Mixed Ca/Sr salt forms of salicylic acid, tuning structure and aqueous solubility

Pamela Allan, Jean-Baptiste Arlin, Alan R. Kennedy* and Aiden Walls

Westchem, Department of Pure & Applied Chemistry, University of Strathclyde, 295 Cathedral Street, Glasgow G1 1XL, Scotland
Correspondence email: a.r.kennedy@strath.ac.uk

Abstract

Ten isostructural single-crystal diffraction studies of mixed cation Ca/Sr salt forms of the salicylate anion are presented, $[Ca_{(1-x)}Sr_x(C_7H_5O_3)_2(OH_2)_2]$, where x = 0, 0.041, 0.083, 0.165, 0.306, 0.529, 0.632, 0.789, 0.835 and 1. The structure of an isostructural Sr/Ba species $[Sr_{0.729}Ba_{0.271}(C_7H_5O_3)_2(OH_2)_2]$, is also described. The Ca/Sr structures form a series where, with increasing Sr content, the unit cell expands in both the crystallographic a and c directions (by 1.80 and 3.18% respectively), but contracts slightly in the b direction (−0.31%). The largest percentage structural expansion lies parallel to the direction of propagation of the one-dimensional coordination polymer that is the primary structural feature. This structural expansion is thus associated with increased M—O distances. Aqueous solubility measurements show that solubility generally increases with increasing Sr content·Thus tuning the composition of these mixed counterion salt forms leads to sytematic structural changes and allows solubility to be tuned to values between those for the pure Ca and Sr species.

1. Comment

Introduction.

The most common way to alter the material properties of acidic Active Pharmaceutical Ingredients (APIs) is to generate salt forms using s-block metal ions (Stahl, 2008). Commonly the material property of prime interest to manufacturers is aqueous solubility, as this has known links to dissolution rate and hence to bioavailability of APIs. We have previously published a study on comparative structure and solubility trends in series of alkaline earth metal salt forms of pharmaceutically relevant benzoic acid derivatives (Arlin *et al.*, 2011). For salts of the API salicylic acid, this study found a rank order solubility of Mg > Ba > Sr > Ca and showed that whilst the Ca and Sr salts were isostructural and isomorphic, the structures of the Mg and Ba salts were very different (Arlin *et al.*, 2011; Debuyst *et al.*, 1979). The structures of the Ca and the Sr salts are both dihydrates with 8-coordinate metal centres and one-dimensional coordination polymer structures that propagate through Ca—O—Ca bridges, where the bridging O atom is from the carboxylate group. In contrast, the structure of the Ba salt is a monohydrate two-dimensional coordination polymer and the Mg salt structure is a discrete tetrahydrate complex of type $[Mg(C_7H_5O_3)_2(OH_2)_4]$.

For crystalline systems the isostructuality of the Ca and Sr salicylate salt forms should, according to the Hume-Rothery rules, favour the possibility of forming solid solutions with mixed Ca/Sr sites (Mizutani, 2011; Hume-Rothery & Powell, 1935). Structures with such mixed-metal formulations are ubiquitous in inorganic systems (*e.g.* minerals or alloys, Sekine *et al.*, 2017; Wahlberg *et al.*, 1965; Davidson *et al.*, 2005; Johnson *et al.*, 1970) but are much less studied in molecular or organic salt species. Whilst molecular structures with sites with mutal substitution of s-block metal ions are known both for mixed group 2 metal species (*e.g.* Trifa *et al.*, 2007) and for mixed group 1 with groups 2 metal species (*e.g.* Kennedy *et al.*, 1998) there are surprisingly few examples of systematic structural studies of this phenomenon. The most relevant work that we are aware of is a report on the structures of Ca and Sr formate, which also gives unit cell data for 3 intermediate mixed Ca/Sr forms (Matsui *et al.*, 1980).

Results.

Eleven samples of salicylate salts were prepared using different initial aqueous Ca/Sr ratios. Of these, ten gave single-crystal samples suitable for accurate structural determination, see Table 1. A l l structures had similar unit cells to the parent "pure" structures. Where both Ca and Sr were present in solution, both metal types were always found incorporated within the structure and sharing one structural site. In all structures, the metal ions occupy a site that is a special position, namely a crystallographic centre of symmetry, Fig. 1. After several trial calculations, all mixed-metal structures were refined with EADP and EXYZ constraints on the metal centres. The composition of the mixed metal site was found by refinement of site occupancy factors, constrained to total 1. The Ca/Sr ratios as measured by diffraction are given in Tables 1 and 13. It can be seen that whilst the single-crystal derived metal ratios do not match the ratios of metals available in the parent solutions, a broad control of crystal composition is possible *i.e.* the greater the proportion of aqueous Sr provided, the greater the incorportaion of Sr into the crystal. Note that all solutions with >50% Ca available gave more Ca incorporation into the solid than expected simply from the solution composition. The equivalent case for the lower % Ca samples is much less clear cut, Table 13.

Attempts were also made to incorporate other group 2 ions into similar structures. No incorporation of Mg was observed, which is perhaps unsurprizing given the large change in ionic radii between Mg and Ca and the fundamentally different structure observed for Mg salicylate as opposed to the Ca and Sr structures (Hume-Rothery & Powell, 1935; Arlin *et al.*, 2011). On both size and structural considerations, the Hume-Rothery rules would suggest that Ba is a more likely candidate for inclusion. Indeed, a 50:50 Sr/Ba solution did give a mixed metal species, Fig. 2, that is isostructural with the Ca and Sr structures described herein. The Sr/Ba occupancy refined to 72.9 (4):27.1 (4). The solid thus has much less Ba present than was available from solution, which perhaps indicates that the larger Ba ion is not such a good fit to the coordination geometry demands of this structural type.

Unit Cell Changes

As expected, the unit cell volume increases as the amount of Sr present in the structure increases. Examination of Fig. 3 shows an overall increase in volume of 4.72%. The increase in volume is relatively linear between approximately 10 and 80% Sr with small discontinuities at either end of this range. Fig. 4 shows the change in length of the individual a, b and c dimensions. With increasing Sr content the structure expands in both the a and c directions (by 1.80 and 3.18% respectively), however the b dimension is relatively invariant and even contracts slightly (−0.31%). The Sr/Ba structure continues these trends with a larger unit cell volume (1529.04 (11) $Å^3$), expansion of a and c (16.8381 (7) and 7.9433 (3) Å respectively) and a relatively large contraction of b (to 11.4349 (5) Å). This pattern of changes to the unit-cell dimensions with changing metal content is obviously different to the unit cell changes caused by thermal expansion of $[Ca(C_7H_5O_3)_2(OH_2)_2]$, Fig. 5, where all axes′ dimensions increase with increasing temperature.

Bond Length Considerations.

A simple driver of unit cell expansion is that increasing the amount of the large Sr ion present leads directly to the observed increase in M—O bond distances (where this observed distance is an average of the component Ca—O and Sr—O distances), Table 14. Of the four structurally independent M—O distances, the bond to the neutral water ligand increases more with increasing Sr content than do the three bonds to formally anionic atoms of carboxylate groups (compare an overall 6.39% increase for M1—O1W compared to 4.63, 5.40 and 4.37% for bonds to O3, $O3^{ii}$ and $O2^{ii}$ respectively, ii = $1 - x, 1 - y, -z$). This fits with the known greater bonding affinity of Ca for neutral water as compared to Sr (Kennedy *et al.*, 2009). It also results in Ca1—O1W being the shortest coordination bond for the Ca species but Sr1—O3 being the shortest coordination bond for the Sr species, the apparent shortest bond lengths swapping at the 50:50 Ca:Sr point. Similarly, further lengthening of the apparent M—O distances occurs in the Sr/Ba structure. Again it is M—O3 that is shortest with distances of 2.5654 (17), 2.5486 (13), 2.6647 (13) and 2.8113 (13) Å for M1—O1W, M1—O3, M1—$O3^{ii}$ and M1—$O2^{ii}$ respectively.

Increasing the average M—O distances causes the metal-to-metal seperations along the coordination polymer to expand. As the coordination polymer propagates parallel to the *c* axis, this explains why it is the c direction that shows the largest percentage expansion. It is harder to explain why the b dimension does not expand but the a dimension does. Fig. 6 illustrates the packing of the coordination polymers. The metal centres define a rhomboid (of side 10.025 Å for calcium salicylate) and with internal M—M—*M* angles of approximately 70 and 110 °. Those M—O vectors that do not lie along the c direction are diagonaly related to both the a and b directions. The hydrogen bonding network follows the same general directions with water-phenol-water interactions linking between coordination chains in both the a and b directions, Tables 2 to 12. The only hydrogen bond interaction that changes systematically with changing metal content is the O1W—H2W···O2^{ii} bond. This lengthens and becomes more linear with increasing Sr content. However, this interaction lies along the chain of the coordination polymer and is thus associated with the expansion of the *c* axis and not the behaviour of a or b. As b is shorter than a, the polymer chains stack closer in the b direction, as measured by *M*···M distances, than in the a direction. A final unique feature of the invariant b direction is that only in this direction are there close hydrophobic contacts (shortest C···C 3.2354 (19) Å) between aromatic rings. These interactions are highlighted in Fig. 6. These are interdigitated interactions that lie alongside a relatively poorly packed region of the structure. It may be these interdigitated features that buffer the *b* axis against expansion.

Aqueous Solubility.

The variation of aqueous solubility with increasing Sr content is illustrated in Fig. 7. Note that here the % Sr is calculated by AA analysis of the bulk powders and does not rely on diffraction analysis of single crystals. It is clear that in general solubility increases with increasing Sr content, with a maximum increase of approximately 50%. Most solubility values lie between those measured for the end points defined by pure calcium salicylate and pure strontium salicylate. Thus it is possible to tune the solubilty of the model API salicylate by using mixed cation formulations. Prior to undertaking this work, we postulated that mixed cation salts may give higher solubility values than their equivalent pure species due to the difficulty of incorporating differently sized "impurity" ions into an energetically minimized lattice. We note that the sample with 82.0% Sr content does indeed give a higher solubility than that found for 100% Sr but that these points have relatively high associated standard deviations and that the difference is thus not significant. There is thus no evidence for enhanced solubility.

2. Synthesis and crystallization

Samples were prepared by dissolving with stirring salicylic acid and the appropriate ratio of calcium carbonate and strontium carbonate in warm water. As an example the Ca:Sr 90:10 sample was prepared from 1.67 g (12.07 mmol) of salicylic acid, 0.55 g (5.49 mmol) of $CaCO_3$ and 0.09 g (0.61 mmol) of $SrCO_3$. Slow evaporation of the solvent gave suitable crystals after 5 to 7 days. These were isolated from the remaining mother liquor by filtration.

Metal ratio of bulk samples was determined by atomic absorption spectrometry as measured by a Thermo Scientific iCE 3300 Series AA spectrometer. A calibration graph was formed using standard solutions containing 1, 2, 2.5, 3, 4 and 5 mg l^{-1} of Sr ions. Samples of salicylate salts were diluted so as to contain approximately 4 mg l^{-1} of Sr each.

Aqueous solubility measurements were performed by forming slurries from approximately 1 g of sample and 8 cm^3 of deionized water. The slurries were placed in an incubator at 298 K and stirred for 10 days. After filtering through 0.2 micron syringe filters, the solutions were diluted to suitable concentration to match a 5 point calibration curve constructed from standard strontium salicylate solutions measured with an Agilent Technologies Cary 60 uv-vis instrument at 295 cm^{-1}. All measurements were performed in duplicate. Solubility results are reported as mol/dm^3 of salicylate ion. The solids isolated from 100% Ca and 100% Sr slurries were checked by powder X-ray diffraction which showed the phases isolated to be consistent with the single-crystal structures described herein (Arlin *et al.*, 2011).

The unit-cell parameters for the variable temperature study are all based on measurements of the same crystal using an Oxford Diffraction Gemini S diffractometer and monochromated λ = 1.54148 Å radiation. All cells were calculated using at least 1326 reflections using the program *CrysAlis PRO* (Agilent, 2014).

3. Refinement

For all structures, H atoms bound to C atoms were placed in the expected geometric positions and treated in riding modes with C–H = 0.95 and $U(H)_{iso} = 1.2U(C)_{eq}$. H atoms bound to O atoms were located by difference synthesis and refined isotropically. For the structures with 100% Ca and 100% Sr it was found neccessary to restrain O–H distances to 0.85 (2) Å.

