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Crystal structures of *catena*-poly[[μ-aqua-diaqua-(μ_3-2-methylpropanoato-κ^4O:O,O':O')calcium] 2-methylpropanoate dihydrate], *catena*-poly[[μ-aqua-diaqua(μ_3-2-methylpropanoato-κ^4O:O,O':O')strontium] 2-methylpropanoate dihydrate] and *catena*-poly[[μ-aqua-diaqua(μ_3-2-methylpropanoato-κ^4O:O,O':O')(calcium/strontium)] 2-methylpropanoate dihydrate]

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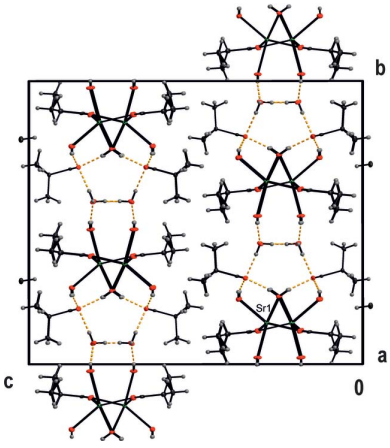
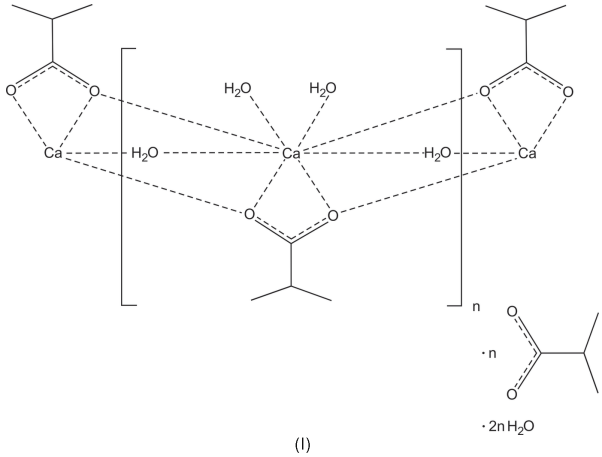
The crystal structures of *catena*-poly[[μ-aqua-diaqua(μ_3-2-methylpropanoato-κ^4O:O,O':O')calcium] 2-methylpropanoate dihydrate], {[Ca($C_4H_7O_2$)(H_2O)$_3$]($C_4H_7O_2$)·2H_2O}$_n$, (I), *catena*-poly[[μ-aqua-diaqua(μ_3-2-methylpropanoato-κ^4O:O,O':O')strontium] 2-methylpropanoate dihydrate], {[Sr($C_4H_7O_2$)(H_2O)$_3$]($C_4H_7O_2$)·2H_2O}$_n$, (II), and *catena*-poly[[μ-aqua-diaqua(μ_3-2-methylpropanoato-κ^4O:O,O':O')(calcium/strontium)] 2-methylpropanoate dihydrate], {[(Ca,Sr)($C_4H_7O_2$)(H_2O)$_3$]($C_4H_7O_2$)·2H_2O}$_n$, (III), are related. (III) can be considered as an Sr-containing solid solution of (I), with Ca^{2+} and Sr^{2+} occupationally disordered in the ratio 0.7936 (16):0.2064 (16). (I)/(III) and (II) are homeotypic with different space groups of *Pbca* and *Cmce*, respectively. All the title crystal structures are composed of hydrophilic sheets containing the cations, carboxylate groups as well as water molecules. The hydrophobic layers, which consist of 2-methylpropanoate chains, surround the hydrophilic sheets from both sides, thus forming a sandwich-like structure extending parallel to (001). The cohesion forces within these sheets are the cation–oxygen bonds and O—H···O hydrogen bonds of moderate strength. Stacking of these sandwiches along [001] is consolidated by van der Waals forces. The structures contain columns defined by the cation–oxygen interactions in which just one symmetry-independent 2-methylpropanoate anion is included, together with three water molecules. These molecules participate in an irregular coordination polyhedron composed of eight O atoms around the cation. Additional water molecules as well as the second 2-methylpropanoate anion are not part of the coordination sphere. These molecules are connected to the above-mentioned columns by O—H···O hydrogen bonds of moderate strength. In (II), the Sr^{2+} cation, two of the coordinating water molecules and both anions are situated on a mirror plane with a concomitant positional disorder of the 2-methylpropyl groups; the non-coordinating water molecule also shows positional disorder of its hydrogen atom.



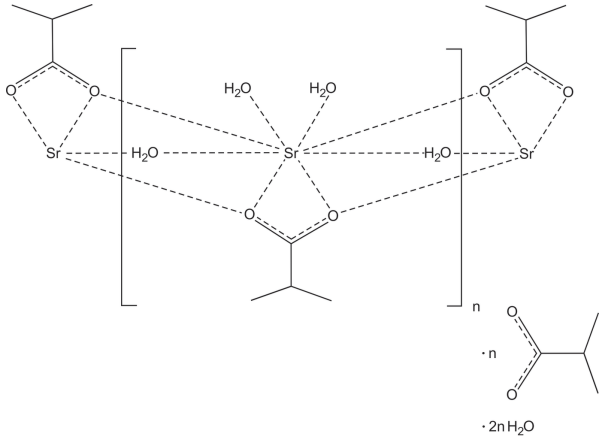
1. Chemical context

A search of the Cambridge Structural Database (Groom *et al.*, 2016; version 5.41 with updates until August 2020) for crystal structures containing solely alkaline earth cations and 2-methylpropanoate (or isobutyrate) anions revealed hexakis-[bis(μ_2-2-methylpropanoato)(2-methylpropanoic acid)mag-

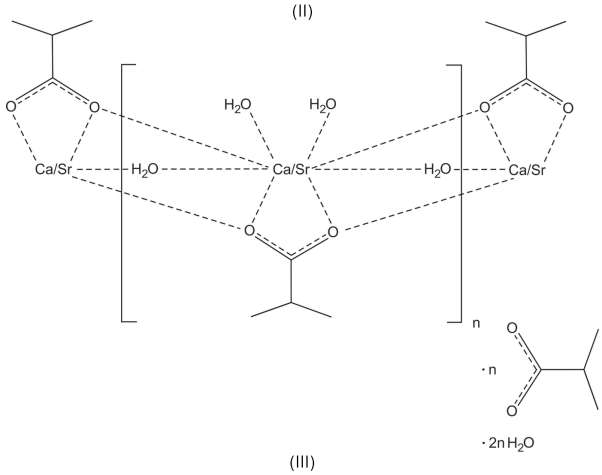
nesium], refcode NAGQUI (Coker *et al.*, 2004) and *catena*-poly[[triaqua(isobutyrato-*kO*)magnesium]-μ-isobutyrato-κ^2O:O'] monohydrate, refcode VIQTOG (Malaestean *et al.*, 2013). Although limited to these two examples, some basic structural features of these compounds can be inferred from other simple carboxylate salts. These features, among others, are illustrated by the series of structures determined by Coker *et al.* (2004), in which the number of carbon atoms in the carboxylate anions gradually increases.



(I)



(II)



(III)

In the crystal structure of *catena*-[tetrakis(μ_2-formato)-tetraaquadimagnesium], MGFORD03 (Coker *et al.*, 2004), no hydrophobic organic chain is present. In the other member of this series, bis(μ_2-acetato-*O*,*O*,*O*′)-tetrakis(μ_2-acetato-*O*,*O*′)-bis(acetic acid)diaquatrimagnesium acetic acid solvate, NAGQOC [Coker *et al.* (2004), see also the redetermination of this structure by Scheurell *et al.* (2012), NAGQOC02], there are sheets within the structure separated into hydrophilic parts (composed of the cations and oxygen atoms) and hydrophobic parts (composed of methyl groups). The remaining free acetic acid molecules are bound by O_{acetic}—H···O hydrogen bonds between the layers. NAGQUI is an example of a structure where the hydrophilic part is surrounded by a hydrophobic layer. The same holds for hexakis[bis(μ_2-3,3-dimethylbutanato)(3,3-dimethylbutanoic acid)magnesium], NAGRET (Coker *et al.*, 2004), as well as for bis(pivalato)tetrakis(pivalic acid)magnesium, VAMCUI01 [Coker *et al.* (2004), see also VAMCUI determined by Troyanov *et al.* (2002)]. Thus, the longer the organic chain, the more important the van der Waals forces become for molecular cohesion in structures with carboxylate anions. The different cohesion forces in the hydrophilic and the hydrophobic parts are the reason for the formation of layer-like structures or structures where an organic part completely surrounds a hydrophilic metal–oxygen sheet or a hydrophilic cluster. Likewise, the longer the hydrophobic chains, the larger is the probability of inclusion of non-coordinating water molecules into the structure because the latter can provide binding bridges between the carboxylate anions, which would otherwise be isolated. Such a situation is realised in VIQTOG where the water molecules complete a column substructure that is defined by the cation–oxygen bonds stemming from the carboxylate groups and water molecules. The growing complexity of water substructures with a growing number of carbon atoms in carboxylate anions has also been observed in the salts of the first five dicarboxylic acids with 4,6-diaminopyrimidine (Matulková *et al.*, 2017).

The present study was undertaken to prepare dicalcium strontium hexakis(2-methylpropanoate) with the intention that the resulting crystal structure might be related to dicalcium strontium hexakis(propionate) (CASRPP06; Mishima, 1984), which exhibits interesting structural and physical properties (*e.g.* Itoh, 1992). However, the synthesis attempt resulted in one of the title structures, *catena*-poly[[μ-aquadiaqua(μ_3-2-methylpropanoato-κ^4O:O,O':O')(calcium/strontium)] 2-methylpropanoate dihydrate], (III). We then also prepared the pure Ca and Sr compounds, *i.e.* (I) and (II), the crystal structures of which are also reported here.

