —Cs1—O3	138.89 (5)	O3 ^{vi} —Cs2—O4 ^{ix}	102.75 (7)
O1 ⁱ —Cs1—O4	46.47 (5)	O3 ^{vi} —Cs2—O4 ^x	146.78 (4)
O1—Cs1—O1 ⁱⁱ	131.38 (5)	O3 ^{vii} —Cs2—O4	147.56 (4)
O1—Cs1—O1 ⁱⁱⁱ	75.17 (6)	O3 ^{vii} —Cs2—O4 ^{viii}	96.57 (7)
O1—Cs1—O3 ⁱ	139.66 (4)	O3 ^{vii} —Cs2—O4 ^{ix}	147.56 (4)
O1—Cs1—O3	82.14 (7)	O3 ^{vii} —Cs2—O4 ^x	96.57 (7)
O1—Cs1—O4	88.43 (6)	O4—Cs2—O4 ^{viii}	77.84 (8)
O1 ⁱⁱ —Cs1—O1 ⁱⁱⁱ	84.96 (7)	O4—Cs2—O4 ^{ix}	61.92 (5)
O1 ⁱⁱ —Cs1—O3 ⁱ	81.03 (6)	O4—Cs2—O4 ^x	106.39 (6)
O1 ⁱⁱ —Cs1—O3	138.89 (5)	O4 ^{viii} —Cs2—O4 ^{ix}	106.39 (6)
O1 ⁱⁱ —Cs1—O4	46.47 (5)	O4 ^{viii} —Cs2—O4 ^x	57.23 (5)
O1 ⁱⁱⁱ —Cs1—O3 ⁱ	139.66 (4)	O4 ^{ix} —Cs2—O4 ^x	77.84 (8)
O1 ⁱⁱⁱ —Cs1—O3	82.14 (7)	Cs1—O1—Cs1 ^{viii}	84.96 (4)
O1 ⁱⁱⁱ —Cs1—O4	88.43 (6)	Cs2—O2—Cs2 ^{viii}	85.68 (3)
O3 ⁱ —Cs1—O3	84.05 (8)	Cs1—O3—Cs1 ^{viii}	84.05 (4)
O3 ⁱ —Cs1—O4	107.86 (8)	Cs1—O3—Cs2 ^{xi}	107.57 (11)
O3—Cs1—O4	168.08 (8)	Cs1—O3—Cs2 ^{xii}	172.44 (11)
O2 ⁱ —Cs2—O2	85.68 (6)	Cs1 ^{viii} —O3—Cs2 ^{xi}	168.38 (11)
O2 ⁱ —Cs2—O2 ^{iv}	74.70 (5)	Cs1 ^{viii} —O3—Cs2 ^{xii}	103.51 (11)
O2 ⁱ —Cs2—O2 ^v	131.48 (4)	H1o3—O3—H1o3 ⁱⁱⁱ	105.0 (10)
O2 ⁱ —Cs2—O3 ^{vi}	45.21 (4)	Cs1—O4—Cs2 ⁱ	137.82 (6)
O2 ⁱ —Cs2—O3 ^{vii}	91.97 (5)	Cs1—O4—Cs2	99.19 (9)
O2 ⁱ —Cs2—O4	62.50 (5)	Cs1—O4—Cs2 ^{xiii}	137.82 (6)
O2 ⁱ —Cs2—O4 ^{viii}	113.38 (5)	Cs1—O4—Cs2 ^{ix}	99.19 (9)
O2 ⁱ —Cs2—O4 ^{ix}	99.35 (7)	Cs2 ⁱ —O4—Cs2	77.84 (4)
O2 ⁱ —Cs2—O4 ^x	167.93 (4)	Cs2 ⁱ —O4—Cs2 ^{xiii}	70.40 (6)
O2—Cs2—O2 ^{iv}	131.48 (4)	Cs2 ⁱ —O4—Cs2 ^{ix}	120.22 (5)
O2—Cs2—O2 ^v	74.89 (5)	Cs2—O4—Cs2 ^{xiii}	120.22 (5)
O2—Cs2—O3 ^{vi}	90.09 (6)	Cs2—O4—Cs2 ^{ix}	76.52 (7)
O2—Cs2—O3 ^{vii}	44.10 (4)	Cs2 ^{xiii} —O4—Cs2 ^{ix}	77.84 (4)
O2—Cs2—O4	110.17 (5)	H1o4—O4—H1o4 ⁱⁱⁱ	105.0 (7)
O2—Cs2—O4 ^{viii}	59.75 (5)	O1—C1—O2	124.0 (2)
O2—Cs2—O4 ^{ix}	166.01 (5)	O1—C1—C2	116.1 (2)
O2—Cs2—O4 ^x	94.51 (7)	O2—C1—C2	119.9 (2)
O2 ^{iv} —Cs2—O2 ^v	85.68 (6)	C1—C2—C3	116.3 (2)
O2 ^{iv} —Cs2—O3 ^{vi}	45.21 (4)	C1—C2—H1c2	109.47
O2 ^{iv} —Cs2—O3 ^{vii}	91.97 (5)	C1—C2—H2c2	109.47
O2 ^{iv} —Cs2—O4	99.35 (7)	C3—C2—H1c2	109.47

O2 ^{iv} —Cs2—O4 ^{viii}	167.93 (4)	C3—C2—H2c2	109.47
O2 ^{iv} —Cs2—O4 ^{ix}	62.50 (5)	H1c2—C2—H2c2	101.72
O2 ^{iv} —Cs2—O4 ^x	113.38 (5)	C2—C3—H1c3	109.47
O2 ^v —Cs2—O3 ^{vi}	90.09 (6)	C2—C3—H2c3	109.47
O2 ^v —Cs2—O3 ^{vii}	44.10 (4)	C2—C3—H3c3	109.47
O2 ^v —Cs2—O4	166.01 (5)	H1c3—C3—H2c3	109.47
O2 ^v —Cs2—O4 ^{viii}	94.51 (7)	H1c3—C3—H3c3	109.47
O2 ^v —Cs2—O4 ^{ix}	110.17 (5)	H2c3—C3—H3c3	109.47

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H1o3 ⁱⁱⁱ ...O2 ^{xiii}	0.820 (9)	1.988 (7)	2.783 (2)	163.3 (19)
O4—H1o4 ⁱⁱⁱ ...O1 ⁱ	0.820 (7)	1.941 (6)	2.748 (2)	168.0 (5)
O4—H1o4 ⁱⁱⁱ ...O2 ⁱ	0.820 (7)	2.646 (5)	3.293 (2)	137.0 (5)
O3—H1o3 ⁱⁱⁱ ...O2 ^{xiv}	0.820 (9)	1.988 (7)	2.783 (2)	163.3 (19)
O4—H1o4 ⁱⁱⁱ ...O1 ⁱⁱ	0.820 (7)	1.941 (6)	2.748 (2)	168.0 (5)
O4—H1o4 ⁱⁱⁱ ...O2 ⁱⁱ	0.820 (7)	2.646 (5)	3.293 (2)	137.0 (5)

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