Table 1

Experimental details

	(CaSal)	(CaSr9010)	(CaSr8020)	(CaSr7030)	(CaSr6040)
Crystal data					
Chemical formula	$C_{14}H_{14}CaO_8$	$C_{14}H_{14}Ca_{0.96}O_8Sr_{0.04}$	$C_{14}H_{14}Ca_{0.92}O_8Sr_{0.08}$	$C_{14}H_{14}Ca_{0.83}O_8Sr_{0.17}$	$C_{14}H_{14}Ca_{0.69}O_8Sr_{0.31}$
M_r	350.33	352.27	354.25	358.18	364.90
Crystal system, space group	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*
Temperature (K)	150	150	150	150	150
a, *b*, *c* (Å)	16.4233 (14), 11.5002 (9), 7.6203 (6)	16.4335 (7), 11.4974 (4), 7.6301 (3)	16.4344 (3), 11.4853 (2), 7.6417 (2)	16.4921 (10), 11.5345 (8), 7.6679 (5)	16.5626 (13), 11.4921 (10), 7.7041 (7)
β (°)	91.914 (7)	91.778 (4)	91.785 (2)	91.838 (6)	91.588 (8)
V (Å^3)	1438.5 (2)	1440.96 (10)	1441.70 (5)	1457.90 (16)	1465.8 (2)
Z	4	4	4	4	4
Radiation type	Mo *Kα*	Mo *Kα*	Mo *Kα*	Mo *Kα*	Mo *Kα*
μ (mm^{-1})	0.48	0.61	0.75	1.01	1.47
Crystal size (mm)	0.30 × 0.25 × 0.10	0.30 × 0.22 × 0.08	0.35 × 0.28 × 0.08	0.26 × 0.22 × 0.12	0.30 × 0.20 × 0.10
Data collection					
Diffractometer	Oxford Diffraction Xcalibur E	Oxford Diffraction Xcalibur E	Oxford Diffraction Xcalibur E	Oxford Diffraction Xcalibur E	Oxford Diffraction Xcalibur E
Absorption correction	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.914, 1.000	0.818, 1.000	0.802, 1.000	0.896, 1.000	0.845, 1.000

No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6630, 1638, 1489	16338, 1640, 1582	16552, 1642, 1568	3241, 1659, 1494	9041, 1656, 1576
R_{int}	0.027	0.036	0.030	0.032	0.035
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.649	0.649	0.650	0.650	0.650
Refinement					
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.068, 1.08	0.021, 0.055, 1.07	0.021, 0.053, 1.08	0.036, 0.093, 1.09	0.024, 0.056, 1.11
No. of reflections	1638	1640	1642	1659	1656
No. of parameters	117	118	118	118	118
No. of restraints	2	0	0	0	0
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	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})	0.34, −0.20	0.29, −0.21	0.31, −0.23	0.37, −0.38	0.28, −0.20

	(CaSr5050)	(CaSr3070)	(CaSr2080)	(CaSr1090)	(Sr100)
Crystal data					
Chemical formula	$C_{14}H_{14}Ca_{0.47}O_8Sr_{0.53}$	$C_{14}H_{14}Ca_{0.37}O_8Sr_{0.63}$	$C_{14}H_{14}Ca_{0.21}O_8Sr_{0.79}$	$C_{14}H_{14}Ca_{0.17}O_8Sr_{0.83}$	$C_{14}H_{14}O_8Sr$
M_r	375.48	380.38	387.85	390.00	397.87
Crystal system, space group	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*
Temperature (K)	150	150	150	150	150
a, *b*, *c* (Å)	16.5994 (10), 11.4832 (6), 7.7650 (5)	16.6319 (6), 11.4995 (4), 7.7729 (3)	16.6650 (11), 11.4816 (7), 7.8105 (5)	16.6693 (9), 11.4865 (7), 7.8446 (4)	16.7182 (6), 11.4644 (4), 7.8627 (3)
β (°)	91.555 (5)	91.599 (4)	91.576 (6)	91.510 (5)	91.660 (3)
V (Å^3)	1479.57 (15)	1486.05 (9)	1493.90 (16)	1501.50 (14)	1506.37 (9)
Z	4	4	4	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	2.17	2.49	2.98	3.11	5.36
Crystal size (mm)	0.30 × 0.20 × 0.10	0.30 × 0.25 × 0.12	0.26 × 0.25 × 0.15	0.30 × 0.15 × 0.06	0.6 × 0.5 × 0.2
Data collection					
Diffractometer	Oxford Diffraction Xcalibur E	Oxford Diffraction Xcalibur E	Oxford Diffraction Xcalibur E	Oxford Diffraction Xcalibur E	Oxford Diffraction Gemini S

Absorption correction	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Analytical *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.847, 1.000	0.735, 1.000	0.896, 1.000	0.462, 1.000	0.120, 0.461
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8207, 1691, 1546	16351, 1704, 1622	6802, 1716, 1594	8538, 1720, 1589	2454, 1272, 1259
R_{int}	0.046	0.036	0.041	0.044	0.016
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.650	0.650	0.649	0.650	0.591
Refinement					
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.058, 1.12	0.021, 0.052, 1.06	0.024, 0.054, 1.06	0.027, 0.065, 1.08	0.027, 0.073, 1.17
No. of reflections	1691	1704	1716	1720	1272
No. of parameters	118	118	118	118	118
No. of restraints	0	0	0	0	3
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	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})	0.25, −0.28	0.49, −0.25	0.31, −0.32	0.70, −0.48	0.68, −0.49

(SrBa)

Crystal data	
Chemical formula	$C_{14}H_{14}Ba_{0.27}O_8Sr_{0.73}$
M_r	411.35
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	16.8381 (7), 11.4349 (5), 7.9433 (3)
β (°)	91.280 (4)
V (Å^3)	1529.04 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.31
Crystal size (mm)	0.28 × 0.25 × 0.15
Data collection	
Diffractometer	Oxford Diffraction Xcalibur E
Absorption correction	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.728, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10452, 1754, 1685
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.021, 0.044, 1.17
No. of reflections	1754
No. of parameters	118
No. of restraints	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.31

Computer programs: *CrysAlis PRO* (Agilent, 2014), *CrysAlis PRO*, *SIR92* (Altomare *et al.*, 1994), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae, 2008), *SHELXL2014*.

Table 2

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.81 (2)	1.90 (2)	2.6256 (13)	148 (2)
O1*W*—H1*W*···O1^{i}	0.82 (2)	2.03 (2)	2.8391 (14)	169 (2)
O1*W*—H2*W*···O2^{ii}	0.84 (2)	2.05 (2)	2.8795 (14)	169 (2)

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

Table 3

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.872 (18)	1.842 (19)	2.6204 (10)	147.6 (16)
O1*W*—H1*W*···O1^{i}	0.864 (19)	1.981 (19)	2.8361 (11)	169.8 (16)
O1*W*—H2*W*···O2^{ii}	0.853 (18)	2.043 (18)	2.8820 (11)	167.6 (15)

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

Table 4

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.865 (18)	1.857 (18)	2.6165 (11)	145.5 (16)
O1*W*—H1*W*···O1^{i}	0.85 (2)	2.00 (2)	2.8350 (11)	169.7 (17)
O1*W*—H2*W*···O2^{ii}	0.836 (19)	2.06 (2)	2.8849 (12)	166.8 (17)

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

Table 5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.87 (3)	1.86 (3)	2.6216 (18)	145 (3)
O1*W*—H1*W*···O1^{i}	0.87 (3)	1.99 (3)	2.8409 (19)	166 (3)
O1*W*—H2*W*···O2^{ii}	0.86 (3)	2.06 (3)	2.891 (2)	161 (3)

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

Table 6

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.87 (2)	1.83 (2)	2.6174 (14)	148 (2)
O1*W*—H1*W*···O1^{i}	0.89 (3)	1.95 (3)	2.8372 (15)	170 (2)
O1*W*—H2*W*···O2^{ii}	0.89 (2)	2.02 (2)	2.8984 (16)	168.7 (19)

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

Table 7

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.90 (3)	1.81 (3)	2.6075 (17)	147 (2)
O1*W*—H1*W*···O1^{i}	0.86 (3)	1.97 (3)	2.8276 (19)	171 (2)
O1*W*—H2*W*···O2^{ii}	0.90 (3)	2.02 (3)	2.906 (2)	169 (2)

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

Table 8

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.90 (3)	1.81 (3)	2.6096 (15)	147 (2)
O1*W*—H1*W*···O1^{i}	0.84 (3)	1.99 (3)	2.8255 (16)	175 (3)
O1*W*—H2*W*···O2^{ii}	0.85 (2)	2.06 (2)	2.9074 (17)	173 (2)

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

Table 9

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.89 (3)	1.84 (3)	2.6031 (17)	142 (2)
O1*W*—H1*W*···O1^{i}	0.88 (3)	1.94 (3)	2.8244 (18)	173 (2)
O1*W*—H2*W*···O2^{ii}	0.85 (3)	2.06 (3)	2.911 (2)	178 (2)

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

Table 10

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.90 (3)	1.80 (3)	2.597 (2)	147 (3)
O1*W*—H1*W*···O1^{i}	0.81 (3)	2.03 (3)	2.827 (2)	173 (3)
O1*W*—H2*W*···O2^{ii}	0.92 (3)	2.01 (3)	2.921 (2)	173 (3)

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

Table 11

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.83 (2)	1.89 (3)	2.604 (2)	145 (4)
O1*W*—H1*W*···O1^{i}	0.82 (2)	2.01 (2)	2.823 (3)	172 (4)
O1*W*—H2*W*···O2^{ii}	0.84 (2)	2.08 (2)	2.925 (3)	178 (4)

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

Table 12

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H7···O2	0.89 (3)	1.80 (3)	2.5938 (18)	148 (3)
O1*W*—H1*W*···O1^{i}	0.82 (3)	2.00 (3)	2.820 (2)	172 (3)
O1*W*—H2*W*···O2^{ii}	0.86 (3)	2.08 (3)	2.923 (2)	169 (3)

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

Table 13

Solubility data and Ca/Sr ratios. The ratios are given as, that available from parent solution, that determined from single-crystal refinement and that determined from AA for bulk sample.

Sr % in Solution	Sr % single-crystal	Sr % bulk AA	Solubility mol/dm^3
0	0	0	0.185 (4)
9.9	4.1 (2)	7.01	0.195 (2)
19.9	8.3 (2)	16.04	0.201 (2)
30.2	16.5 (3)	23.67	0.209 (2)
39.7	30.6 (3)	36.13	0.235 (10)
49.5	52.9 (3)	51.88	0.231 (4)
60.3		56.67	0.242 (8)
69.8	63.2 (4)	75.59	0.235 (6)
80.7	78.9 (4)	82.01	0.279 (20)
88.8	83.5 (5)	90.28	0.257 (8)
100	100	100	0.257 (10)

Table 14

Variation in apparent *M*-O bond lengths (Å) for different Ca:Sr ratios. ii = $1 - x$, $1 - y$, $-z$.

Sr % from single-crystal	M-O1W	M-O3	M-O3^{ii}	M-O2^{ii}
0	2.3761 (10)	2.4005 (9)	2.4781 (9)	2.6333 (9)′
4.1 (2)	2.3814 (8)	2.4027 (7)	2.4910 (7)	2.6458 (7)
8.3 (2)	2.3830 (9)	2.4062 (8)	2.4968 (8)	2.6506 (8)
16.5 (3)	2.3968 (15)	2.4224 (13)	2.5166 (14)	2.6739 (13)
30.6 (3)	2.4211 (11)	2.4324 (10)	2.5336 (10)	2.6907 (10)
52.9 (3)	2.4608 (15)	2.4596 (13)	2.5621 (13)	2.7143 (12)
63.2 (4)	2.4777 (12)	2.4686 (10)	2.5749 (10)	2.7260 (10)
78.9 (4)	2.5020 (14)	2.4849 (12)	2.5902 (12)	2.7368 (12)
83.5 (5)	2.5091 (17)	2.4953 (13)	2.5990 (14)	2.7400 (15)
100	2.528 (2)	2.5116 (17)	2.6120 (17)	2.7484 (17)

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Figure 1

Top, contents of the asymmetric unit of the 69:31 Ca:Sr species with non-H atoms shown as 50% probability ellipsoids. Atom label M1 is the mixed metal site occupied by Ca1 and Sr1. Bottom, for the same structure, part of the one-dimensional coordination polymer that extends in the crystallographic c direction. H atoms are omitted for clarity.

Figure 2

Top, contents of the asymmetric unit for the 73:27 Sr:Ba species, with non-H atoms shown as 50% probability ellipsoids. Atom label M1 is the mixed metal site occupied by Sr1 and Ba1. Bottom, for the same structure, part of the one-dimensional coordination polymer that extends in the crystallographic c direction. H atoms are omitted for clarity.

Figure 3

Expansion of unit cell volume with increasing Sr content. For comparison, the unit cell volume of the 72.9:27.1 Sr:Ba species is 1529.04 (11) Å^3.

Figure 4

Change in length of unit cell axes with increase in Sr content. All percentages are given as change from the 100% Ca species. Black = *a* axis, green = *b* axis and blue = *c* axis.