2. Structural commentary

The structures have the same features and are composed of the respective cation, two carboxylate molecules and additional water molecules. One of the carboxylate anions and three water molecules coordinate to the cation, the remaining molecules form a substructure interconnected by hydrogen bonds only. Compound (III) is an Sr-containing solid solution of (I), and the two structures are crystal-chemically isotypic. The refined ratio of the occupationally disordered cation site is Ca:Sr = 0.7936 (16):0.2064 (16). The crystal structures of (I)/(III) and (II) are homeotypic (Lima-de-Faria *et al.*, 1990), with

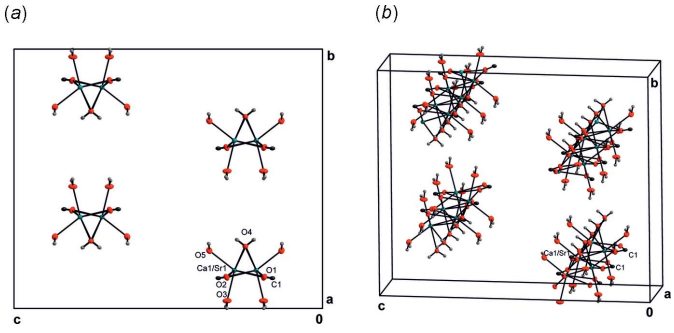


Figure 1
(*a*) View of the columns along the *a* axis in the crystal structure of (III). The columns depicted are formed by (Ca1/Sr1) (green) and O atoms (red); the latter are also depicted with bonds to carbon C atoms (grey) and H atoms (light-grey spheres of arbitrary radius). Displacement ellipsoids are shown at the 30% probability level. (*b*) Perspective view of the columns in (III).

similar lattice parameters and crystal-chemical features, but different space-group types.

There are three main cohesion forces present in the title structures: The first cohesion force regards the cation–oxygen interactions. For each of the crystal structures, there are eight oxygen atoms in the coordination sphere, defined by one carboxylate molecule in a bidentate bridging mode. (In VIQTOG there are two carboxylate anions coordinating in a monodentate mode and bridging to other Mg^{2+} cations.) In the title structures, the cation-coordinating atoms are symmetry-equivalent atoms O1 in (II), and O1 and O2 in (I) and (III), respectively. Other coordinating O atoms are the water O atoms O2, O3 and O4 in (II), and the water O atoms O3, O4 and O5 in (I) and (III). [The Sr^{2+} cation in (II) is located on a mirror plane (Wyckoff position 8*f*)]. Numerical values of the cation–oxygen bonds are listed in Tables 1, 2 and 3 for structures (I), (II) and (III), respectively. The coordination polyhedra form columns oriented parallel to the *a* axis. Because of the similarity of the three structures, (III) was chosen as a representative (Fig. 1*a*,*b*).

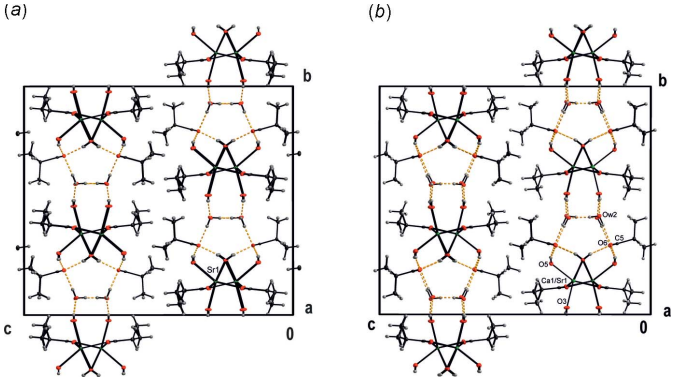


Figure 2
View of the unit-cell content of (*a*) (II) and (*b*) (III). Hydrogen bonds are shown as yellow dashed lines; colour code as in Fig. 1. The substructures with the hydrophilic sheets and hydrogen-bonded system, which connects the columns and water molecules, are clearly discernible from the hydrophobic part of the structure composed of 2-methylethyl chains.

Table 1
Selected bond lengths (Å) for (I).

Ca1—O3	2.3479 (12)	Ca1—O2	2.4993 (11)
Ca1—O2^{i}	2.3653 (10)	Ca1—O1	2.5308 (11)
Ca1—O1^{ii}	2.3938 (10)	Ca1—O4^{ii}	2.5446 (11)
Ca1—O5	2.4085 (12)	Ca1—O4	2.6019 (11)

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

Table 2
Selected bond lengths (Å) for (II).

Sr1—O1^{i}	2.4788 (10)	Sr1—O1	2.6561 (11)
Sr1—O1^{ii}	2.4788 (10)	Sr1—O1^{iii}	2.6561 (11)
Sr1—O3	2.4899 (16)	Sr1—O2	2.6796 (11)
Sr1—O4	2.5593 (18)	Sr1—O2^{ii}	2.6796 (11)

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

Table 3
Selected bond lengths (Å) for (III).

Ca1—O3	2.3719 (10)	Ca1—O2	2.5457 (9)
Ca1—O2^{i}	2.3845 (9)	Ca1—O1	2.5714 (9)
Ca1—O1^{ii}	2.4091 (8)	Ca1—O4^{ii}	2.5747 (9)
Ca1—O5	2.4209 (10)	Ca1—O4	2.6271 (9)

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

The second type of a cohesion force in the title structures originates from O—H···O hydrogen bonds of moderate strength (Gilli & Gilli, 2009) that link the above mentioned columns into hydrophilic sheets parallel to (001) (Fig. 2*a*,*b*). Within a sheet, the coordinating water molecules are solely engaged as donor groups whereas the non-coordinating water molecules (O*w*1 and O*w*2 in (I) and (III), and O*w*1 in (II)) have the functions both as donor and acceptor groups. The carboxylate acceptor atoms O6 and O7 in the structure of (I) and (III) and the pair of equivalent atoms O5 (x, y, z and $1-x, y, z$) in the structure of (II) stem from the second, non-coordinating carboxylate anion. Each of these carboxylate oxygen atoms is an acceptor of three hydrogen bonds that are donated by two coordinating and by one non-coordinating water molecules. Numerical values of these interactions are collated in Tables 4, 5 and 6 for structures (I), (II) and (III)), respectively. Fig. 3*a*,*b* depict the hydrogen-bonded substructures in (II) and (III). The graph-set motifs are $R_5^5(10)$ (Etter *et*

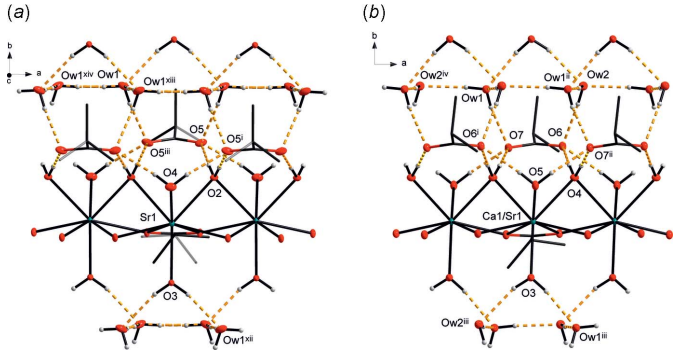


Figure 3
View of the hydrogen-bonded substructures in (*a*) (II) and (*b*) (III). The symmetry codes correspond to those given in Tables 5 and 6, respectively. Colour code is as in Fig. 1.

Table 4
Hydrogen-bond geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1*o*3···O*w*2^{iii}	0.840 (13)	2.063 (15)	2.8754 (16)	162.5 (15)
O3—H2*o*3···O*w*1^{iii}	0.840 (14)	1.954 (15)	2.7829 (17)	168.8 (15)
O4—H1*o*4···O6	0.840 (13)	1.936 (13)	2.7560 (15)	165.1 (14)
O4—H2*o*4···O7^{i}	0.840 (14)	1.925 (13)	2.7431 (15)	164.4 (14)
O5—H1*o*5···O6^{ii}	0.840 (13)	1.966 (13)	2.7805 (15)	163.0 (18)
O5—H2*o*5···O7^{i}	0.840 (13)	1.935 (13)	2.7597 (15)	166.9 (18)
O*w*1—H1*ow*1···O*w*2^{iv}	0.840 (5)	1.882 (4)	2.7192 (17)	174 (2)
O*w*1—H2*ow*1···O7	0.840 (13)	1.960 (13)	2.7872 (17)	168.0 (18)
O*w*2—H1*ow*2···O6	0.840 (13)	1.969 (13)	2.8070 (17)	175.1 (17)
O*w*2—H2*ow*2···O*w*1^{i}	0.840 (7)	1.886 (7)	2.7242 (18)	175 (2)

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

Table 5
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1*o*2···O5	0.820 (16)	1.936 (15)	2.7465 (14)	169.3 (17)
O3—H1*o*3···O*w*1^{iv}	0.827 (17)	2.022 (17)	2.8339 (18)	167.1 (18)
O4—H1*o*4···O5^{i}	0.844 (18)	1.964 (17)	2.7887 (16)	165.3 (19)
O*w*1—H1*ow*1···O5^{iii}	0.818 (18)	1.976 (19)	2.7913 (18)	174 (2)
O*w*1—H2*ow*1···O*w*1^{v}	0.82 (2)	1.92 (3)	2.736 (2)	176 (5)
O*w*1—H3*ow*1···O*w*1^{vi}	0.803 (17)	1.946 (17)	2.747 (2)	176 (5)

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

al., 1990), which include these atoms: O*w*1–O*w*1^{xiii}($-x+\frac{1}{2}, y, -z+\frac{1}{2}$)–O*w*1^{xiv}($x+\frac{1}{2}, y, -z+\frac{1}{2}$)–O*w*1^{iii}($-x+1, y, z$)–O3^{xv}($-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$) for (II) and O*w*1–O*w*2^{v}($-x-\frac{1}{2}, y, -z+\frac{1}{2}$)–O*w*1^{ii}($x+\frac{1}{2}, y, -z+\frac{1}{2}$)–O*w*2–O3^{vi}($-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$) for (III), respectively. Note the disorder of the hydrogen atoms H2*ow*1 and H3*ow*1 bound to O*w*1 in the structure of (II).