Figure 5

Change in unit cell volume and length of unit cell axes with change in temperature for calcium salicylate. All percentages are given as change from the corresponding values at 123 K. Black = *a* axis, green = *b* axis and blue = *c* axis.

Figure 6

Packing diagram of 100% Ca structure viewed along the *c* axis and hence down the length of the coordination polymers. Hydrogen bond contacts are drawn as dotted lines and hydrogen atoms are omitted for clarity. The purple ring highlights one area of the hydrophobic contacts discussed in the main text.

Figure 7

Aqueous solubility *versus* increasing Sr content, as measured by AA analysis of bulk powders.

supporting information

Mixed Ca/Sr salt forms of salicylic acid, tuning structure and aqueous solubility

Computing details

For all structures, data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *Mercury* (Macrae, 2008); software used to prepare material for publication: *SHELXL2014*.

(CaSal)

Crystal data

$C_{14}H_{14}CaO_8$
$M_r = 350.33$
Monoclinic, $C2/c$
$a = 16.4233$ (14) Å
$b = 11.5002$ (9) Å
$c = 7.6203$ (6) Å
$\beta = 91.914$ (7)°
$V = 1438.5$ (2) Å^3
$Z = 4$
$F(000) = 728$
$D_x = 1.618$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3540 reflections
$\theta = 3.4$–30.3°
$\mu = 0.48$ mm^{-1}
$T = 150$ K
Prism, colourless
0.30 × 0.25 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: sealed tube
ω scans
Absorption correction: multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
$T_{min} = 0.914$, $T_{max} = 1.000$
6630 measured reflections
1638 independent reflections
1489 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -21\rightarrow19$
$k = -14\rightarrow14$
$l = -9\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.068$
$S = 1.08$
1638 reflections
117 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 1.0416P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ca1	0.5000	0.45083 (3)	−0.2500	0.01114 (11)
O1	0.25618 (6)	0.25378 (9)	0.26849 (13)	0.0177 (2)
O2	0.37861 (6)	0.40061 (8)	0.26911 (12)	0.0153 (2)
O3	0.45483 (6)	0.39842 (8)	0.03573 (12)	0.0148 (2)
O1W	0.39906 (6)	0.32390 (9)	−0.37242 (13)	0.0196 (2)
C1	0.30186 (8)	0.18870 (11)	0.15844 (16)	0.0135 (3)
C2	0.27321 (9)	0.07827 (12)	0.11389 (17)	0.0180 (3)
H2	0.2225	0.0518	0.1550	0.022*
C3	0.31936 (9)	0.00752 (12)	0.00916 (18)	0.0206 (3)
H3	0.3005	−0.0685	−0.0191	0.025*
C4	0.39285 (9)	0.04591 (12)	−0.05540 (19)	0.0201 (3)
H4	0.4244	−0.0039	−0.1257	0.024*
C5	0.41968 (8)	0.15710 (11)	−0.01649 (17)	0.0164 (3)
H5	0.4692	0.1842	−0.0630	0.020*
C6	0.37466 (8)	0.23026 (11)	0.09084 (16)	0.0126 (3)
C7	0.40414 (8)	0.34989 (11)	0.13286 (16)	0.0116 (3)
H1O	0.2805 (13)	0.3137 (18)	0.288 (3)	0.041 (6)*
H1W	0.3577 (10)	0.2942 (16)	−0.336 (2)	0.037 (5)*
H2W	0.3917 (12)	0.3364 (16)	−0.481 (2)	0.035 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.01109 (19)	0.01165 (18)	0.01080 (19)	0.000	0.00189 (13)	0.000
O1	0.0145 (5)	0.0186 (5)	0.0203 (5)	−0.0045 (4)	0.0060 (4)	−0.0023 (4)
O2	0.0163 (5)	0.0156 (5)	0.0143 (5)	−0.0024 (4)	0.0034 (4)	−0.0028 (4)
O3	0.0149 (5)	0.0144 (4)	0.0154 (5)	−0.0032 (3)	0.0037 (4)	0.0011 (4)
O1W	0.0171 (6)	0.0261 (6)	0.0156 (5)	−0.0084 (4)	0.0024 (4)	0.0007 (4)
C1	0.0134 (7)	0.0158 (6)	0.0111 (6)	−0.0005 (5)	−0.0005 (5)	0.0016 (5)
C2	0.0189 (7)	0.0187 (7)	0.0164 (6)	−0.0074 (5)	−0.0007 (5)	0.0035 (5)
C3	0.0302 (8)	0.0141 (6)	0.0173 (7)	−0.0054 (6)	−0.0030 (6)	0.0004 (6)
C4	0.0259 (8)	0.0161 (7)	0.0185 (7)	0.0022 (5)	0.0027 (6)	−0.0032 (6)
C5	0.0154 (7)	0.0180 (7)	0.0158 (6)	0.0002 (5)	0.0023 (5)	0.0006 (5)
C6	0.0141 (6)	0.0122 (6)	0.0116 (6)	−0.0014 (5)	−0.0012 (5)	0.0013 (5)
C7	0.0098 (6)	0.0133 (6)	0.0116 (6)	0.0008 (4)	−0.0014 (4)	0.0015 (5)

Geometric parameters (Å, º)

Ca1—O1W^{i}	2.3761 (10)	O3—C7	1.2624 (15)
Ca1—O1W	2.3761 (10)	O3—Ca1^{ii}	2.4781 (9)
Ca1—O3	2.4005 (9)	O1W—H1W	0.819 (15)
Ca1—O3^{i}	2.4005 (9)	O1W—H2W	0.842 (15)
Ca1—O3^{ii}	2.4781 (9)	C1—C2	1.3924 (18)

Ca1—O3^{iii}	2.4781 (9)	C1—C6	1.4016 (18)
Ca1—O2^{ii}	2.6333 (9)	C2—C3	1.383 (2)
Ca1—O2^{iii}	2.6333 (9)	C2—H2	0.9500
Ca1—C7^{ii}	2.9041 (13)	C3—C4	1.390 (2)
Ca1—C7^{iii}	2.9041 (13)	C3—H3	0.9500
Ca1—Ca1^{ii}	3.9745 (4)	C4—C5	1.3814 (19)
Ca1—Ca1^{iv}	3.9745 (4)	C4—H4	0.9500
Ca1—H2W	2.789 (17)	C5—C6	1.4013 (18)
O1—C1	1.3669 (16)	C5—H5	0.9500
O1—H1O	0.81 (2)	C6—C7	1.4898 (17)
O2—C7	1.2740 (15)	C7—Ca1^{ii}	2.9041 (13)
O2—Ca1^{ii}	2.6333 (9)		

O1W^{i}—Ca1—O1W	104.19 (5)	O1W^{i}—Ca1—Ca1^{iv}	121.93 (3)
O1W^{i}—Ca1—O3	73.88 (3)	O1W—Ca1—Ca1^{iv}	79.67 (3)
O1W—Ca1—O3	88.24 (3)	O3—Ca1—Ca1^{iv}	161.97 (2)
O1W^{i}—Ca1—O3^{i}	88.24 (3)	O3^{i}—Ca1—Ca1^{iv}	36.10 (2)
O1W—Ca1—O3^{i}	73.88 (3)	O3^{ii}—Ca1—Ca1^{iv}	115.02 (3)
O3—Ca1—O3^{i}	150.92 (5)	O3^{iii}—Ca1—Ca1^{iv}	34.80 (2)
O1W^{i}—Ca1—O3^{ii}	88.94 (3)	O2^{ii}—Ca1—Ca1^{iv}	74.82 (2)
O1W—Ca1—O3^{ii}	151.41 (3)	O2^{iii}—Ca1—Ca1^{iv}	83.84 (2)
O3—Ca1—O3^{ii}	70.90 (3)	C7^{ii}—Ca1—Ca1^{iv}	93.02 (3)
O3^{i}—Ca1—O3^{ii}	132.73 (3)	C7^{iii}—Ca1—Ca1^{iv}	59.88 (3)
O1W^{i}—Ca1—O3^{iii}	151.41 (3)	Ca1^{ii}—Ca1—Ca1^{iv}	146.93 (2)
O1W—Ca1—O3^{iii}	88.94 (3)	O1W^{i}—Ca1—H2W	112.3 (4)
O3—Ca1—O3^{iii}	132.73 (3)	O1W—Ca1—H2W	16.4 (3)
O3^{i}—Ca1—O3^{iii}	70.90 (3)	O3—Ca1—H2W	104.1 (3)
O3^{ii}—Ca1—O3^{iii}	91.21 (4)	O3^{i}—Ca1—H2W	61.3 (4)
O1W^{i}—Ca1—O2^{ii}	84.30 (3)	O3^{ii}—Ca1—H2W	156.4 (4)
O1W—Ca1—O2^{ii}	153.69 (3)	O3^{iii}—Ca1—H2W	75.2 (4)
O3—Ca1—O2^{ii}	118.07 (3)	O2^{ii}—Ca1—H2W	137.7 (3)
O3^{i}—Ca1—O2^{ii}	81.68 (3)	O2^{iii}—Ca1—H2W	82.7 (4)
O3^{ii}—Ca1—O2^{ii}	51.10 (3)	C7^{ii}—Ca1—H2W	153.4 (3)
O3^{iii}—Ca1—O2^{ii}	73.75 (3)	C7^{iii}—Ca1—H2W	81.4 (4)
O1W^{i}—Ca1—O2^{iii}	153.69 (3)	Ca1^{ii}—Ca1—H2W	135.9 (4)
O1W—Ca1—O2^{iii}	84.30 (3)	Ca1^{iv}—Ca1—H2W	63.3 (3)
O3—Ca1—O2^{iii}	81.68 (3)	C1—O1—H1O	107.4 (15)
O3^{i}—Ca1—O2^{iii}	118.07 (3)	C7—O2—Ca1^{ii}	88.94 (7)
O3^{ii}—Ca1—O2^{iii}	73.75 (3)	C7—O3—Ca1	150.77 (8)
O3^{iii}—Ca1—O2^{iii}	51.10 (3)	C7—O3—Ca1^{ii}	96.42 (7)
O2^{ii}—Ca1—O2^{iii}	99.10 (4)	Ca1—O3—Ca1^{ii}	109.10 (3)
O1W^{i}—Ca1—C7^{ii}	90.01 (4)	Ca1—O1W—H1W	134.2 (13)
O1W—Ca1—C7^{ii}	165.80 (4)	Ca1—O1W—H2W	110.8 (13)
O3—Ca1—C7^{ii}	95.75 (3)	H1W—O1W—H2W	108.3 (18)
O3^{i}—Ca1—C7^{ii}	107.23 (3)	O1—C1—C2	117.45 (12)
O3^{ii}—Ca1—C7^{ii}	25.59 (3)	O1—C1—C6	122.09 (11)
O3^{iii}—Ca1—C7^{ii}	78.33 (3)	C2—C1—C6	120.46 (12)
O2^{ii}—Ca1—C7^{ii}	26.01 (3)	C3—C2—C1	119.33 (13)
O2^{iii}—Ca1—C7^{ii}	82.80 (3)	C3—C2—H2	120.3
O1W^{i}—Ca1—C7^{iii}	165.80 (4)	C1—C2—H2	120.3
O1W—Ca1—C7^{iii}	90.01 (4)	C2—C3—C4	121.08 (13)
O3—Ca1—C7^{iii}	107.23 (3)	C2—C3—H3	119.5