The third type of cohesion force is related to van der Waals interactions between the hydrophobic parts of the layers involving the methylene and methyl groups. The shortest C···C distances observed in (I) and (III) are C4···C7($x+\frac{1}{2}, -y, z+\frac{1}{2}$), which are 3.762 (2) and 3.746 (2) Å, respectively. The shortest C···C interactions in (II) for C3*b*···C6 ($x+\frac{1}{2}, -y+\frac{1}{2}, -z$) and C3*b*···C7 ($-x+\frac{3}{2}, -y+\frac{1}{2}, -z$) are 3.569 (4) and 3.146 (5) Å, respectively. These comparatively shorter distances indicate positional disorder (see *Refinement* section). As a general rule, it can be inferred that the shorter the C···C distances between adjacent groups, the greater is the probability for the occurrence of positional disorder of the 1-methylethyl group. See also the discussion regarding the observed disorder in barium dicalcium hexakis(propanoate) (CABAPN) by Stadnicka & Glazer (1980) where, however, the methyl carbons get as close as 4.05 (2) Å.

3. Synthesis and crystallization

For (III), two molar equivalents of $CaCO_3$ and one molar equivalent of $SrCO_3$ were neutralized by six molar equivalents of 2-methylpropionic acid (using 0.76 g of $CaCO_3$, 0.56 g of $SrCO_3$ and about 2.50 g of 2-methylpropionic acid). The solution was heated at 343 K, an excess of the acid was then added until the pH was between 5 and 6. The solution was filtered and then heated at 313 K until needle-like colourless crystals appeared. The pure Ca compound, (I), and the pure Sr compound, (II), were prepared for the sake of comparison. 0.85 g of $CaCO_3$ were neutralized by 1.5 g of 2-methylpropionic acid and 1.26 g of $SrCO_3$ were neutralized by 1.5 g of 2-methylpropionic acid, respectively; in each case these values correspond to the molar ratio of 1:2. The solutions were heated at 343 K, an excess of the acid was then added until the pH was between 5 and 6. The solutions were filtered and then heated at 313 K until needle-like colourless crystals appeared.

We have also tried to prepare magnesium 2-methylpropanoate and barium 2-methylpropanoate in a similar way as for (I)–(III). However, it turned out that the obtained crystals of the former compound correspond to VIQTOG, while the crystal structure of the latter compound is modulated and is being solved at present. Provided that we obtain a satisfactory model, the results will be published elsewhere.

Table 6
Hydrogen-bond geometry (Å, °) for (III).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1*o*3···O*w*2^{iii}	0.840 (11)	2.061 (12)	2.8767 (14)	163.6 (13)
O3—H2*o*3···O*w*1^{iii}	0.840 (12)	1.953 (12)	2.7842 (14)	169.8 (13)
O4—H1*o*4···O6	0.840 (11)	1.932 (10)	2.7498 (13)	164.2 (11)
O4—H2*o*4···O7^{i}	0.840 (11)	1.920 (10)	2.7382 (13)	164.2 (11)
O5—H1*o*5···O6^{ii}	0.840 (11)	1.964 (11)	2.7831 (13)	164.9 (15)
O5—H2*o*5···O7^{i}	0.840 (11)	1.944 (11)	2.7636 (13)	165.0 (14)
O*w*1—H1*ow*1···O*w*2^{iv}	0.840 (4)	1.888 (3)	2.7233 (14)	172.8 (16)
O*w*1—H2*ow*1···O7	0.840 (10)	1.951 (11)	2.7836 (14)	170.7 (15)
O*w*2—H1*ow*2···O6	0.840 (10)	1.967 (10)	2.8050 (14)	175.3 (15)
O*w*2—H2*ow*2···O*w*1^{i}	0.840 (5)	1.887 (5)	2.7248 (15)	175.2 (17)

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

4. Structure determination and refinement

Crystal data, data collection and structure refinement details are summarized in Table 7. In all structures, the methanetriyl hydrogen atoms were placed in calculated positions and refined with $C_{methanetriyl}$—$H_{methanetriyl}$ = 1.00 Å, $U_{iso}(H_{methanetriyl}) = 1.2U_{eq}(C_{methanetriyl})$. Methyl hydrogen atoms were discernible in difference electron-density maps and were refined with C_{methyl}—H_{methyl} = 0.98 Å, $U_{iso}(H_{methyl}) = 1.5U_{eq}(C_{methyl})$. Finally, difference electron density maps revealed the water hydrogen atoms, which were refined with restraints of O_{water}—H_{water} = 0.840 (1) Å.

For (II), difference electron-density maps revealed positional disorder of the 2-methylpropyl entity in both anions. This positional disorder affects the non-oxygen atoms that are not situated on the mirror plane (Wyckoff position 8*f*). In addition, methyl atoms C3*a* and C3*b* with their attached hydrogen atoms were first subjected to a trial refinement of their occupancies, which resulted in 0.510 (5) and 0.490 (5) for C3*a* and C3*b* and the attached hydrogen atoms, respectively. In the final model, the occupancies were fixed at 0.50 for these groups. O*w*1 is situated in a general position like its hydrogen atoms. As a result of the local environment, H1*ow*1 was assumed to be fully occupied while H2*ow*1 and H3*ow*1 were

Table 7
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$[Ca(C_4H_7O_2)(H_2O)_3]\cdot C_4H_7O_2\cdot 2H_2O$	$[Sr(C_4H_7O_2)(H_2O)_3]\cdot C_4H_7O_2\cdot 2H_2O$	$[Ca_{0.794}Sr_{0.206}(C_4H_7O_2)(H_2O)_3]\cdot C_4H_7O_2\cdot 2H_2O$
M_r	304.4	351.9	314.2
Crystal system, space group	Orthorhombic, *Pbca*	Orthorhombic, *Cmce*	Orthorhombic, *Pbca*
Temperature (K)	120	120	120
a, *b*, *c* (Å)	6.6662 (2), 19.5903 (7), 23.4286 (8)	6.8801 (3), 19.7520 (11), 23.2734 (13)	6.7153 (3), 19.6061 (10), 23.3498 (11)
V (Å^3)	3059.61 (18)	3162.8 (3)	3074.3 (3)
Z	8	8	8
Radiation type	Mo *Kα*	Mo *Kα*	Mo *Kα*
μ (mm^{-1})	0.44	3.44	1.08
Crystal size (mm)	0.27 × 0.17 × 0.05	0.24 × 0.12 × 0.08	0.59 × 0.18 × 0.08
Data collection			
Diffractometer	Bruker D8 VENTURE Kappa Duo PHOTON 100 CMOS	Bruker D8 VENTURE Kappa Duo PHOTON 100 CMOS	Bruker D8 VENTURE Kappa Duo PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2017)	Multi-scan (*SADABS*; Bruker, 2017)	Multi-scan (*SADABS*; Bruker, 2017)
T_{min}, T_{max}	0.889, 0.980	0.491, 0.770	0.573, 0.917
No. of measured, independent and observed [$I > 3\sigma(I)$] reflections	25865, 3511, 2955	21213, 1965, 1762	25462, 3533, 2787
R_{int}	0.033	0.032	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649	0.649	0.651
Refinement			
$R[F > 3\sigma(F)]$, $wR(F)$, S	0.039, 0.081, 1.99	0.021, 0.055, 1.79	0.026, 0.062, 1.54
No. of reflections	3511	1965	3533
No. of parameters	193	126	195
No. of restraints	10	9	10
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.38	0.37, −0.30	0.27, −0.25

Computer programs: *APEX2* and *SAINT* (Bruker, 2017), *SUPERFLIP* (Palatinus & Chapuis, 2007), *SHELXT* (Sheldrick, 2015), *JANA*2006 (Petříček *et al.*, 2014), *DIAMOND* (Brandenburg, 2015) and *publCIF* (Westrip, 2010).

supposed to be equally disordered over two positions. This assumption turned out to be in agreement with a trial refinement of their occupational parameters despite the very low scattering power of the hydrogen atoms.

For (III), the Ca/Sr occupation was refined [ratio 0.7936 (16):0.2064 (16)] under the assumption of the same position and the same displacement parameters for Ca and Sr and a fully occupied site. A B-C type 1 Lorentzian isotropic (Becker & Coppens, 1974) extinction correction was applied.

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supporting information

Acta Cryst. (2020). E**76**, 1684-1688 [https://doi.org/10.1107/S2056989020012888]

Crystal structures of *catena*-poly[[μ-aqua-diaqua(μ_3-2-methylpropanoato-κ^4O:O,O':O')calcium] 2-methylpropanoate dihydrate], *catena*-poly[[μ-aqua-diaqua(μ_3-2-methylpropanoato-κ^4O:O,O':O')strontium] 2-methylpropanoate dihydrate] and *catena*-poly[[μ-aqua-diaqua(μ_3-2-methylpropanoato-κ^4O:O,O':O')(calcium/strontium)] 2-methylpropanoate dihydrate]

Erika Samolová and Jan Fábry

Computing details

For all structures, data collection: *APEX2* (Bruker, 2017); cell refinement: *SAINT* (Bruker, 2017); data reduction: *SAINT* (Bruker, 2017). Program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007) for (I), (III); *SHELXT* (Sheldrick, 2015) for (II). For all structures, program(s) used to refine structure: *JANA*2006 (Petříček *et al.*, 2014); molecular graphics: *DIAMOND* (Brandenburg, 2015); software used to prepare material for publication: *publCIF* (Westrip, 2010).

\ *catena*-Poly[[μ-aqua-diaqua(μ_3-2-methylpropanoato-\ κ^4O:O,O':O')calcium] 2-methylpropanoate dihydrate] (I)

Crystal data

$[Ca(C_4H_7O_2)(H_2O)_3]\cdot C_4H_7O_2\cdot 2H_2O$
M_r = 304.4
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 6.6662 (2) Å
b = 19.5903 (7) Å
c = 23.4286 (8) Å
V = 3059.61 (18) Å^3
Z = 8
$F(000)$ = 1312
There have been used diffractions with I/σ(I)>20 for the unit cell determination.
D_x = 1.321 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9916 reflections
θ = 2.3–27.5°
μ = 0.44 mm^{-1}
T = 120 K
Prism, colourless
0.27 × 0.17 × 0.05 mm

Data collection

Bruker D8 VENTURE Kappa Duo PHOTON 100 CMOS diffractometer
Radiation source: X-ray tube
Quazar Mo multilayer optic monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2017)
T_{min} = 0.889, T_{max} = 0.980
25865 measured reflections
3511 independent reflections
2955 reflections with $I > 3\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°, θ_{min} = 2.1°
h = −8→8
k = −24→25
l = −30→30

Refinement

Refinement on F^2
$R[F > 3\sigma(F)] = 0.039$
$wR(F) = 0.081$
$S = 1.99$
3511 reflections
193 parameters
10 restraints
66 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 $w = 1/(\sigma^2(I) + 0.0004I^2)$
$(\Delta/\sigma)_{max} = 0.015$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ca1	0.51243 (4)	0.148107 (15)	0.283542 (12)	0.01153 (9)
O1	0.67506 (14)	0.12357 (6)	0.18811 (5)	0.0155 (3)
O2	0.34606 (14)	0.12092 (6)	0.19069 (4)	0.0161 (3)
C1	0.5086 (2)	0.11831 (8)	0.16303 (6)	0.0129 (4)
C2	0.4989 (2)	0.10975 (8)	0.09862 (7)	0.0165 (4)
H1c2	0.446418	0.153868	0.083208	0.0198*
C3	0.3552 (3)	0.05243 (10)	0.08221 (7)	0.0284 (6)
H1c3	0.349227	0.048592	0.040536	0.0426*
H2c3	0.403026	0.009271	0.098419	0.0426*
H3c3	0.221179	0.06258	0.097119	0.0426*
C4	0.7039 (2)	0.09872 (10)	0.07130 (7)	0.0238 (5)
H1c4	0.689212	0.096932	0.029701	0.0357*
H2c4	0.793135	0.136497	0.081634	0.0357*
H3c4	0.761063	0.055638	0.084979	0.0357*
O3	0.49949 (16)	0.03175 (6)	0.30728 (6)	0.0229 (4)
H1o3	0.3920 (16)	0.0098 (9)	0.3109 (8)	0.0343*
H2o3	0.594 (2)	0.0035 (8)	0.3078 (8)	0.0343*
O4	0.76674 (16)	0.23978 (6)	0.24860 (5)	0.0156 (3)
H1o4	0.737 (3)	0.2657 (8)	0.2213 (5)	0.0233*
H2o4	0.804 (3)	0.2649 (8)	0.2756 (5)	0.0233*
O5	0.52665 (15)	0.22166 (6)	0.36582 (5)	0.0168 (3)
H1o5	0.4273 (17)	0.2477 (8)	0.3694 (8)	0.0252*
H2o5	0.6286 (17)	0.2468 (8)	0.3667 (8)	0.0252*
O6	0.69414 (15)	0.30599 (6)	0.14688 (4)	0.0181 (3)
O7	0.36106 (15)	0.30246 (6)	0.15020 (5)	0.0180 (3)
C5	0.5238 (2)	0.31076 (8)	0.12347 (6)	0.0137 (4)
C6	0.5131 (2)	0.33159 (9)	0.06102 (7)	0.0179 (4)
H1c6	0.379623	0.317605	0.045454	0.0215*
C7	0.5390 (3)	0.40883 (9)	0.05774 (7)	0.0268 (5)
H1c7	0.530688	0.42353	0.017824	0.0403*
H2c7	0.432769	0.431102	0.079868	0.0403*
H3c7	0.670091	0.421507	0.073409	0.0403*
C8	0.6681 (3)	0.29543 (10)	0.02414 (7)	0.0295 (6)
H1c8	0.651725	0.309588	−0.015704	0.0443*
H2c8	0.803143	0.307466	0.037273	0.0443*
H3c8	0.649309	0.245941	0.02711	0.0443*

Ow1	0.22518 (17)	0.42507 (7)	0.19654 (5)	0.0225 (4)
H1ow1	0.1005 (5)	0.4296 (11)	0.1931 (8)	0.0337*
H2ow1	0.253 (3)	0.3889 (6)	0.1790 (8)	0.0337*
Ow2	0.81843 (18)	0.43259 (7)	0.19043 (5)	0.0229 (4)
H1ow2	0.782 (3)	0.3957 (5)	0.1754 (8)	0.0344*
H2ow2	0.791 (3)	0.4276 (11)	0.2252 (2)	0.0344*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.00793 (14)	0.01282 (15)	0.01385 (16)	0.00014 (12)	−0.00009 (12)	−0.00034 (11)
O1	0.0097 (5)	0.0190 (6)	0.0176 (6)	−0.0006 (4)	−0.0018 (4)	−0.0019 (5)
O2	0.0099 (5)	0.0213 (6)	0.0173 (6)	0.0007 (5)	0.0010 (4)	−0.0039 (5)
C1	0.0124 (7)	0.0089 (7)	0.0175 (7)	0.0007 (6)	−0.0003 (6)	0.0006 (6)
C2	0.0153 (7)	0.0187 (8)	0.0154 (7)	−0.0004 (7)	−0.0001 (6)	0.0011 (6)
C3	0.0300 (10)	0.0383 (12)	0.0169 (9)	−0.0148 (9)	−0.0002 (7)	−0.0072 (8)
C4	0.0217 (8)	0.0315 (11)	0.0182 (9)	−0.0031 (8)	0.0042 (7)	−0.0065 (8)
O3	0.0121 (5)	0.0141 (6)	0.0424 (7)	0.0006 (5)	0.0006 (5)	0.0027 (5)
O4	0.0172 (5)	0.0150 (6)	0.0145 (6)	0.0002 (5)	−0.0009 (4)	0.0004 (5)
O5	0.0114 (5)	0.0183 (6)	0.0207 (6)	−0.0007 (4)	0.0009 (5)	−0.0028 (5)
O6	0.0151 (5)	0.0217 (7)	0.0175 (6)	0.0018 (5)	−0.0029 (4)	0.0010 (5)
O7	0.0142 (5)	0.0200 (6)	0.0198 (6)	−0.0016 (5)	0.0029 (4)	0.0009 (5)
C5	0.0160 (7)	0.0078 (7)	0.0173 (7)	0.0001 (6)	0.0002 (6)	−0.0013 (6)
C6	0.0149 (7)	0.0217 (8)	0.0170 (8)	−0.0021 (7)	−0.0017 (6)	0.0014 (6)
C7	0.0380 (10)	0.0210 (9)	0.0215 (9)	0.0040 (8)	−0.0008 (8)	0.0061 (7)
C8	0.0419 (11)	0.0276 (11)	0.0191 (9)	0.0059 (9)	0.0078 (8)	0.0003 (8)
Ow1	0.0164 (6)	0.0178 (7)	0.0333 (7)	0.0000 (5)	0.0021 (5)	−0.0035 (5)
Ow2	0.0213 (6)	0.0194 (7)	0.0280 (7)	0.0000 (5)	−0.0028 (5)	−0.0035 (6)

Geometric parameters (Å, º)

Ca1—O3	2.3479 (12)	C8—H1c8	0.98
Ca1—O2^{i}	2.3653 (10)	C8—H2c8	0.98
Ca1—O1^{ii}	2.3938 (10)	C8—H3c8	0.98
Ca1—O5	2.4085 (12)	O3—H1o3	0.840 (13)
Ca1—O2	2.4993 (11)	O3—H2o3	0.840 (14)
Ca1—O1	2.5308 (11)	O4—H1o4	0.840 (13)
Ca1—O4^{ii}	2.5446 (11)	O4—H2o4	0.840 (14)
Ca1—O4	2.6019 (11)	O5—H1o5	0.840 (13)
O1—C1	1.2597 (17)	O5—H2o5	0.840 (13)
O2—C1	1.2637 (17)	Ow1—H1ow1	0.840 (5)
C1—C2	1.520 (2)	Ow1—H2ow1	0.840 (13)
C2—H1c2	1	Ow2—H1ow2	0.840 (13)
C2—C3	1.525 (2)	Ow2—H2ow2	0.840 (7)
C2—C4	1.524 (2)	C2—C6	4.435 (2)
C3—H1c3	0.98	C2—C8	4.189 (2)
C3—H2c3	0.98	C2—C8^{iii}	4.073 (2)
C3—H3c3	0.98	C3—C4^{iv}	4.443 (2)

C4—H1c4	0.98	C3—C7^{iii}	3.971 (2)
C4—H2c4	0.98	C3—C7^{v}	3.892 (3)
C4—H3c4	0.98	C3—C8^{iii}	4.080 (3)
O6—C5	1.2643 (18)	C4—C6^{vi}	3.965 (2)
O7—C5	1.2634 (18)	C4—C7^{vi}	3.762 (2)
C5—C6	1.520 (2)	C4—C7^{vii}	4.108 (3)
C6—H1c6	1	C4—C8	4.016 (3)
C6—C7	1.525 (2)	C4—C8^{vi}	4.345 (2)
C6—C8	1.522 (2)	C6—C8^{iii}	3.932 (2)
C7—H1c7	0.98	C8—C8^{iii}	3.944 (3)
C7—H2c7	0.98	C8—C8^{vi}	3.944 (3)
C7—H3c7	0.98		