O3^{i}—Ca1—C7^{iii}	95.75 (3)	C4—C3—H3	119.5
O3^{ii}—Ca1—C7^{iii}	78.33 (3)	C5—C4—C3	119.50 (13)
O3^{iii}—Ca1—C7^{iii}	25.59 (3)	C5—C4—H4	120.3
O2^{ii}—Ca1—C7^{iii}	82.80 (3)	C3—C4—H4	120.3
O2^{iii}—Ca1—C7^{iii}	26.01 (3)	C4—C5—C6	120.68 (13)
C7^{ii}—Ca1—C7^{iii}	75.79 (5)	C4—C5—H5	119.7
O1W^{i}—Ca1—Ca1^{ii}	79.68 (3)	C6—C5—H5	119.7
O1W—Ca1—Ca1^{ii}	121.93 (3)	C5—C6—C1	118.88 (12)
O3—Ca1—Ca1^{ii}	36.10 (2)	C5—C6—C7	120.39 (12)
O3^{i}—Ca1—Ca1^{ii}	161.97 (2)	C1—C6—C7	120.73 (11)
O3^{ii}—Ca1—Ca1^{ii}	34.80 (2)	O3—C7—O2	121.12 (11)
O3^{iii}—Ca1—Ca1^{ii}	115.02 (3)	O3—C7—C6	119.88 (11)
O2^{ii}—Ca1—Ca1^{ii}	83.84 (2)	O2—C7—C6	118.98 (11)
O2^{iii}—Ca1—Ca1^{ii}	74.82 (2)	O3—C7—Ca1^{ii}	57.99 (6)
C7^{ii}—Ca1—Ca1^{ii}	59.88 (3)	O2—C7—Ca1^{ii}	65.04 (7)
C7^{iii}—Ca1—Ca1^{ii}	93.02 (3)	C6—C7—Ca1^{ii}	164.53 (9)
O1—C1—C2—C3	−177.15 (12)	Ca1^{ii}—O3—C7—O2	16.52 (13)
C6—C1—C2—C3	3.2 (2)	Ca1—O3—C7—C6	46.8 (2)
C1—C2—C3—C4	−1.5 (2)	Ca1^{ii}—O3—C7—C6	−162.11 (10)
C2—C3—C4—C5	−0.9 (2)	Ca1—O3—C7—Ca1^{ii}	−151.07 (18)
C3—C4—C5—C6	1.6 (2)	Ca1^{ii}—O2—C7—O3	−15.42 (12)
C4—C5—C6—C1	0.08 (19)	Ca1^{ii}—O2—C7—C6	163.22 (10)
C4—C5—C6—C7	179.75 (12)	C5—C6—C7—O3	20.62 (18)
O1—C1—C6—C5	177.86 (11)	C1—C6—C7—O3	−159.71 (12)
C2—C1—C6—C5	−2.53 (19)	C5—C6—C7—O2	−158.04 (12)
O1—C1—C6—C7	−1.81 (19)	C1—C6—C7—O2	21.63 (18)
C2—C1—C6—C7	177.80 (12)	C5—C6—C7—Ca1^{ii}	−56.9 (4)
Ca1—O3—C7—O2	−134.55 (14)	C1—C6—C7—Ca1^{ii}	122.8 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.81 (2)	1.90 (2)	2.6256 (13)	148 (2)
O1*W*—H1*W*···O1^{v}	0.82 (2)	2.03 (2)	2.8391 (14)	169 (2)
O1*W*—H2*W*···O2^{vi}	0.84 (2)	2.05 (2)	2.8795 (14)	169 (2)

Symmetry codes: (v) −*x*+1/2, −*y*+1/2, −*z*; (vi) *x*, *y*, *z*−1.

(CaSr9010)

Crystal data

$C_{14}H_{14}Ca_{0.96}O_8Sr_{0.04}$
M_r = 352.27
Monoclinic, *C*2/*c*
a = 16.4335 (7) Å
b = 11.4974 (4) Å
c = 7.6301 (3) Å
β = 91.778 (4)°
V = 1440.96 (10) Å^3
Z = 4

F(000) = 731
D_x = 1.624 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 11617 reflections
θ = 3.4–29.5°
μ = 0.61 mm^{-1}
T = 150 K
Prism, colourless
0.30 × 0.22 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: sealed tube
ω scans

Absorption correction: multi-scan
CrysAlis PRO, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.818, T_{max} = 1.000
16338 measured reflections
1640 independent reflections
1582 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −21→21
k = −14→14
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.055
S = 1.07
1640 reflections
118 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 0.9927P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.5000	0.44977 (2)	−0.2500	0.01035 (10)	0.041 (2)
Ca1	0.5000	0.44977 (2)	−0.2500	0.01035 (10)	0.959 (2)
O1	0.25621 (5)	0.25393 (7)	0.26840 (10)	0.01890 (18)	
O2	0.37837 (4)	0.40042 (6)	0.26872 (9)	0.01685 (18)	
O3	0.45479 (4)	0.39796 (6)	0.03611 (10)	0.01647 (17)	
O1W	0.39881 (5)	0.32319 (7)	−0.37328 (11)	0.02102 (19)	
C1	0.30173 (6)	0.18873 (9)	0.15848 (13)	0.0145 (2)	
C2	0.27303 (7)	0.07831 (9)	0.11382 (14)	0.0187 (2)	
H2	0.2222	0.0520	0.1548	0.022*	
C3	0.31912 (7)	0.00729 (9)	0.00925 (15)	0.0216 (2)	
H3	0.3002	−0.0687	−0.0189	0.026*	
C4	0.39272 (7)	0.04548 (9)	−0.05531 (15)	0.0215 (2)	
H4	0.4243	−0.0044	−0.1255	0.026*	
C5	0.41952 (7)	0.15686 (9)	−0.01624 (14)	0.0176 (2)	
H5	0.4690	0.1840	−0.0627	0.021*	
C6	0.37455 (6)	0.23004 (8)	0.09104 (13)	0.0136 (2)	
C7	0.40399 (6)	0.34951 (8)	0.13303 (13)	0.0129 (2)	
H1O	0.2824 (11)	0.3190 (16)	0.286 (2)	0.042 (5)*	
H1W	0.3548 (11)	0.2929 (15)	−0.334 (2)	0.044 (5)*	

H2W	0.3914 (10)	0.3352 (14)	−0.483 (2)	0.037 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01016 (15)	0.01078 (14)	0.01022 (15)	0.000	0.00204 (9)	0.000
Ca1	0.01016 (15)	0.01078 (14)	0.01022 (15)	0.000	0.00204 (9)	0.000
O1	0.0163 (4)	0.0196 (4)	0.0212 (4)	−0.0039 (3)	0.0068 (3)	−0.0021 (3)
O2	0.0179 (4)	0.0163 (4)	0.0165 (4)	−0.0021 (3)	0.0038 (3)	−0.0025 (3)
O3	0.0163 (4)	0.0154 (4)	0.0180 (4)	−0.0034 (3)	0.0046 (3)	0.0007 (3)
O1W	0.0187 (4)	0.0272 (4)	0.0173 (4)	−0.0072 (3)	0.0031 (3)	0.0015 (3)
C1	0.0151 (5)	0.0161 (5)	0.0124 (4)	−0.0009 (4)	−0.0004 (4)	0.0020 (4)
C2	0.0205 (5)	0.0183 (5)	0.0172 (5)	−0.0071 (4)	−0.0006 (4)	0.0027 (4)
C3	0.0317 (6)	0.0147 (5)	0.0183 (5)	−0.0062 (4)	−0.0022 (4)	−0.0002 (4)
C4	0.0278 (6)	0.0169 (5)	0.0201 (5)	0.0023 (4)	0.0025 (4)	−0.0036 (4)
C5	0.0179 (5)	0.0180 (5)	0.0171 (5)	−0.0002 (4)	0.0024 (4)	0.0001 (4)
C6	0.0144 (5)	0.0131 (4)	0.0131 (4)	−0.0013 (4)	−0.0002 (4)	0.0009 (4)
C7	0.0110 (4)	0.0134 (4)	0.0142 (4)	0.0004 (3)	−0.0004 (3)	0.0012 (3)

Geometric parameters (Å, º)

Sr1—O1W^{i}	2.3814 (8)	O3—C7	1.2620 (12)
Sr1—O1W	2.3814 (8)	O3—Ca1^{ii}	2.4910 (7)
Sr1—O3^{i}	2.4027 (7)	O3—Sr1^{ii}	2.4910 (7)
Sr1—O3	2.4027 (7)	O1W—H1W	0.864 (19)
Sr1—O3^{ii}	2.4910 (7)	O1W—H2W	0.853 (18)
Sr1—O3^{iii}	2.4910 (7)	C1—C2	1.3929 (14)
Sr1—O2^{ii}	2.6458 (7)	C1—C6	1.4002 (14)
Sr1—O2^{iii}	2.6458 (7)	C2—C3	1.3838 (16)
Sr1—C7^{ii}	2.9198 (10)	C2—H2	0.9500
Sr1—C7^{iii}	2.9198 (10)	C3—C4	1.3911 (17)
Sr1—Sr1^{ii}	3.9861 (2)	C3—H3	0.9500
Sr1—Ca1^{ii}	3.9861 (2)	C4—C5	1.3836 (15)
Sr1—H2W	2.807 (17)	C4—H4	0.9500
O1—C1	1.3652 (12)	C5—C6	1.4007 (14)
O1—H1O	0.872 (18)	C5—H5	0.9500
O2—C7	1.2724 (12)	C6—C7	1.4878 (13)
O2—Ca1^{ii}	2.6458 (7)	C7—Ca1^{ii}	2.9197 (10)
O2—Sr1^{ii}	2.6458 (7)	C7—Sr1^{ii}	2.9197 (10)
O1W^{i}—Sr1—O1W	104.66 (4)	O3^{iii}—Sr1—Ca1^{ii}	114.49 (2)
O1W^{i}—Sr1—O3^{i}	88.60 (3)	O2^{ii}—Sr1—Ca1^{ii}	83.423 (17)
O1W—Sr1—O3^{i}	73.82 (3)	O2^{iii}—Sr1—Ca1^{ii}	74.766 (17)
O1W^{i}—Sr1—O3	73.82 (3)	C7^{ii}—Sr1—Ca1^{ii}	59.63 (2)
O1W—Sr1—O3	88.60 (3)	C7^{iii}—Sr1—Ca1^{ii}	92.72 (2)
O3^{i}—Sr1—O3	151.29 (4)	Sr1^{ii}—Sr1—Ca1^{ii}	0.000 (7)
O1W^{i}—Sr1—O3^{ii}	88.87 (3)	O1W^{i}—Sr1—H2W	112.7 (3)
O1W—Sr1—O3^{ii}	151.49 (3)	O1W—Sr1—H2W	16.4 (4)
O3^{i}—Sr1—O3^{ii}	132.47 (3)	O3^{i}—Sr1—H2W	61.1 (4)
O3—Sr1—O3^{ii}	70.93 (3)	O3—Sr1—H2W	104.5 (4)
O1W^{i}—Sr1—O3^{iii}	151.49 (3)	O3^{ii}—Sr1—H2W	156.3 (3)
O1W—Sr1—O3^{iii}	88.87 (3)	O3^{iii}—Sr1—H2W	75.2 (3)

O3^{i}—Sr1—O3^{iii}	70.93 (3)	O2^{ii}—Sr1—H2W	137.5 (4)
O3—Sr1—O3^{iii}	132.47 (3)	O2^{iii}—Sr1—H2W	82.7 (3)
O3^{ii}—Sr1—O3^{iii}	90.69 (4)	C7^{ii}—Sr1—H2W	153.0 (4)
O1W^{i}—Sr1—O2^{ii}	84.25 (3)	C7^{iii}—Sr1—H2W	81.4 (3)
O1W—Sr1—O2^{ii}	153.63 (3)	Sr1^{ii}—Sr1—H2W	136.3 (4)
O3^{i}—Sr1—O2^{ii}	81.77 (2)	Ca1^{ii}—Sr1—H2W	136.3 (4)
O3—Sr1—O2^{ii}	117.77 (2)	C1—O1—H1O	106.9 (12)
O3^{ii}—Sr1—O2^{ii}	50.76 (2)	C7—O2—Ca1^{ii}	89.20 (6)
O3^{iii}—Sr1—O2^{ii}	73.59 (2)	C7—O2—Sr1^{ii}	89.20 (6)
O1W^{i}—Sr1—O2^{iii}	153.63 (3)	Ca1^{ii}—O2—Sr1^{ii}	0.0
O1W—Sr1—O2^{iii}	84.25 (3)	C7—O3—Sr1	150.54 (7)
O3^{i}—Sr1—O2^{iii}	117.76 (2)	C7—O3—Ca1^{ii}	96.64 (6)
O3—Sr1—O2^{iii}	81.77 (2)	Sr1—O3—Ca1^{ii}	109.1
O3^{ii}—Sr1—O2^{iii}	73.59 (2)	C7—O3—Sr1^{ii}	96.64 (6)
O3^{iii}—Sr1—O2^{iii}	50.76 (2)	Sr1—O3—Sr1^{ii}	109.07 (3)
O2^{ii}—Sr1—O2^{iii}	98.76 (3)	Ca1^{ii}—O3—Sr1^{ii}	0.0
O1W^{i}—Sr1—C7^{ii}	89.90 (3)	Sr1—O1W—H1W	133.8 (11)
O1W—Sr1—C7^{ii}	165.45 (3)	Sr1—O1W—H2W	111.4 (11)
O3^{i}—Sr1—C7^{ii}	107.12 (3)	H1W—O1W—H2W	107.9 (15)
O3—Sr1—C7^{ii}	95.60 (3)	O1—C1—C2	117.57 (9)
O3^{ii}—Sr1—C7^{ii}	25.43 (3)	O1—C1—C6	122.02 (9)
O3^{iii}—Sr1—C7^{ii}	78.00 (3)	C2—C1—C6	120.40 (10)
O2^{ii}—Sr1—C7^{ii}	25.83 (2)	C3—C2—C1	119.44 (10)
O2^{iii}—Sr1—C7^{ii}	82.58 (3)	C3—C2—H2	120.3
O1W^{i}—Sr1—C7^{iii}	165.45 (3)	C1—C2—H2	120.3
O1W—Sr1—C7^{iii}	89.90 (3)	C2—C3—C4	121.03 (10)
O3^{i}—Sr1—C7^{iii}	95.60 (3)	C2—C3—H3	119.5
O3—Sr1—C7^{iii}	107.12 (3)	C4—C3—H3	119.5
O3^{ii}—Sr1—C7^{iii}	78.00 (3)	C5—C4—C3	119.35 (10)
O3^{iii}—Sr1—C7^{iii}	25.43 (3)	C5—C4—H4	120.3
O2^{ii}—Sr1—C7^{iii}	82.58 (3)	C3—C4—H4	120.3
O2^{iii}—Sr1—C7^{iii}	25.83 (2)	C4—C5—C6	120.78 (10)
C7^{ii}—Sr1—C7^{iii}	75.55 (4)	C4—C5—H5	119.6
O1W^{i}—Sr1—Sr1^{ii}	79.62 (2)	C6—C5—H5	119.6
O1W—Sr1—Sr1^{ii}	122.30 (2)	C1—C6—C5	118.91 (9)
O3^{i}—Sr1—Sr1^{ii}	161.918 (18)	C1—C6—C7	120.66 (9)
O3—Sr1—Sr1^{ii}	36.203 (17)	C5—C6—C7	120.43 (9)
O3^{ii}—Sr1—Sr1^{ii}	34.729 (16)	O3—C7—O2	121.02 (9)
O3^{iii}—Sr1—Sr1^{ii}	114.49 (2)	O3—C7—C6	119.87 (9)
O2^{ii}—Sr1—Sr1^{ii}	83.423 (17)	O2—C7—C6	119.10 (9)
O2^{iii}—Sr1—Sr1^{ii}	74.766 (17)	O3—C7—Ca1^{ii}	57.93 (5)
C7^{ii}—Sr1—Sr1^{ii}	59.63 (2)	O2—C7—Ca1^{ii}	64.97 (5)
C7^{iii}—Sr1—Sr1^{ii}	92.72 (2)	C6—C7—Ca1^{ii}	164.70 (7)
O1W^{i}—Sr1—Ca1^{ii}	79.62 (2)	O3—C7—Sr1^{ii}	57.93 (5)
O1W—Sr1—Ca1^{ii}	122.30 (2)	O2—C7—Sr1^{ii}	64.97 (5)
O3^{i}—Sr1—Ca1^{ii}	161.918 (18)	C6—C7—Sr1^{ii}	164.70 (7)
O3—Sr1—Ca1^{ii}	36.203 (17)	Ca1^{ii}—C7—Sr1^{ii}	0.0
O3^{ii}—Sr1—Ca1^{ii}	34.729 (16)		

O1—C1—C2—C3	−177.05 (9)	Sr1^{ii}—O3—C7—Ca1^{ii}	0.0
C6—C1—C2—C3	3.26 (15)	Sr1—O3—C7—Sr1^{ii}	−151.02 (14)
C1—C2—C3—C4	−1.53 (16)	Ca1^{ii}—O3—C7—Sr1^{ii}	0.0

C2—C3—C4—C5	−0.95 (17)	Ca1^{ii}—O2—C7—O3	−15.32 (9)
C3—C4—C5—C6	1.72 (17)	Sr1^{ii}—O2—C7—O3	−15.32 (9)
O1—C1—C6—C5	177.84 (9)	Ca1^{ii}—O2—C7—C6	163.42 (8)
C2—C1—C6—C5	−2.49 (15)	Sr1^{ii}—O2—C7—C6	163.42 (8)
O1—C1—C6—C7	−1.91 (14)	Sr1^{ii}—O2—C7—Ca1^{ii}	0.0
C2—C1—C6—C7	177.76 (9)	Ca1^{ii}—O2—C7—Sr1^{ii}	0.0
C4—C5—C6—C1	−0.02 (15)	C1—C6—C7—O3	−159.70 (9)
C4—C5—C6—C7	179.73 (10)	C5—C6—C7—O3	20.55 (14)
Sr1—O3—C7—O2	−134.61 (11)	C1—C6—C7—O2	21.55 (14)
Ca1^{ii}—O3—C7—O2	16.41 (10)	C5—C6—C7—O2	−158.20 (10)
Sr1^{ii}—O3—C7—O2	16.41 (10)	C1—C6—C7—Ca1^{ii}	123.1 (2)
Sr1—O3—C7—C6	46.66 (18)	C5—C6—C7—Ca1^{ii}	−56.7 (3)
Ca1^{ii}—O3—C7—C6	−162.32 (7)	C1—C6—C7—Sr1^{ii}	123.1 (2)
Sr1^{ii}—O3—C7—C6	−162.32 (7)	C5—C6—C7—Sr1^{ii}	−56.7 (3)
Sr1—O3—C7—Ca1^{ii}	−151.02 (14)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.872 (18)	1.842 (19)	2.6204 (10)	147.6 (16)
O1*W*—H1*W*···O1^{iv}	0.864 (19)	1.981 (19)	2.8361 (11)	169.8 (16)
O1*W*—H2*W*···O2^{v}	0.853 (18)	2.043 (18)	2.8820 (11)	167.6 (15)

Symmetry codes: (iv) −*x*+1/2, −*y*+1/2, −*z*; (v) *x*, *y*, *z*−1.

(CaSr8020)

Crystal data

$C_{14}H_{14}Ca_{0.92}O_8Sr_{0.08}$
M_r = 354.25
Monoclinic, *C*2/*c*
a = 16.4344 (3) Å
b = 11.4853 (2) Å
c = 7.6417 (2) Å
β = 91.785 (2)°
V = 1441.70 (5) Å^3
Z = 4
F(000) = 734
D_x = 1.632 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 11379 reflections
θ = 3.4–30.4°
μ = 0.75 mm^{-1}
T = 150 K
Prism, colourless
0.35 × 0.28 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: sealed tube
ω scans
Absorption correction: multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.802, T_{max} = 1.000
16552 measured reflections
1642 independent reflections
1568 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −21→21
k = −14→14
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.053$
$S = 1.08$
1642 reflections
118 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0238P)^2 + 1.0809P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.5000	0.44923 (2)	−0.2500	0.01030 (10)	0.083 (2)
Ca1	0.5000	0.44923 (2)	−0.2500	0.01030 (10)	0.917 (2)
O1	0.25630 (5)	0.25391 (7)	0.26823 (11)	0.01854 (19)	
O2	0.37832 (5)	0.40026 (7)	0.26855 (10)	0.01658 (18)	
O3	0.45479 (5)	0.39771 (7)	0.03630 (10)	0.01642 (18)	
O1W	0.39865 (5)	0.32276 (8)	−0.37365 (12)	0.0213 (2)	
C1	0.30175 (6)	0.18861 (9)	0.15851 (13)	0.0141 (2)	
C2	0.27301 (7)	0.07823 (10)	0.11382 (14)	0.0183 (2)	
H2	0.2222	0.0519	0.1549	0.022*	
C3	0.31889 (8)	0.00733 (10)	0.00931 (15)	0.0214 (3)	
H3	0.2998	−0.0687	−0.0191	0.026*	
C4	0.39251 (8)	0.04538 (10)	−0.05506 (16)	0.0215 (3)	
H4	0.4240	−0.0047	−0.1251	0.026*	
C5	0.41944 (7)	0.15671 (10)	−0.01621 (14)	0.0171 (2)	
H5	0.4689	0.1839	−0.0627	0.021*	
C6	0.37448 (6)	0.22991 (9)	0.09118 (13)	0.0133 (2)	
C7	0.40395 (6)	0.34932 (9)	0.13318 (13)	0.0129 (2)	
H1O	0.2813 (11)	0.3191 (16)	0.288 (2)	0.039 (5)*	
H1W	0.3551 (12)	0.2915 (16)	−0.339 (2)	0.043 (5)*	
H2W	0.3914 (11)	0.3337 (15)	−0.481 (3)	0.043 (5)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.00968 (14)	0.01105 (15)	0.01028 (15)	0.000	0.00222 (9)	0.000
Ca1	0.00968 (14)	0.01105 (15)	0.01028 (15)	0.000	0.00222 (9)	0.000
O1	0.0159 (4)	0.0194 (4)	0.0207 (4)	−0.0038 (3)	0.0065 (3)	−0.0023 (3)
O2	0.0174 (4)	0.0164 (4)	0.0161 (4)	−0.0018 (3)	0.0038 (3)	−0.0029 (3)
O3	0.0156 (4)	0.0154 (4)	0.0186 (4)	−0.0035 (3)	0.0049 (3)	0.0004 (3)
O1W	0.0182 (4)	0.0283 (5)	0.0176 (4)	−0.0069 (3)	0.0036 (3)	0.0018 (3)
C1	0.0147 (5)	0.0159 (5)	0.0117 (5)	−0.0006 (4)	−0.0001 (4)	0.0020 (4)
C2	0.0196 (5)	0.0187 (5)	0.0165 (5)	−0.0071 (4)	−0.0007 (4)	0.0029 (4)
C3	0.0309 (6)	0.0146 (5)	0.0186 (6)	−0.0063 (5)	−0.0024 (5)	−0.0004 (4)
C4	0.0280 (6)	0.0173 (5)	0.0193 (6)	0.0020 (5)	0.0025 (5)	−0.0036 (4)

C5	0.0176 (5)	0.0173 (5)	0.0165 (5)	−0.0002 (4)	0.0030 (4)	0.0000 (4)
C6	0.0136 (5)	0.0130 (5)	0.0131 (5)	−0.0010 (4)	−0.0004 (4)	0.0010 (4)
C7	0.0104 (4)	0.0142 (5)	0.0140 (5)	0.0006 (4)	−0.0008 (4)	0.0013 (4)

Geometric parameters (Å, º)

Sr1—O1W^{i}	2.3830 (9)	O3—C7	1.2624 (13)
Sr1—O1W	2.3830 (9)	O3—Ca1^{ii}	2.4968 (8)
Sr1—O3	2.4062 (8)	O3—Sr1^{ii}	2.4968 (8)
Sr1—O3^{i}	2.4062 (8)	O1W—H1W	0.85 (2)
Sr1—O3^{ii}	2.4968 (8)	O1W—H2W	0.836 (19)
Sr1—O3^{iii}	2.4968 (8)	C1—C2	1.3917 (15)
Sr1—O2^{ii}	2.6506 (8)	C1—C6	1.3989 (15)
Sr1—O2^{iii}	2.6506 (8)	C2—C3	1.3809 (17)
Sr1—C7^{ii}	2.9247 (11)	C2—H2	0.9500
Sr1—C7^{iii}	2.9247 (11)	C3—C4	1.3907 (17)
Sr1—Sr1^{ii}	3.9949 (2)	C3—H3	0.9500
Sr1—Ca1^{ii}	3.9949 (2)	C4—C5	1.3824 (16)
Sr1—H2W	2.805 (18)	C4—H4	0.9500
O1—C1	1.3647 (13)	C5—C6	1.4015 (15)
O1—H1O	0.865 (18)	C5—H5	0.9500
O2—C7	1.2716 (13)	C6—C7	1.4862 (14)
O2—Ca1^{ii}	2.6505 (8)	C7—Ca1^{ii}	2.9247 (11)
O2—Sr1^{ii}	2.6505 (8)	C7—Sr1^{ii}	2.9247 (11)
O1W^{i}—Sr1—O1W	104.89 (5)	O3^{iii}—Sr1—Ca1^{ii}	114.28 (2)
O1W^{i}—Sr1—O3	73.82 (3)	O2^{ii}—Sr1—Ca1^{ii}	83.294 (17)
O1W—Sr1—O3	88.79 (3)	O2^{iii}—Sr1—Ca1^{ii}	74.689 (17)
O1W^{i}—Sr1—O3^{i}	88.79 (3)	C7^{ii}—Sr1—Ca1^{ii}	59.55 (2)
O1W—Sr1—O3^{i}	73.82 (3)	C7^{iii}—Sr1—Ca1^{ii}	92.57 (2)
O3—Sr1—O3^{i}	151.53 (4)	Sr1^{ii}—Sr1—Ca1^{ii}	0.000 (7)
O1W^{i}—Sr1—O3^{ii}	88.84 (3)	O1W^{i}—Sr1—H2W	112.6 (4)
O1W—Sr1—O3^{ii}	151.47 (3)	O1W—Sr1—H2W	16.0 (4)
O3—Sr1—O3^{ii}	70.88 (3)	O3—Sr1—H2W	104.4 (4)
O3^{i}—Sr1—O3^{ii}	132.36 (3)	O3^{i}—Sr1—H2W	61.3 (4)
O1W^{i}—Sr1—O3^{iii}	151.47 (3)	O3^{ii}—Sr1—H2W	156.3 (4)
O1W—Sr1—O3^{iii}	88.84 (3)	O3^{iii}—Sr1—H2W	75.6 (4)
O3—Sr1—O3^{iii}	132.36 (3)	O2^{ii}—Sr1—H2W	137.8 (4)
O3^{i}—Sr1—O3^{iii}	70.88 (3)	O2^{iii}—Sr1—H2W	82.9 (4)
O3^{ii}—Sr1—O3^{iii}	90.48 (4)	C7^{ii}—Sr1—H2W	153.3 (4)
O1W^{i}—Sr1—O2^{ii}	84.24 (3)	C7^{iii}—Sr1—H2W	81.7 (4)
O1W—Sr1—O2^{ii}	153.57 (3)	Sr1^{ii}—Sr1—H2W	136.2 (4)
O3—Sr1—O2^{ii}	117.64 (2)	Ca1^{ii}—Sr1—H2W	136.2 (4)
O3^{i}—Sr1—O2^{ii}	81.77 (2)	C1—O1—H1O	108.5 (12)
O3^{ii}—Sr1—O2^{ii}	50.66 (2)	C7—O2—Ca1^{ii}	89.25 (6)
O3^{iii}—Sr1—O2^{ii}	73.47 (3)	C7—O2—Sr1^{ii}	89.25 (6)
O1W^{i}—Sr1—O2^{iii}	153.57 (3)	Ca1^{ii}—O2—Sr1^{ii}	0.0
O1W—Sr1—O2^{iii}	84.24 (3)	C7—O3—Sr1	150.49 (7)
O3—Sr1—O2^{iii}	81.77 (2)	C7—O3—Ca1^{ii}	96.62 (6)
O3^{i}—Sr1—O2^{iii}	117.64 (2)	Sr1—O3—Ca1^{ii}	109.1
O3^{ii}—Sr1—O2^{iii}	73.47 (3)	C7—O3—Sr1^{ii}	96.62 (6)
O3^{iii}—Sr1—O2^{iii}	50.66 (2)	Sr1—O3—Sr1^{ii}	109.12 (3)