O1—Ca1—O1^{ii}	127.55 (4)	H1c2—C2—C4	106.53
O1—Ca1—O2	51.73 (3)	C3—C2—C4	110.65 (14)
O1—Ca1—O2^{i}	77.29 (3)	C2—C3—H1c3	109.47
O1—Ca1—O3	92.33 (4)	C2—C3—H2c3	109.47
O1—Ca1—O4	64.79 (4)	C2—C3—H3c3	109.47
O1—Ca1—O4^{ii}	98.53 (4)	H1c3—C3—H2c3	109.47
O1—Ca1—O5	143.49 (4)	H1c3—C3—H3c3	109.47
O1^{ii}—Ca1—O2	77.40 (3)	H2c3—C3—H3c3	109.47
O1^{ii}—Ca1—O2^{i}	140.12 (4)	C2—C4—H1c4	109.47
O1^{ii}—Ca1—O3	72.83 (4)	C2—C4—H2c4	109.47
O1^{ii}—Ca1—O4	146.94 (4)	C2—C4—H3c4	109.47
O1^{ii}—Ca1—O4^{ii}	67.61 (4)	H1c4—C4—H2c4	109.47
O1^{ii}—Ca1—O5	86.28 (4)	H1c4—C4—H3c4	109.47
O2—Ca1—O2^{i}	126.26 (4)	H2c4—C4—H3c4	109.47
O2—Ca1—O3	89.03 (4)	C5—C6—H1c6	108.62
O2—Ca1—O4	99.34 (4)	C5—C6—C7	108.04 (13)
O2—Ca1—O4^{ii}	66.87 (4)	C5—C6—C8	112.92 (13)
O2—Ca1—O5	147.31 (4)	H1c6—C6—C7	110.74
O2^{i}—Ca1—O3	75.85 (4)	H1c6—C6—C8	105.64
O2^{i}—Ca1—O4	67.86 (4)	C7—C6—C8	110.89 (14)
O2^{i}—Ca1—O4^{ii}	147.11 (4)	C6—C7—H1c7	109.47
O2^{i}—Ca1—O5	83.88 (4)	C6—C7—H2c7	109.47
O3—Ca1—O4	140.23 (4)	C6—C7—H3c7	109.47
O3—Ca1—O4^{ii}	137.03 (4)	H1c7—C7—H2c7	109.47
O3—Ca1—O5	113.12 (4)	H1c7—C7—H3c7	109.47
O4—Ca1—O4^{ii}	80.74 (3)	H2c7—C7—H3c7	109.47
O4—Ca1—O5	79.23 (4)	C6—C8—H1c8	109.47
O4^{ii}—Ca1—O5	80.79 (4)	C6—C8—H2c8	109.47
Ca1—O1—Ca1^{i}	96.85 (4)	C6—C8—H3c8	109.47
Ca1—O2—Ca1^{ii}	98.46 (4)	H1c8—C8—H2c8	109.47
Ca1—O4—Ca1^{i}	91.45 (4)	H1c8—C8—H3c8	109.47
O1—C1—O2	120.85 (13)	H2c8—C8—H3c8	109.47
O1—C1—C2	120.64 (12)	H1o3—O3—H2o3	107.6 (15)
O2—C1—C2	118.50 (12)	H1o4—O4—H2o4	106.8 (14)
C1—C2—H1c2	106.15	H1o5—O5—H2o5	106.3 (14)

C1—C2—C3	111.00 (13)	H1ow1—Ow1—H2ow1	105 (2)
C1—C2—C4	113.24 (12)	H1ow2—Ow2—H2ow2	104.1 (19)
H1c2—C2—C3	108.99		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1*o*3···O*w*2^{viii}	0.840 (13)	2.063 (15)	2.8754 (16)	162.5 (15)
O3—H2*o*3···O*w*1^{viii}	0.840 (14)	1.954 (15)	2.7829 (17)	168.8 (15)
O4—H1*o*4···O6	0.840 (13)	1.936 (13)	2.7560 (15)	165.1 (14)
O4—H2*o*4···O7^{i}	0.840 (14)	1.925 (13)	2.7431 (15)	164.4 (14)
O5—H1*o*5···O6^{ii}	0.840 (13)	1.966 (13)	2.7805 (15)	163.0 (18)
O5—H2*o*5···O7^{i}	0.840 (13)	1.935 (13)	2.7597 (15)	166.9 (18)
O*w*1—H1*ow*1···O*w*2^{iv}	0.840 (5)	1.882 (4)	2.7192 (17)	174 (2)
O*w*1—H2*ow*1···O7	0.840 (13)	1.960 (13)	2.7872 (17)	168.0 (18)
O*w*2—H1*ow*2···O6	0.840 (13)	1.969 (13)	2.8070 (17)	175.1 (17)
O*w*2—H2*ow*2···O*w*1^{i}	0.840 (7)	1.886 (7)	2.7242 (18)	175 (2)

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

catena-Poly[[*μ*-aqua-diaqua(*μ*$_3$-2-methylpropanoato-\ *κ*^{4}*O*:*O*,*O*′:*O*′)strontium] 2-methylpropanoate dihydrate] (II)

Crystal data

$[Sr(C_4H_7O_2)(H_2O)_3]\cdot C_4H_7O_2\cdot 2H_2O$
M_r = 351.9
Orthorhombic, *Cmce*
Hall symbol: -C 2bc 2
a = 6.8801 (3) Å
b = 19.7520 (11) Å
c = 23.2734 (13) Å
V = 3162.8 (3) Å^3
Z = 8
F(000) = 1456
There have been used diffractions with I/*σ*(I)>20 for the unit cell determination.
D_x = 1.478 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9972 reflections
θ = 2.2–27.5°
μ = 3.44 mm^{-1}
T = 120 K
Prism, colourless
0.24 × 0.12 × 0.08 mm

Data collection

Bruker D8 VENTURE Kappa Duo PHOTON 100 CMOS diffractometer
Radiation source: X-ray tube
Quazar Mo multilayer optic monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2017)
T_{min} = 0.491, T_{max} = 0.770
21213 measured reflections
1965 independent reflections
1762 reflections with $I > 3\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°, θ_{min} = 2.2°
h = −8→8
k = −25→25
l = −30→27

Refinement

Refinement on F^2
$R[F > 3\sigma(F)]$ = 0.021
wR(*F*) = 0.055
S = 1.79
1965 reflections
126 parameters

9 restraints
62 constraints
Primary atom site location: dual-space method
H atoms treated by a mixture of independent and constrained refinement

Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(I) + 0.0004I^2)$
$(\Delta/\sigma)_{max} = 0.050$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Special details

Refinement. The positions of the methyl hydrogen atoms s H1C6, H2C6 and H3C6 were restrained by the angle restraints 56.250?(1) ° for the angles H1c6—C6—H2c6iii, H2c6—C6—H2c6iii, H2c6—C6—H2c6iii, H3c6—C6—H3c6iii ((iii) x + 1, y, z).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.5	0.145526 (9)	0.287511 (8)	0.01228 (6)	
O1	0.65991 (15)	0.11785 (5)	0.18632 (5)	0.0166 (3)	
C1	0.5	0.11399 (10)	0.15989 (9)	0.0130 (6)	
C2	0.5	0.10609 (11)	0.09535 (10)	0.0163 (6)	
H1c2	0.44623	0.149367	0.079711	0.0196*	0.5
C3a	0.3722 (5)	0.04613 (19)	0.07858 (15)	0.0299 (11)	0.5
H1c3a	0.429281	0.004234	0.093548	0.0448*	0.5
H2c3a	0.241896	0.052214	0.094806	0.0448*	0.5
H3c3a	0.363233	0.043419	0.036618	0.0448*	0.5
C3b	0.7010 (5)	0.09931 (18)	0.06811 (14)	0.0233 (10)	0.5
H1c3b	0.778228	0.139682	0.076891	0.035*	0.5
H2c3b	0.766218	0.059155	0.08359	0.035*	0.5
H3c3b	0.687385	0.094733	0.026376	0.035*	0.5
O2	0.75	0.23969 (8)	0.25	0.0159 (4)	
H1o2	0.717 (3)	0.2627 (9)	0.2223 (6)	0.0238*	
O3	0.5	0.02368 (8)	0.31496 (8)	0.0218 (5)	
H1o3	0.599 (2)	−0.0003 (10)	0.3152 (9)	0.0328*	
O4	0.5	0.22986 (9)	0.37100 (8)	0.0276 (6)	
H1o4	0.597 (2)	0.2558 (10)	0.3707 (9)	0.0414*	
O5	0.66149 (19)	0.30397 (6)	0.14868 (5)	0.0267 (4)	
C4	0.5	0.31058 (11)	0.12363 (10)	0.0204 (7)	
C5	0.5	0.33102 (9)	0.06050 (8)	0.0185 (6)	
H1c5	0.378186	0.314569	0.041672	0.0222*	0.5
C6	0.5	0.40764 (9)	0.05703 (8)	0.0570 (13)	
H1c6	0.365706	0.424153	0.056282	0.0855*	0.5
H2c6	0.56715	0.426313	0.090613	0.0855*	0.5
H3c6	0.567143	0.421994	0.021948	0.0855*	0.5
C7	0.6601 (5)	0.2941 (2)	0.02353 (15)	0.0302 (12)	0.5
H1c7	0.788041	0.313174	0.032479	0.0452*	0.5
H2c7	0.659677	0.245607	0.032529	0.0452*	0.5
H3c7	0.632122	0.300485	−0.017398	0.0452*	0.5
Ow1	0.1996 (2)	0.42598 (7)	0.19314 (6)	0.0323 (4)	
H1ow1	0.233 (3)	0.3890 (8)	0.1810 (10)	0.0484*	
H2ow1	0.228 (8)	0.424 (2)	0.2273 (9)	0.0484*	0.5
H3ow1	0.083 (2)	0.424 (2)	0.1927 (19)	0.0484*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01072 (11)	0.01255 (11)	0.01357 (12)	0	0	−0.00006 (8)
O1	0.0105 (5)	0.0232 (6)	0.0160 (6)	0.0002 (4)	−0.0021 (4)	−0.0048 (5)
C1	0.0139 (10)	0.0088 (9)	0.0163 (11)	0	0	−0.0014 (8)
C2	0.0160 (11)	0.0193 (11)	0.0137 (11)	0	0	0.0003 (9)
C3a	0.0282 (19)	0.044 (2)	0.0176 (17)	−0.0197 (17)	0.0033 (15)	−0.0109 (16)
C3b	0.0209 (16)	0.0328 (19)	0.0164 (16)	−0.0053 (14)	0.0062 (13)	−0.0033 (14)
O2	0.0209 (8)	0.0128 (7)	0.0140 (8)	0	−0.0028 (7)	0
O3	0.0114 (8)	0.0127 (8)	0.0415 (11)	0	0	0.0013 (7)
O4	0.0419 (12)	0.0215 (9)	0.0194 (9)	0	0	−0.0014 (7)
O5	0.0430 (8)	0.0199 (6)	0.0172 (6)	0.0072 (6)	−0.0088 (5)	0.0004 (5)
C4	0.0384 (14)	0.0081 (9)	0.0145 (11)	0	0	−0.0002 (8)
C5	0.0226 (12)	0.0198 (11)	0.0132 (11)	0	0	0.0012 (9)
C6	0.128 (3)	0.0216 (14)	0.0217 (15)	0	0	0.0094 (12)
C7	0.041 (2)	0.034 (2)	0.0162 (17)	0.0110 (17)	0.0050 (16)	−0.0005 (15)
Ow1	0.0426 (8)	0.0220 (7)	0.0322 (7)	−0.0113 (6)	0.0130 (7)	−0.0072 (6