O2^{ii}—Sr1—O2^{iii}	98.58 (3)	Ca1^{ii}—O3—Sr1^{ii}	0.0
O1W^{i}—Sr1—C7^{ii}	89.84 (3)	Sr1—O1W—H1W	136.1 (12)
O1W—Sr1—C7^{ii}	165.27 (3)	Sr1—O1W—H2W	112.0 (12)
O3—Sr1—C7^{ii}	95.51 (3)	H1W—O1W—H2W	105.8 (16)
O3^{i}—Sr1—C7^{ii}	107.04 (3)	O1—C1—C2	117.60 (10)
O3^{ii}—Sr1—C7^{ii}	25.39 (3)	O1—C1—C6	122.00 (9)
O3^{iii}—Sr1—C7^{ii}	77.84 (3)	C2—C1—C6	120.40 (10)
O2^{ii}—Sr1—C7^{ii}	25.77 (3)	C3—C2—C1	119.46 (10)
O2^{iii}—Sr1—C7^{ii}	82.45 (3)	C3—C2—H2	120.3
O1W^{i}—Sr1—C7^{iii}	165.27 (3)	C1—C2—H2	120.3
O1W—Sr1—C7^{iii}	89.84 (3)	C2—C3—C4	121.07 (10)
O3—Sr1—C7^{iii}	107.04 (3)	C2—C3—H3	119.5
O3^{i}—Sr1—C7^{iii}	95.51 (3)	C4—C3—H3	119.5
O3^{ii}—Sr1—C7^{iii}	77.84 (3)	C5—C4—C3	119.40 (11)
O3^{iii}—Sr1—C7^{iii}	25.39 (3)	C5—C4—H4	120.3
O2^{ii}—Sr1—C7^{iii}	82.45 (3)	C3—C4—H4	120.3
O2^{iii}—Sr1—C7^{iii}	25.77 (3)	C4—C5—C6	120.63 (10)
C7^{ii}—Sr1—C7^{iii}	75.42 (4)	C4—C5—H5	119.7
O1W^{i}—Sr1—Sr1^{ii}	79.60 (2)	C6—C5—H5	119.7
O1W—Sr1—Sr1^{ii}	122.44 (2)	C1—C6—C5	118.95 (10)
O3—Sr1—Sr1^{ii}	36.194 (18)	C1—C6—C7	120.66 (9)
O3^{i}—Sr1—Sr1^{ii}	161.916 (19)	C5—C6—C7	120.39 (9)
O3^{ii}—Sr1—Sr1^{ii}	34.688 (17)	O3—C7—O2	121.11 (10)
O3^{iii}—Sr1—Sr1^{ii}	114.28 (2)	O3—C7—C6	119.79 (9)
O2^{ii}—Sr1—Sr1^{ii}	83.294 (17)	O2—C7—C6	119.09 (9)
O2^{iii}—Sr1—Sr1^{ii}	74.689 (17)	O3—C7—Ca1^{ii}	57.99 (5)
C7^{ii}—Sr1—Sr1^{ii}	59.55 (2)	O2—C7—Ca1^{ii}	64.98 (5)
C7^{iii}—Sr1—Sr1^{ii}	92.57 (2)	C6—C7—Ca1^{ii}	164.81 (7)
O1W^{i}—Sr1—Ca1^{ii}	79.60 (2)	O3—C7—Sr1^{ii}	57.99 (5)
O1W—Sr1—Ca1^{ii}	122.44 (2)	O2—C7—Sr1^{ii}	64.98 (5)
O3—Sr1—Ca1^{ii}	36.194 (18)	C6—C7—Sr1^{ii}	164.81 (7)
O3^{i}—Sr1—Ca1^{ii}	161.916 (19)	Ca1^{ii}—C7—Sr1^{ii}	0.0
O3^{ii}—Sr1—Ca1^{ii}	34.688 (17)		

O1—C1—C2—C3	−177.19 (10)	Sr1^{ii}—O3—C7—Ca1^{ii}	0.0
C6—C1—C2—C3	3.20 (16)	Sr1—O3—C7—Sr1^{ii}	−150.97 (15)
C1—C2—C3—C4	−1.38 (17)	Ca1^{ii}—O3—C7—Sr1^{ii}	0.0
C2—C3—C4—C5	−1.13 (18)	Ca1^{ii}—O2—C7—O3	−15.25 (10)
C3—C4—C5—C6	1.85 (17)	Sr1^{ii}—O2—C7—O3	−15.25 (10)
O1—C1—C6—C5	177.92 (10)	Ca1^{ii}—O2—C7—C6	163.56 (8)
C2—C1—C6—C5	−2.49 (15)	Sr1^{ii}—O2—C7—C6	163.56 (8)
O1—C1—C6—C7	−1.84 (15)	Sr1^{ii}—O2—C7—Ca1^{ii}	0.0
C2—C1—C6—C7	177.75 (9)	Ca1^{ii}—O2—C7—Sr1^{ii}	0.0
C4—C5—C6—C1	−0.05 (16)	C1—C6—C7—O3	−159.75 (10)
C4—C5—C6—C7	179.71 (10)	C5—C6—C7—O3	20.50 (15)
Sr1—O3—C7—O2	−134.65 (12)	C1—C6—C7—O2	21.43 (15)
Ca1^{ii}—O3—C7—O2	16.32 (11)	C5—C6—C7—O2	−158.32 (10)
Sr1^{ii}—O3—C7—O2	16.32 (11)	C1—C6—C7—Ca1^{ii}	123.1 (3)
Sr1—O3—C7—C6	46.55 (19)	C5—C6—C7—Ca1^{ii}	−56.6 (3)
Ca1^{ii}—O3—C7—C6	−162.47 (8)	C1—C6—C7—Sr1^{ii}	123.1 (3)

Sr1^{ii}—O3—C7—C6	−162.47 (8)	C5—C6—C7—Sr1^{ii}	−56.6 (3)
Sr1—O3—C7—Ca1^{ii}	−150.97 (15)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.865 (18)	1.857 (18)	2.6165 (11)	145.5 (16)
O1*W*—H1*W*···O1^{iv}	0.85 (2)	2.00 (2)	2.8350 (11)	169.7 (17)
O1*W*—H2*W*···O2^{v}	0.836 (19)	2.06 (2)	2.8849 (12)	166.8 (17)

Symmetry codes: (iv) −*x*+1/2, −*y*+1/2, −*z*; (v) *x*, *y*, *z*−1.

(CaSr7030)

Crystal data

$C_{14}H_{14}Ca_{0.83}O_8Sr_{0.17}$
M_r = 358.18
Monoclinic, *C*2/*c*
a = 16.4921 (10) Å
b = 11.5345 (8) Å
c = 7.6679 (5) Å
β = 91.838 (6)°
V = 1457.90 (16) Å^3
Z = 4
F(000) = 740
D_x = 1.632 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 2211 reflections
θ = 3.4–30.1°
μ = 1.01 mm^{-1}
T = 150 K
Cut prism, colourless
0.26 × 0.22 × 0.12 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: sealed tube
ω scans
Absorption correction: multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.896, T_{max} = 1.000
3241 measured reflections
1659 independent reflections
1494 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −21→18
k = −12→14
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.093
S = 1.09
1659 reflections
118 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.5000	0.44817 (4)	−0.2500	0.01289 (17)	0.165 (3)
Ca1	0.5000	0.44817 (4)	−0.2500	0.01289 (17)	0.835 (3)
O1	0.25637 (7)	0.25373 (13)	0.26791 (18)	0.0219 (3)	
O2	0.37813 (7)	0.39984 (12)	0.26805 (17)	0.0196 (3)	
O3	0.45477 (7)	0.39682 (12)	0.03736 (17)	0.0205 (3)	
O1W	0.39825 (8)	0.32205 (14)	−0.3747 (2)	0.0264 (4)	
C1	0.30155 (10)	0.18853 (17)	0.1580 (2)	0.0176 (4)	
C2	0.27293 (11)	0.07830 (19)	0.1139 (2)	0.0217 (4)	
H2	0.2225	0.0520	0.1553	0.026*	
C3	0.31847 (12)	0.00760 (18)	0.0095 (3)	0.0238 (5)	
H3	0.2993	−0.0680	−0.0189	0.029*	
C4	0.39199 (13)	0.04538 (18)	−0.0547 (3)	0.0248 (5)	
H4	0.4233	−0.0044	−0.1247	0.030*	
C5	0.41889 (11)	0.15622 (17)	−0.0154 (2)	0.0203 (4)	
H5	0.4683	0.1830	−0.0615	0.024*	
C6	0.37431 (10)	0.22961 (17)	0.0915 (2)	0.0162 (4)	
C7	0.40362 (10)	0.34874 (16)	0.1336 (2)	0.0158 (4)	
H1O	0.2801 (18)	0.321 (3)	0.280 (4)	0.056 (9)*	
H1W	0.3554 (16)	0.290 (2)	−0.331 (3)	0.046 (8)*	
H2W	0.3898 (16)	0.329 (2)	−0.486 (4)	0.046 (8)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0097 (2)	0.0165 (3)	0.0126 (2)	0.000	0.00114 (15)	0.000
Ca1	0.0097 (2)	0.0165 (3)	0.0126 (2)	0.000	0.00114 (15)	0.000
O1	0.0170 (6)	0.0246 (8)	0.0244 (7)	−0.0032 (6)	0.0064 (5)	−0.0028 (6)
O2	0.0178 (6)	0.0214 (8)	0.0196 (7)	−0.0031 (6)	0.0032 (5)	−0.0026 (6)
O3	0.0155 (6)	0.0224 (8)	0.0238 (7)	−0.0032 (5)	0.0042 (5)	0.0006 (6)
O1W	0.0192 (7)	0.0375 (9)	0.0226 (8)	−0.0068 (7)	0.0032 (6)	0.0037 (7)
C1	0.0160 (8)	0.0213 (10)	0.0153 (8)	0.0006 (8)	−0.0014 (7)	0.0019 (8)
C2	0.0202 (9)	0.0258 (10)	0.0190 (9)	−0.0072 (8)	−0.0010 (7)	0.0032 (9)
C3	0.0322 (10)	0.0177 (10)	0.0211 (10)	−0.0061 (9)	−0.0057 (8)	0.0012 (9)
C4	0.0309 (11)	0.0229 (11)	0.0207 (10)	0.0027 (8)	0.0020 (9)	−0.0028 (8)
C5	0.0189 (8)	0.0224 (10)	0.0197 (9)	−0.0002 (8)	0.0015 (7)	0.0004 (8)
C6	0.0147 (8)	0.0185 (9)	0.0154 (8)	−0.0011 (7)	−0.0015 (7)	0.0006 (8)
C7	0.0097 (7)	0.0191 (9)	0.0182 (9)	0.0020 (7)	−0.0029 (7)	0.0006 (8)

Geometric parameters (Å, º)

Sr1—O1W	2.3968 (15)	O3—C7	1.266 (2)
Sr1—O1W^{i}	2.3968 (15)	O3—Ca1^{ii}	2.5166 (14)
Sr1—O3	2.4224 (13)	O3—Sr1^{ii}	2.5166 (14)