Geometric parameters (Å, º)

Sr1—O1^{i}	2.4788 (10)	C5—C7^{iii}	1.577 (4)
Sr1—O1^{ii}	2.4788 (10)	C6—H1c6	0.98
Sr1—O3	2.4899 (16)	C6—H1c6^{iii}	0.98
Sr1—O4	2.5593 (18)	C6—H2c6	0.98
Sr1—O1	2.6561 (11)	C6—H2c6^{iii}	0.98
Sr1—O1^{iii}	2.6561 (11)	C6—H3c6	0.98
Sr1—O2	2.6796 (11)	C6—H3c6^{iii}	0.98
Sr1—O2^{ii}	2.6796 (11)	C7—H1c7	0.98
O1—C1	1.2629 (15)	C7—H2c7	0.98
C1—C2	1.510 (3)	C7—H3c7	0.98
C2—H1c2	1	Ow1—H1ow1	0.818 (18)
C2—H1c2^{iii}	1	Ow1—H2ow1	0.82 (2)
C2—C3a	1.526 (4)	Ow1—H3ow1	0.803 (17)
C2—C3a^{iii}	1.526 (4)	C2—C7	4.217 (4)
C2—C3b	1.527 (3)	C2—C7^{iv}	4.124 (4)
C2—C3b^{iii}	1.527 (3)	C2—C7^{v}	4.124 (4)
C3a—H1c3a	0.98	C2—C7^{iii}	4.217 (4)
C3a—H2c3a	0.98	C3a—C3a^{vi}	4.087 (5)
C3a—H3c3a	0.98	C3a—C3a^{vii}	4.449 (5)
C3b—H1c3b	0.98	C3a—C3b^{vii}	4.491 (5)
C3b—H2c3b	0.98	C3a—C6^{viii}	3.781 (4)
C3b—H3c3b	0.98	C3a—C6^{iv}	4.166 (4)
O2—H1o2	0.820 (16)	C3a—C7^{iv}	4.212 (5)
O2—H1o2^{i}	0.820 (16)	C3b—C3b^{ix}	4.115 (5)
O3—H1o3	0.827 (17)	C3b—C5^{x}	3.884 (4)
O3—H1o3^{iii}	0.827 (17)	C3b—C6^{xi}	4.317 (4)
O4—H1o4	0.844 (18)	C3b—C6^{x}	3.569 (4)

O4—H1o4^{iii}	0.844 (18)	C3b—C7	3.993 (5)
O5—C4	1.2615 (16)	C3b—C7^{x}	4.356 (5)
C4—C5	1.524 (3)	C3b—C7^{v}	3.146 (5)
C5—H1c5	1	C5—C7^{iv}	3.923 (4)
C5—H1c5^{iii}	1	C5—C7^{v}	3.923 (4)
C5—C6	1.516 (3)	C7—C7^{iv}	4.007 (5)
C5—C7	1.577 (4)	C7—C7^{x}	4.007 (5)

O1—Sr1—O1^{i}	77.38 (3)	C2—C3a—H3c3a	109.47
O1—Sr1—O1^{ii}	124.29 (3)	H1c3a—C3a—H2c3a	109.47
O1—Sr1—O1^{iii}	48.94 (3)	H1c3a—C3a—H3c3a	109.47
O1—Sr1—O2	65.67 (3)	H1c3a^{iii}—C3a—H3c3a	103.72
O1—Sr1—O2^{ii}	96.88 (2)	H2c3a—C3a—H3c3a	109.47
O1—Sr1—O3	91.64 (5)	C2—C3b—H1c3b	109.47
O1—Sr1—O4	143.81 (4)	C2—C3b—H2c3b	109.47
O1^{i}—Sr1—O1^{ii}	141.45 (4)	C2—C3b—H3c3b	109.47
O1^{i}—Sr1—O1^{iii}	124.29 (3)	H1c3b—C3b—H2c3b	109.47
O1^{i}—Sr1—O2	68.11 (3)	H1c3b—C3b—H3c3b	109.47
O1^{i}—Sr1—O2^{ii}	147.04 (3)	H2c3b—C3b—H3c3b	109.47
O1^{i}—Sr1—O3	73.97 (3)	H1o2—O2—H1o2^{i}	112.6 (16)
O1^{i}—Sr1—O4	87.54 (3)	H1o3—O3—H1o3^{iii}	110.2 (17)
O1^{ii}—Sr1—O1^{iii}	77.38 (3)	H1o4—O4—H1o4^{iii}	105.2 (18)
O1^{ii}—Sr1—O2	147.04 (3)	O5—C4—O5^{iii}	123.46 (19)
O1^{ii}—Sr1—O2^{ii}	68.11 (3)	O5—C4—C5	118.23 (10)
O1^{ii}—Sr1—O3	73.97 (3)	O5^{iii}—C4—C5	118.23 (10)
O1^{ii}—Sr1—O4	87.54 (3)	C4—C5—H1c5	109.66
O1^{iii}—Sr1—O2	96.88 (2)	C4—C5—H1c5^{iii}	109.66
O1^{iii}—Sr1—O2^{ii}	65.67 (3)	C4—C5—C6	108.42 (15)
O1^{iii}—Sr1—O3	91.64 (5)	C4—C5—C7	113.80 (17)
O1^{iii}—Sr1—O4	143.81 (4)	C4—C5—C7^{iii}	113.80 (17)
O2—Sr1—O2^{ii}	79.87 (3)	H1c5—C5—H1c5^{iii}	113.88
O2—Sr1—O3	138.98 (2)	H1c5—C5—C6	107.52
O2—Sr1—O4	78.21 (3)	C5—C6—H1c6	109.47
O2^{ii}—Sr1—O3	138.98 (2)	C5—C6—H1c6^{iii}	109.47
O2^{ii}—Sr1—O4	78.21 (3)	C5—C6—H2c6	109.47
O3—Sr1—O4	115.74 (6)	C5—C6—H2c6^{iii}	109.47
Sr1—O1—Sr1^{i}	97.34 (4)	C5—C6—H3c6	109.47
Sr1—O2—Sr1^{i}	92.08 (5)	C5—C6—H3c6^{iii}	109.47
O1—C1—O1^{iii}	121.20 (18)	H1c6—C6—H2c6	109.47
O1—C1—C2	119.39 (10)	H1c6—C6—H3c6	109.47
O1^{iii}—C1—C2	119.39 (10)	H1c6^{iii}—C6—H2c6^{iii}	109.47
C1—C2—H1c2	105.88	H1c6^{iii}—C6—H3c6^{iii}	109.47
C1—C2—H1c2^{iii}	105.88	H2c6—C6—H3c6	109.47
C1—C2—C3a	109.54 (19)	H2c6^{iii}—C6—H3c6^{iii}	109.47
C1—C2—C3a^{iii}	109.54 (19)	H1c7—C7—H2c7	109.47
C1—C2—C3b	114.96 (14)	H1c7—C7—H3c7	109.47
C1—C2—C3b^{iii}	114.96 (14)	H2c7—C7—H3c7	109.47
H1c2—C2—C3a	110.93	H1c7—H3c7—H2c7	60

H1c2—C2—C3b	105.01	H1ow1—Ow1—H2ow1	103 (4)
H1c2^{iii}—C2—C3a^{iii}	110.93	H1ow1—Ow1—H3ow1	104 (4)
C2—C3a—H1c3a	109.47	H2ow1—Ow1—H3ow1	104 (5)
C2—C3a—H2c3a	109.47		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*o*2···O5	0.820 (16)	1.936 (15)	2.7465 (14)	169.3 (17)
O3—H1*o*3···O*w*1^{xii}	0.827 (17)	2.022 (17)	2.8339 (18)	167.1 (18)
O4—H1*o*4···O5^{i}	0.844 (18)	1.964 (17)	2.7887 (16)	165.3 (19)
O*w*1—H1*ow*1···O5^{iii}	0.818 (18)	1.976 (19)	2.7913 (18)	174 (2)
O*w*1—H2*ow*1···O*w*1^{xiii}	0.82 (2)	1.92 (3)	2.736 (2)	176 (5)
O*w*1—H3*ow*1···O*w*1^{xiv}	0.803 (17)	1.946 (17)	2.747 (2)	176 (5)