Sr1—O3^{i}	2.4224 (13)	O1W—H1W	0.87 (3)
Sr1—O3^{ii}	2.5166 (14)	O1W—H2W	0.86 (3)
Sr1—O3^{iii}	2.5166 (14)	C1—C2	1.394 (3)
Sr1—O2^{ii}	2.6739 (13)	C1—C6	1.401 (2)
Sr1—O2^{iii}	2.6739 (13)	C2—C3	1.381 (3)
Sr1—C7^{ii}	2.9529 (19)	C2—H2	0.9500
Sr1—C7^{iii}	2.9529 (19)	C3—C4	1.393 (3)
Sr1—Sr1^{ii}	4.0160 (4)	C3—H3	0.9500
Sr1—Ca1^{ii}	4.0160 (4)	C4—C5	1.383 (3)
Sr1—H2W	2.87 (3)	C4—H4	0.9500
O1—C1	1.368 (2)	C5—C6	1.403 (3)
O1—H1O	0.87 (3)	C5—H5	0.9500
O2—C7	1.271 (2)	C6—C7	1.489 (3)
O2—Ca1^{ii}	2.6740 (13)	C7—Ca1^{ii}	2.9529 (19)
O2—Sr1^{ii}	2.6740 (13)	C7—Sr1^{ii}	2.9529 (19)

O1W—Sr1—O1W^{i}	105.26 (8)	O3^{iii}—Sr1—Ca1^{ii}	113.45 (4)
O1W—Sr1—O3	89.00 (5)	O2^{ii}—Sr1—Ca1^{ii}	82.95 (3)
O1W^{i}—Sr1—O3	73.78 (5)	O2^{iii}—Sr1—Ca1^{ii}	74.48 (3)
O1W—Sr1—O3^{i}	73.78 (5)	C7^{ii}—Sr1—Ca1^{ii}	59.45 (4)
O1W^{i}—Sr1—O3^{i}	89.00 (5)	C7^{iii}—Sr1—Ca1^{ii}	92.06 (4)
O3—Sr1—O3^{i}	151.69 (7)	Sr1^{ii}—Sr1—Ca1^{ii}	0.0
O1W—Sr1—O3^{ii}	151.52 (4)	O1W—Sr1—H2W	15.7 (6)
O1W^{i}—Sr1—O3^{ii}	89.05 (5)	O1W^{i}—Sr1—H2W	112.4 (6)
O3—Sr1—O3^{ii}	71.21 (5)	O3—Sr1—H2W	104.4 (6)
O3^{i}—Sr1—O3^{ii}	132.03 (5)	O3^{i}—Sr1—H2W	61.2 (5)
O1W—Sr1—O3^{iii}	89.05 (5)	O3^{ii}—Sr1—H2W	156.4 (6)
O1W^{i}—Sr1—O3^{iii}	151.52 (5)	O3^{iii}—Sr1—H2W	76.4 (6)
O3—Sr1—O3^{iii}	132.03 (5)	O2^{ii}—Sr1—H2W	138.0 (6)
O3^{i}—Sr1—O3^{iii}	71.21 (5)	O2^{iii}—Sr1—H2W	83.4 (6)
O3^{ii}—Sr1—O3^{iii}	89.46 (7)	C7^{ii}—Sr1—H2W	153.4 (6)
O1W—Sr1—O2^{ii}	153.52 (5)	C7^{iii}—Sr1—H2W	82.3 (6)
O1W^{i}—Sr1—O2^{ii}	84.31 (5)	Sr1^{ii}—Sr1—H2W	136.4 (5)
O3—Sr1—O2^{ii}	117.47 (4)	Ca1^{ii}—Sr1—H2W	136.4 (5)
O3^{i}—Sr1—O2^{ii}	81.91 (4)	C1—O1—H1O	107.5 (19)
O3^{ii}—Sr1—O2^{ii}	50.21 (4)	C7—O2—Ca1^{ii}	89.62 (10)
O3^{iii}—Sr1—O2^{ii}	73.04 (4)	C7—O2—Sr1^{ii}	89.62 (10)
O1W—Sr1—O2^{iii}	84.31 (5)	Ca1^{ii}—O2—Sr1^{ii}	0.0
O1W^{i}—Sr1—O2^{iii}	153.52 (5)	C7—O3—Sr1	150.16 (12)
O3—Sr1—O2^{iii}	81.91 (4)	C7—O3—Ca1^{ii}	97.05 (11)
O3^{i}—Sr1—O2^{iii}	117.47 (4)	Sr1—O3—Ca1^{ii}	108.8
O3^{ii}—Sr1—O2^{iii}	73.04 (4)	C7—O3—Sr1^{ii}	97.05 (11)
O3^{iii}—Sr1—O2^{iii}	50.21 (4)	Sr1—O3—Sr1^{ii}	108.79 (5)
O2^{ii}—Sr1—O2^{iii}	98.07 (6)	Ca1^{ii}—O3—Sr1^{ii}	0.0
O1W—Sr1—C7^{ii}	164.87 (5)	Sr1—O1W—H1W	132.2 (17)
O1W^{i}—Sr1—C7^{ii}	89.87 (5)	Sr1—O1W—H2W	115.4 (18)
O3—Sr1—C7^{ii}	95.59 (5)	H1W—O1W—H2W	108 (2)
O3^{i}—Sr1—C7^{ii}	106.89 (5)	O1—C1—C2	117.64 (16)
O3^{ii}—Sr1—C7^{ii}	25.19 (4)	O1—C1—C6	121.87 (17)
O3^{iii}—Sr1—C7^{ii}	77.16 (5)	C2—C1—C6	120.48 (18)
O2^{ii}—Sr1—C7^{ii}	25.49 (4)	C3—C2—C1	119.53 (17)
O2^{iii}—Sr1—C7^{ii}	82.09 (5)	C3—C2—H2	120.2

O1W—Sr1—C7^{iii}	89.87 (5)	C1—C2—H2	120.2
O1W^{i}—Sr1—C7^{iii}	164.87 (5)	C2—C3—C4	121.04 (19)
O3—Sr1—C7^{iii}	106.89 (5)	C2—C3—H3	119.5
O3^{i}—Sr1—C7^{iii}	95.60 (5)	C4—C3—H3	119.5
O3^{ii}—Sr1—C7^{iii}	77.16 (5)	C5—C4—C3	119.26 (19)
O3^{iii}—Sr1—C7^{iii}	25.19 (4)	C5—C4—H4	120.4
O2^{ii}—Sr1—C7^{iii}	82.09 (5)	C3—C4—H4	120.4
O2^{iii}—Sr1—C7^{iii}	25.49 (4)	C4—C5—C6	120.96 (17)
C7^{ii}—Sr1—C7^{iii}	75.01 (7)	C4—C5—H5	119.5
O1W—Sr1—Sr1^{ii}	122.70 (4)	C6—C5—H5	119.5
O1W^{i}—Sr1—Sr1^{ii}	79.70 (4)	C1—C6—C5	118.66 (17)
O3—Sr1—Sr1^{ii}	36.39 (3)	C1—C6—C7	120.61 (16)
O3^{i}—Sr1—Sr1^{ii}	161.92 (3)	C5—C6—C7	120.73 (16)
O3^{ii}—Sr1—Sr1^{ii}	34.82 (3)	O3—C7—O2	120.89 (17)
O3^{iii}—Sr1—Sr1^{ii}	113.45 (4)	O3—C7—C6	119.73 (16)
O2^{ii}—Sr1—Sr1^{ii}	82.95 (3)	O2—C7—C6	119.36 (15)
O2^{iii}—Sr1—Sr1^{ii}	74.48 (3)	O3—C7—Ca1^{ii}	57.76 (9)
C7^{ii}—Sr1—Sr1^{ii}	59.45 (4)	O2—C7—Ca1^{ii}	64.89 (9)
C7^{iii}—Sr1—Sr1^{ii}	92.06 (4)	C6—C7—Ca1^{ii}	164.95 (11)
O1W—Sr1—Ca1^{ii}	122.70 (4)	O3—C7—Sr1^{ii}	57.76 (9)
O1W^{i}—Sr1—Ca1^{ii}	79.70 (4)	O2—C7—Sr1^{ii}	64.89 (9)
O3—Sr1—Ca1^{ii}	36.39 (3)	C6—C7—Sr1^{ii}	164.95 (11)
O3^{i}—Sr1—Ca1^{ii}	161.92 (3)	Ca1^{ii}—C7—Sr1^{ii}	0.0
O3^{ii}—Sr1—Ca1^{ii}	34.82 (3)		

O1—C1—C2—C3	−177.15 (17)	Sr1^{ii}—O3—C7—Ca1^{ii}	0.0
C6—C1—C2—C3	2.6 (3)	Sr1—O3—C7—Sr1^{ii}	−150.2 (3)
C1—C2—C3—C4	−1.0 (3)	Ca1^{ii}—O3—C7—Sr1^{ii}	0.0
C2—C3—C4—C5	−1.1 (3)	Ca1^{ii}—O2—C7—O3	−14.77 (16)
C3—C4—C5—C6	1.7 (3)	Sr1^{ii}—O2—C7—O3	−14.77 (16)
O1—C1—C6—C5	177.71 (16)	Ca1^{ii}—O2—C7—C6	163.75 (14)
C2—C1—C6—C5	−2.0 (3)	Sr1^{ii}—O2—C7—C6	163.75 (14)
O1—C1—C6—C7	−2.3 (3)	Sr1^{ii}—O2—C7—Ca1^{ii}	0.0
C2—C1—C6—C7	177.94 (16)	Ca1^{ii}—O2—C7—Sr1^{ii}	0.0
C4—C5—C6—C1	−0.1 (3)	C1—C6—C7—O3	−159.89 (17)
C4—C5—C6—C7	179.91 (17)	C5—C6—C7—O3	20.1 (3)
Sr1—O3—C7—O2	−134.4 (2)	C1—C6—C7—O2	21.6 (3)
Ca1^{ii}—O3—C7—O2	15.83 (17)	C5—C6—C7—O2	−158.43 (17)
Sr1^{ii}—O3—C7—O2	15.83 (17)	C1—C6—C7—Ca1^{ii}	124.1 (4)
Sr1—O3—C7—C6	47.1 (3)	C5—C6—C7—Ca1^{ii}	−55.9 (5)
Ca1^{ii}—O3—C7—C6	−162.68 (13)	C1—C6—C7—Sr1^{ii}	124.1 (4)
Sr1^{ii}—O3—C7—C6	−162.68 (13)	C5—C6—C7—Sr1^{ii}	−55.9 (5)
Sr1—O3—C7—Ca1^{ii}	−150.2 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.87 (3)	1.86 (3)	2.6216 (18)	145 (3)

O1*W*—H1*W*···O1^{iv}	0.87 (3)	1.99 (3)	2.8409 (19)	166 (3)
O1*W*—H2*W*···O2^{v}	0.86 (3)	2.06 (3)	2.891 (2)	161 (3)

Symmetry codes: (iv) −*x*+1/2, −*y*+1/2, −*z*; (v) *x*, *y*, *z*−1.