Symmetry codes: (i) −*x*+3/2, *y*, −*z*+1/2; (iii) −*x*+1, *y*, *z*; (xii) −*x*+1, *y*−1/2, −*z*+1/2; (xiii) −*x*+1/2, *y*, −*z*+1/2; (xiv) −*x*, *y*, *z*.

catena-Poly[[*μ*-aqua-diaqua(*μ*$_3$-2-methylpropanoato-\ *κ*^{4}*O*:*O*,*O*′:*O*′)(calcium/strontium)] 2-methylpropanoate dihydrate] (III)

Crystal data

$[Ca_{0.794}Sr_{0.206}(C_4H_7O_2)(H_2O)_3]\cdot C_4H_7O_2\cdot 2H_2O$
M_r = 314.2
Orthorhombic, *Pbca*
Hall symbol: –P 2ac 2ab
a = 6.7153 (3) Å
b = 19.6061 (10) Å
c = 23.3498 (11) Å
V = 3074.3 (3) Å^3
Z = 8
F(000) = 1342
There have been used diffractions with I/*σ*(I)>20 for the unit cell determination.
D_x = 1.358 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9952 reflections
θ = 2.3–27.5°
μ = 1.08 mm^{-1}
T = 120 K
Prism, colourless
0.59 × 0.18 × 0.08 mm

Data collection

Bruker D8 VENTURE Kappa Duo PHOTON 100 CMOS diffractometer
Radiation source: X-ray tube
Quazar Mo multilayer optic monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2017)
T_{min} = 0.573, T_{max} = 0.917
25462 measured reflections
3533 independent reflections
2787 reflections with *I* > 3*σ*(*I*)
R_{int} = 0.030
θ_{max} = 27.5°, θ_{min} = 2.1°
h = −8→8
k = −25→24
l = −30→30

Refinement

Refinement on F^2
$R[F > 3\sigma(F)]$ = 0.026
wR(*F*) = 0.062
S = 1.54
3533 reflections
195 parameters
10 restraints
75 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 $w = 1/(\sigma^2(I) + 0.0004I^2)$
$(\Delta/\sigma)_{max}$ = 0.041

$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Extinction correction: B-C type 1 Lorentzian isotropic (Becker & Coppens, 1974)
Extinction coefficient: 3100 (900)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ca1	0.51172 (3)	0.147275 (10)	0.285280 (8)	0.01318 (7)	0.7936 (16)
Sr1	0.51172 (3)	0.147275 (10)	0.285280 (8)	0.01318 (7)	0.2064 (16)
O1	0.67331 (12)	0.12224 (5)	0.18768 (4)	0.0183 (3)	
O2	0.34659 (12)	0.11963 (5)	0.18993 (4)	0.0193 (3)	
C1	0.50850 (17)	0.11708 (6)	0.16238 (5)	0.0157 (4)	
C2	0.49970 (18)	0.10867 (7)	0.09788 (6)	0.0197 (4)	
H1c2	0.446005	0.152571	0.082499	0.0236*	
C3	0.3591 (2)	0.05083 (8)	0.08122 (6)	0.0329 (5)	
H1c3	0.350464	0.047978	0.039391	0.0494*	
H2c3	0.410119	0.00765	0.096456	0.0494*	
H3c3	0.22658	0.059708	0.097106	0.0494*	
C4	0.7032 (2)	0.09886 (8)	0.07048 (6)	0.0271 (5)	
H1c4	0.688453	0.096553	0.02877	0.0407*	
H2c4	0.789504	0.137344	0.080535	0.0407*	
H3c4	0.762668	0.056376	0.084481	0.0407*	
O3	0.49864 (13)	0.02977 (5)	0.30914 (5)	0.0278 (3)	
H1o3	0.3934 (13)	0.0071 (7)	0.3132 (7)	0.0417*	
H2o3	0.5919 (16)	0.0012 (6)	0.3097 (7)	0.0417*	
O4	0.76561 (13)	0.23946 (5)	0.24874 (4)	0.0186 (3)	
H1o4	0.734 (2)	0.2655 (6)	0.2217 (4)	0.0279*	
H2o4	0.807 (2)	0.2641 (6)	0.2757 (4)	0.0279*	
O5	0.52603 (13)	0.22321 (5)	0.36693 (4)	0.0223 (3)	
H1o5	0.4290 (15)	0.2502 (6)	0.3690 (7)	0.0335*	
H2o5	0.6251 (14)	0.2493 (6)	0.3680 (6)	0.0335*	
O6	0.69194 (12)	0.30554 (5)	0.14705 (4)	0.0194 (3)	
O7	0.36161 (13)	0.30221 (5)	0.15020 (4)	0.0197 (3)	
C5	0.52316 (17)	0.31043 (6)	0.12361 (5)	0.0151 (3)	
C6	0.51349 (18)	0.33128 (7)	0.06086 (5)	0.0198 (4)	
H1c6	0.381257	0.317376	0.044996	0.0237*	
C7	0.5386 (2)	0.40842 (7)	0.05757 (6)	0.0296 (5)	
H1c7	0.434506	0.430552	0.080392	0.0444*	
H2c7	0.669669	0.421115	0.072612	0.0444*	
H3c7	0.527634	0.423207	0.017606	0.0444*	
C8	0.6670 (2)	0.29505 (8)	0.02419 (6)	0.0333 (5)	
H1c8	0.649839	0.308533	−0.015923	0.05*	
H2c8	0.800974	0.307583	0.037063	0.05*	
H3c8	0.649318	0.245608	0.027732	0.05*	
Ow1	0.22415 (14)	0.42437 (5)	0.19632 (5)	0.0245 (3)	
H1ow1	0.1006 (4)	0.4288 (9)	0.1920 (7)	0.0368*	
H2ow1	0.253 (2)	0.3873 (4)	0.1804 (6)	0.0368*	
Ow2	0.81968 (14)	0.43158 (5)	0.19043 (4)	0.0247 (3)	

H1ow2	0.787 (2)	0.3938 (4)	0.1763 (6)	0.0371*
H2ow2	0.793 (2)	0.4272 (9)	0.22542 (17)	0.0371*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.01013 (11)	0.01378 (12)	0.01565 (12)	0.00007 (8)	−0.00019 (8)	−0.00028 (8)
Sr1	0.01013 (11)	0.01378 (12)	0.01565 (12)	0.00007 (8)	−0.00019 (8)	−0.00028 (8)
O1	0.0151 (4)	0.0226 (5)	0.0172 (5)	−0.0002 (4)	−0.0021 (4)	−0.0025 (4)
O2	0.0155 (5)	0.0251 (5)	0.0174 (5)	−0.0001 (4)	0.0011 (4)	−0.0033 (4)
C1	0.0187 (6)	0.0096 (6)	0.0190 (6)	0.0001 (5)	−0.0004 (5)	−0.0004 (5)
C2	0.0224 (7)	0.0211 (7)	0.0155 (6)	−0.0011 (6)	−0.0007 (5)	0.0007 (5)
C3	0.0371 (9)	0.0443 (10)	0.0173 (7)	−0.0170 (8)	−0.0002 (6)	−0.0081 (7)
C4	0.0282 (8)	0.0356 (9)	0.0174 (7)	−0.0058 (7)	0.0041 (6)	−0.0059 (7)
O3	0.0155 (5)	0.0175 (5)	0.0504 (7)	0.0009 (4)	−0.0001 (5)	−0.0016 (5)
O4	0.0240 (5)	0.0167 (5)	0.0151 (5)	−0.0007 (4)	−0.0006 (4)	0.0003 (4)
O5	0.0154 (5)	0.0276 (6)	0.0240 (5)	−0.0002 (4)	0.0007 (4)	0.0028 (4)
O6	0.0168 (4)	0.0239 (5)	0.0176 (5)	0.0003 (4)	−0.0022 (4)	0.0013 (4)
O7	0.0174 (5)	0.0223 (5)	0.0194 (5)	−0.0011 (4)	0.0029 (4)	0.0017 (4)
C5	0.0179 (6)	0.0107 (6)	0.0167 (6)	−0.0006 (5)	0.0000 (5)	−0.0013 (5)
C6	0.0187 (6)	0.0247 (7)	0.0159 (6)	−0.0023 (6)	−0.0016 (5)	0.0012 (5)
C7	0.0421 (9)	0.0257 (8)	0.0210 (7)	0.0039 (7)	−0.0007 (6)	0.0075 (6)
C8	0.0479 (9)	0.0339 (9)	0.0181 (7)	0.0067 (8)	0.0086 (7)	0.0007 (7)
Ow1	0.0189 (5)	0.0206 (6)	0.0341 (6)	−0.0002 (4)	0.0022 (4)	−0.0031 (5)
Ow2	0.0237 (5)	0.0235 (6)	0.0269 (6)	0.0002 (4)	−0.0025 (4)	−0.0035 (5)

Geometric parameters (Å, º)

Ca1—Sr1	0	C6—C7	1.524 (2)
Ca1—O3	2.3719 (10)	C6—C8	1.517 (2)
Ca1—O2^{i}	2.3845 (9)	C7—H1c7	0.98
Ca1—O1^{ii}	2.4091 (8)	C7—H2c7	0.98
Ca1—O5	2.4209 (10)	C7—H3c7	0.98
Ca1—O2	2.5457 (9)	C8—H1c8	0.98
Ca1—O1	2.5714 (9)	C8—H2c8	0.98
Ca1—O4^{ii}	2.5747 (9)	C8—H3c8	0.98
Ca1—O4	2.6271 (9)	O3—H1o3	0.840 (11)
Sr1—O1	2.5714 (9)	O3—H2o3	0.840 (12)
Sr1—O1^{ii}	2.4091 (8)	O4—H1o4	0.840 (11)
Sr1—O2	2.5457 (9)	O4—H2o4	0.840 (11)
Sr1—O2^{i}	2.3845 (9)	O5—H1o5	0.840 (11)
Sr1—O3	2.3719 (10)	O5—H2o5	0.840 (11)
Sr1—O4	2.6271 (9)	Ow1—H1ow1	0.840 (4)
Sr1—O4^{ii}	2.5747 (9)	Ow1—H2ow1	0.840 (10)
Sr1—O5	2.4209 (10)	Ow2—H1ow2	0.840 (10)
O1—C1	1.2587 (14)	Ow2—H2ow2	0.840 (5)
O2—C1	1.2644 (15)	C2—C6	4.450 (2)
C1—C2	1.5160 (18)	C2—C8	4.192 (2)

C2—H1c2	1	C2—C8^{iii}	4.084 (2)
C2—C3	1.526 (2)	C3—C7^{iii}	3.972 (2)
C2—C4	1.5210 (18)	C3—C7^{iv}	3.903 (2)
C3—H1c3	0.98	C3—C8^{iii}	4.105 (2)
C3—H2c3	0.98	C4—C6^{v}	3.9526 (19)
C3—H3c3	0.98	C4—C7^{v}	3.746 (2)
C4—H1c4	0.98	C4—C7^{vi}	4.128 (2)
C4—H2c4	0.98	C4—C8	4.003 (2)
C4—H3c4	0.98	C4—C8^{v}	4.349 (2)
O6—C5	1.2624 (14)	C6—C8^{iii}	3.936 (2)
O7—C5	1.2603 (15)	C8—C8^{iii}	3.959 (2)
C5—C6	1.5225 (18)	C8—C8^{v}	3.959 (2)
C6—H1c6	1		

O1—Ca1—O1^{ii}	126.26 (3)	Ca1—O2—Ca1^{ii}	98.63 (3)
O1—Ca1—O2	50.81 (3)	Ca1—O2—Sr1^{ii}	98.63 (3)
O1—Ca1—O2^{i}	76.93 (3)	Ca1^{ii}—O2—Sr1	98.63 (3)
O1—Ca1—O3	92.20 (3)	Ca1^{ii}—O2—O1	160.57 (5)
O1—Ca1—O4	64.51 (3)	Ca1^{ii}—O2—O1^{ii}	54.25 (2)
O1—Ca1—O4^{ii}	97.55 (3)	Ca1^{ii}—O2—O3^{ii}	51.84 (3)
O1—Ca1—O5	143.00 (3)	Ca1^{ii}—O2—O4^{ii}	60.18 (3)
O1^{ii}—Ca1—O2	76.99 (3)	Ca1^{ii}—O2—O5^{ii}	48.02 (2)
O1^{ii}—Ca1—O2^{i}	141.23 (3)	Sr1—O2—Sr1^{ii}	98.63 (3)
O1^{ii}—Ca1—O3	72.88 (3)	Ca1—O4—Ca1^{i}	91.94 (3)
O1^{ii}—Ca1—O4	146.87 (3)	Ca1—O4—Sr1^{i}	91.94 (3)
O1^{ii}—Ca1—O4^{ii}	67.56 (3)	Ca1^{i}—O4—Sr1	91.94 (3)
O1^{ii}—Ca1—O5	87.50 (3)	Sr1—O4—Sr1^{i}	91.94 (3)
O2—Ca1—O2^{i}	125.08 (3)	O1—C1—O2	120.94 (11)
O2—Ca1—O3	89.00 (3)	O1—C1—C2	120.62 (11)
O2—Ca1—O4	98.35 (3)	O2—C1—C2	118.44 (10)
O2—Ca1—O4^{ii}	66.42 (3)	C1—C2—H1c2	106.1
O2—Ca1—O5	146.83 (3)	C1—C2—C3	110.99 (11)
O2^{i}—Ca1—O3	75.94 (3)	C1—C2—C4	113.37 (10)
O2^{i}—Ca1—O4	67.86 (3)	H1c2—C2—C3	108.97
O2^{i}—Ca1—O4^{ii}	147.12 (3)	H1c2—C2—C4	106.36
O2^{i}—Ca1—O5	84.90 (3)	C3—C2—C4	110.76 (11)
O3—Ca1—O4	140.23 (3)	C2—C3—H1c3	109.47
O3—Ca1—O4^{ii}	136.93 (3)	C2—C3—H2c3	109.47
O3—Ca1—O5	114.44 (4)	C2—C3—H3c3	109.47
O4—Ca1—O4^{ii}	80.41 (3)	H1c3—C3—H2c3	109.47
O4—Ca1—O5	78.87 (3)	H1c3—C3—H3c3	109.47
O4^{ii}—Ca1—O5	80.60 (3)	H2c3—C3—H3c3	109.47
O1—Sr1—O1^{ii}	126.26 (3)	C2—C4—H1c4	109.47
O1—Sr1—O2	50.81 (3)	C2—C4—H2c4	109.47
O1—Sr1—O2^{i}	76.93 (3)	C2—C4—H3c4	109.47
O1—Sr1—O3	92.20 (3)	H1c4—C4—H2c4	109.47
O1—Sr1—O4	64.51 (3)	H1c4—C4—H3c4	109.47
O1—Sr1—O4^{ii}	97.55 (3)	H2c4—C4—H3c4	109.47

O1—Sr1—O5	143.00 (3)	O6—C5—O7	123.33 (11)
O1^{ii}—Sr1—O2	76.99 (3)	O6—C5—C6	118.43 (10)
O1^{ii}—Sr1—O2^{i}	141.23 (3)	O7—C5—C6	118.14 (10)
O1^{ii}—Sr1—O3	72.88 (3)	C5—C6—H1c6	108.73
O1^{ii}—Sr1—O4	146.87 (3)	C5—C6—C7	108.08 (11)
O1^{ii}—Sr1—O4^{ii}	67.56 (3)	C5—C6—C8	112.86 (11)
O1^{ii}—Sr1—O5	87.50 (3)	H1c6—C6—C7	110.49
O2—Sr1—O2^{i}	125.08 (3)	H1c6—C6—C8	105.47
O2—Sr1—O3	89.00 (3)	C7—C6—C8	111.19 (11)
O2—Sr1—O4	98.35 (3)	C6—C7—H1c7	109.47
O2—Sr1—O4^{ii}	66.42 (3)	C6—C7—H2c7	109.47
O2—Sr1—O5	146.83 (3)	C6—C7—H3c7	109.47
O2^{i}—Sr1—O3	75.94 (3)	H1c7—C7—H2c7	109.47
O2^{i}—Sr1—O4	67.86 (3)	H1c7—C7—H3c7	109.47
O2^{i}—Sr1—O4^{ii}	147.12 (3)	H2c7—C7—H3c7	109.47
O2^{i}—Sr1—O5	84.90 (3)	C6—C8—H1c8	109.47
O3—Sr1—O4	140.23 (3)	C6—C8—H2c8	109.47
O3—Sr1—O4^{ii}	136.93 (3)	C6—C8—H3c8	109.47
O3—Sr1—O5	114.44 (4)	H1c8—C8—H2c8	109.47
O4—Sr1—O4^{ii}	80.41 (3)	H1c8—C8—H3c8	109.47
O4—Sr1—O5	78.87 (3)	H2c8—C8—H3c8	109.47
O4^{ii}—Sr1—O5	80.60 (3)	H1o3—O3—H2o3	105.9 (12)
Ca1—O1—Ca1^{i}	97.29 (3)	H1o4—O4—H2o4	107.3 (11)
Ca1—O1—Sr1^{i}	97.29 (3)	H1o5—O5—H2o5	103.2 (11)
Ca1^{i}—O1—Sr1	97.29 (3)	H1ow1—Ow1—H2ow1	105.5 (15)
Ca1^{i}—O1—O2	160.27 (5)	H1ow2—Ow2—H2ow2	103.8 (15)
Sr1—O1—Sr1^{i}	97.29 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1*o*3···O*w*2^{vii}	0.840 (11)	2.061 (12)	2.8767 (14)	163.6 (13)
O3—H2*o*3···O*w*1^{vii}	0.840 (12)	1.953 (12)	2.7842 (14)	169.8 (13)
O4—H1*o*4···O6	0.840 (11)	1.932 (10)	2.7498 (13)	164.2 (11)
O4—H2*o*4···O7^{i}	0.840 (11)	1.920 (10)	2.7382 (13)	164.2 (11)
O5—H1*o*5···O6^{ii}	0.840 (11)	1.964 (11)	2.7831 (13)	164.9 (15)
O5—H2*o*5···O7^{i}	0.840 (11)	1.944 (11)	2.7636 (13)	165.0 (14)
O*w*1—H1*ow*1···O*w*2^{viii}	0.840 (4)	1.888 (3)	2.7233 (14)	172.8 (16)
O*w*1—H2*ow*1···O7	0.840 (10)	1.951 (11)	2.7836 (14)	170.7 (15)
O*w*2—H1*ow*2···O6	0.840 (10)	1.967 (10)	2.8050 (14)	175.3 (15)
O*w*2—H2*ow*2···O*w*1^{i}	0.840 (5)	1.887 (5)	2.7248 (15)	175.2 (17)

Symmetry codes: (i) $x+1/2, y, -z+1/2$; (ii) $x-1/2, y, -z+1/2$; (vii) $-x+1, y-1/2, -z+1/2$; (viii) $x-1, y, z$.