(CaSr6040)

Crystal data

$C_{14}H_{14}Ca_{0.69}O_8Sr_{0.31}$
M_r = 364.90
Monoclinic, *C*2/*c*
a = 16.5626 (13) Å
b = 11.4921 (10) Å
c = 7.7041 (7) Å
β = 91.588 (8)°
V = 1465.8 (2) Å^3
Z = 4
F(000) = 750
D_x = 1.653 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5800 reflections
θ = 3.4–28.9°
μ = 1.47 mm^{-1}
T = 150 K
Cut prism, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: sealed tube
ω scans
Absorption correction: multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.845, T_{max} = 1.000
9041 measured reflections
1656 independent reflections
1576 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −21→21
k = −14→14
l = −9→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.056
S = 1.11
1656 reflections
118 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0227P)^2 + 0.9652P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.5000	0.44698 (2)	−0.2500	0.01216 (10)	0.306 (3)
Ca1	0.5000	0.44698 (2)	−0.2500	0.01216 (10)	0.694 (3)
O1	0.25637 (6)	0.25381 (9)	0.26752 (13)	0.0210 (2)	

O2	0.37777 (6)	0.39961 (8)	0.26740 (13)	0.0196 (2)
O3	0.45477 (6)	0.39600 (8)	0.03791 (13)	0.0201 (2)
O1W	0.39752 (7)	0.32033 (10)	−0.37681 (16)	0.0260 (3)
C1	0.30144 (8)	0.18819 (12)	0.15846 (17)	0.0160 (3)
C2	0.27255 (9)	0.07810 (12)	0.11375 (19)	0.0201 (3)
H2	0.2220	0.0521	0.1544	0.024*
C3	0.31787 (10)	0.00708 (13)	0.00995 (19)	0.0238 (3)
H3	0.2988	−0.0687	−0.0182	0.029*
C4	0.39121 (9)	0.04474 (13)	−0.0543 (2)	0.0237 (3)
H4	0.4222	−0.0052	−0.1246	0.028*
C5	0.41838 (9)	0.15549 (12)	−0.01466 (19)	0.0196 (3)
H5	0.4678	0.1821	−0.0603	0.023*
C6	0.37401 (8)	0.22901 (12)	0.09187 (17)	0.0152 (3)
C7	0.40357 (8)	0.34819 (11)	0.13391 (18)	0.0152 (3)
H1O	0.2827 (13)	0.3191 (19)	0.284 (3)	0.049 (6)*
H1W	0.3521 (15)	0.290 (2)	−0.337 (3)	0.062 (7)*
H2W	0.3920 (12)	0.3345 (18)	−0.490 (3)	0.046 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01084 (15)	0.01233 (15)	0.01342 (16)	0.000	0.00272 (10)	0.000
Ca1	0.01084 (15)	0.01233 (15)	0.01342 (16)	0.000	0.00272 (10)	0.000
O1	0.0183 (5)	0.0206 (5)	0.0245 (6)	−0.0042 (4)	0.0069 (4)	−0.0028 (4)
O2	0.0191 (5)	0.0178 (5)	0.0222 (5)	−0.0023 (4)	0.0040 (4)	−0.0033 (4)
O3	0.0178 (5)	0.0169 (5)	0.0260 (6)	−0.0037 (4)	0.0066 (4)	0.0000 (4)
O1W	0.0217 (6)	0.0334 (6)	0.0232 (6)	−0.0055 (5)	0.0052 (5)	0.0041 (5)
C1	0.0163 (6)	0.0175 (7)	0.0140 (7)	−0.0003 (5)	0.0002 (5)	0.0024 (5)
C2	0.0219 (7)	0.0199 (7)	0.0185 (7)	−0.0068 (6)	−0.0002 (6)	0.0033 (6)
C3	0.0355 (8)	0.0159 (7)	0.0199 (8)	−0.0068 (6)	−0.0022 (6)	−0.0001 (6)
C4	0.0301 (8)	0.0194 (7)	0.0217 (8)	0.0018 (6)	0.0032 (6)	−0.0031 (6)
C5	0.0188 (7)	0.0196 (7)	0.0204 (7)	0.0002 (5)	0.0028 (6)	0.0003 (6)
C6	0.0150 (6)	0.0149 (6)	0.0157 (7)	−0.0012 (5)	−0.0001 (5)	0.0013 (5)
C7	0.0114 (6)	0.0151 (6)	0.0192 (7)	0.0004 (5)	−0.0006 (5)	0.0014 (5)

Geometric parameters (Å, º)

Sr1—O1W^{i}	2.4211 (11)	O3—C7	1.2660 (16)
Sr1—O1W	2.4211 (11)	O3—Ca1^{ii}	2.5336 (10)
Sr1—O3	2.4324 (10)	O3—Sr1^{ii}	2.5336 (10)
Sr1—O3^{i}	2.4324 (10)	O1W—H1W	0.89 (3)
Sr1—O3^{ii}	2.5336 (10)	O1W—H2W	0.89 (2)
Sr1—O3^{iii}	2.5336 (10)	C1—C2	1.3925 (19)
Sr1—O2^{ii}	2.6907 (10)	C1—C6	1.4008 (19)
Sr1—O2^{iii}	2.6907 (10)	C2—C3	1.379 (2)
Sr1—C7^{ii}	2.9686 (13)	C2—H2	0.9500
Sr1—C7^{iii}	2.9686 (13)	C3—C4	1.393 (2)
Sr1—Sr1^{ii}	4.0402 (4)	C3—H3	0.9500
Sr1—Ca1^{ii}	4.0402 (4)	C4—C5	1.381 (2)
Sr1—H2W	2.85 (2)	C4—H4	0.9500
O1—C1	1.3662 (17)	C5—C6	1.4002 (19)
O1—H1O	0.87 (2)	C5—H5	0.9500

O2—C7	1.2703 (17)	C6—C7	1.4872 (18)
O2—Ca1^{ii}	2.6906 (10)	C7—Ca1^{ii}	2.9686 (13)
O2—Sr1^{ii}	2.6906 (10)	C7—Sr1^{ii}	2.9686 (13)
O1W^{i}—Sr1—O1W	106.09 (6)	O3^{iii}—Sr1—Ca1^{ii}	113.09 (3)
O1W^{i}—Sr1—O3	73.59 (4)	O2^{ii}—Sr1—Ca1^{ii}	82.52 (2)
O1W—Sr1—O3	89.60 (4)	O2^{iii}—Sr1—Ca1^{ii}	74.63 (2)
O1W^{i}—Sr1—O3^{i}	89.60 (4)	C7^{ii}—Sr1—Ca1^{ii}	59.19 (3)
O1W—Sr1—O3^{i}	73.59 (4)	C7^{iii}—Sr1—Ca1^{ii}	91.94 (3)
O3—Sr1—O3^{i}	152.13 (5)	Sr1^{ii}—Sr1—Ca1^{ii}	0.0
O1W^{i}—Sr1—O3^{ii}	88.65 (4)	O1W^{i}—Sr1—H2W	114.2 (4)
O1W—Sr1—O3^{ii}	151.62 (4)	O1W—Sr1—H2W	17.1 (4)
O3—Sr1—O3^{ii}	71.12 (4)	O3—Sr1—H2W	106.2 (5)
O3^{i}—Sr1—O3^{ii}	131.81 (3)	O3^{i}—Sr1—H2W	60.1 (4)
O1W^{i}—Sr1—O3^{iii}	151.62 (4)	O3^{ii}—Sr1—H2W	155.7 (4)
O1W—Sr1—O3^{iii}	88.65 (4)	O3^{iii}—Sr1—H2W	74.6 (4)
O3—Sr1—O3^{iii}	131.81 (3)	O2^{ii}—Sr1—H2W	136.4 (5)
O3^{i}—Sr1—O3^{iii}	71.12 (4)	O2^{iii}—Sr1—H2W	82.5 (4)
O3^{ii}—Sr1—O3^{iii}	89.17 (5)	C7^{ii}—Sr1—H2W	151.5 (4)
O1W^{i}—Sr1—O2^{ii}	83.91 (3)	C7^{iii}—Sr1—H2W	80.9 (4)
O1W—Sr1—O2^{ii}	153.36 (4)	Sr1^{ii}—Sr1—H2W	137.7 (4)
O3—Sr1—O2^{ii}	117.03 (3)	Ca1^{ii}—Sr1—H2W	137.7 (4)
O3^{i}—Sr1—O2^{ii}	82.02 (3)	C1—O1—H1O	106.5 (14)
O3^{ii}—Sr1—O2^{ii}	49.91 (3)	C7—O2—Ca1^{ii}	89.66 (8)
O3^{iii}—Sr1—O2^{ii}	73.18 (3)	C7—O2—Sr1^{ii}	89.66 (8)
O1W^{i}—Sr1—O2^{iii}	153.36 (4)	Ca1^{ii}—O2—Sr1^{ii}	0.0
O1W—Sr1—O2^{iii}	83.92 (3)	C7—O3—Sr1	149.93 (9)
O3—Sr1—O2^{iii}	82.02 (3)	C7—O3—Ca1^{ii}	97.08 (8)
O3^{i}—Sr1—O2^{iii}	117.03 (3)	Sr1—O3—Ca1^{ii}	108.9
O3^{ii}—Sr1—O2^{iii}	73.18 (3)	C7—O3—Sr1^{ii}	97.08 (8)
O3^{iii}—Sr1—O2^{iii}	49.91 (3)	Sr1—O3—Sr1^{ii}	108.88 (4)
O2^{ii}—Sr1—O2^{iii}	98.12 (4)	Ca1^{ii}—O3—Sr1^{ii}	0.0
O1W^{i}—Sr1—C7^{ii}	89.42 (4)	Sr1—O1W—H1W	133.3 (15)
O1W—Sr1—C7^{ii}	164.48 (4)	Sr1—O1W—H2W	109.7 (13)
O3—Sr1—C7^{ii}	95.33 (3)	H1W—O1W—H2W	110.1 (19)
O3^{i}—Sr1—C7^{ii}	106.80 (4)	O1—C1—C2	117.63 (12)
O3^{ii}—Sr1—C7^{ii}	25.04 (3)	O1—C1—C6	121.97 (12)
O3^{iii}—Sr1—C7^{ii}	77.09 (4)	C2—C1—C6	120.40 (13)
O2^{ii}—Sr1—C7^{ii}	25.34 (3)	C3—C2—C1	119.48 (13)
O2^{iii}—Sr1—C7^{ii}	82.22 (3)	C3—C2—H2	120.3
O1W^{i}—Sr1—C7^{iii}	164.48 (4)	C1—C2—H2	120.3
O1W—Sr1—C7^{iii}	89.42 (4)	C2—C3—C4	121.07 (14)
O3—Sr1—C7^{iii}	106.80 (4)	C2—C3—H3	119.5
O3^{i}—Sr1—C7^{iii}	95.33 (4)	C4—C3—H3	119.5
O3^{ii}—Sr1—C7^{iii}	77.09 (4)	C5—C4—C3	119.32 (14)
O3^{iii}—Sr1—C7^{iii}	25.04 (3)	C5—C4—H4	120.3
O2^{ii}—Sr1—C7^{iii}	82.22 (3)	C3—C4—H4	120.3
O2^{iii}—Sr1—C7^{iii}	25.34 (3)	C4—C5—C6	120.82 (13)
C7^{ii}—Sr1—C7^{iii}	75.08 (5)	C4—C5—H5	119.6
O1W^{i}—Sr1—Sr1^{ii}	79.35 (3)	C6—C5—H5	119.6
O1W—Sr1—Sr1^{ii}	123.20 (3)	C5—C6—C1	118.83 (13)
O3—Sr1—Sr1^{ii}	36.40 (2)	C5—C6—C7	120.56 (12)

O3^{i}—Sr1—Sr1^{ii}	161.85 (2)	C1—C6—C7	120.62 (12)
O3^{ii}—Sr1—Sr1^{ii}	34.73 (2)	O3—C7—O2	121.12 (12)
O3^{iii}—Sr1—Sr1^{ii}	113.09 (3)	O3—C7—C6	119.62 (12)
O2^{ii}—Sr1—Sr1^{ii}	82.52 (2)	O2—C7—C6	119.25 (12)
O2^{iii}—Sr1—Sr1^{ii}	74.63 (2)	O3—C7—Ca1^{ii}	57.88 (7)
C7^{ii}—Sr1—Sr1^{ii}	59.19 (3)	O2—C7—Ca1^{ii}	65.01 (7)
C7^{iii}—Sr1—Sr1^{ii}	91.94 (3)	C6—C7—Ca1^{ii}	165.24 (9)
O1W^{i}—Sr1—Ca1^{ii}	79.35 (3)	O3—C7—Sr1^{ii}	57.88 (7)
O1W—Sr1—Ca1^{ii}	123.20 (3)	O2—C7—Sr1^{ii}	65.01 (7)
O3—Sr1—Ca1^{ii}	36.40 (2)	C6—C7—Sr1^{ii}	165.24 (9)
O3^{i}—Sr1—Ca1^{ii}	161.85 (2)	Ca1^{ii}—C7—Sr1^{ii}	0.0
O3^{ii}—Sr1—Ca1^{ii}	34.73 (2)		
O1—C1—C2—C3	−177.25 (13)	Sr1^{ii}—O3—C7—Ca1^{ii}	0.0
C6—C1—C2—C3	3.1 (2)	Sr1—O3—C7—Sr1^{ii}	−149.92 (19)
C1—C2—C3—C4	−1.5 (2)	Ca1^{ii}—O3—C7—Sr1^{ii}	0.0
C2—C3—C4—C5	−0.7 (2)	Ca1^{ii}—O2—C7—O3	−14.85 (13)
C3—C4—C5—C6	1.4 (2)	Sr1^{ii}—O2—C7—O3	−14.85 (13)
C4—C5—C6—C1	0.2 (2)	Ca1^{ii}—O2—C7—C6	164.10 (10)
C4—C5—C6—C7	−179.95 (13)	Sr1^{ii}—O2—C7—C6	164.10 (10)
O1—C1—C6—C5	177.92 (12)	Sr1^{ii}—O2—C7—Ca1^{ii}	0.0
C2—C1—C6—C5	−2.5 (2)	Ca1^{ii}—O2—C7—Sr1^{ii}	0.0
O1—C1—C6—C7	−1.9 (2)	C5—C6—C7—O3	20.16 (19)
C2—C1—C6—C7	177.69 (12)	C1—C6—C7—O3	−160.01 (13)
Sr1—O3—C7—O2	−134.00 (15)	C5—C6—C7—O2	−158.80 (13)
Ca1^{ii}—O3—C7—O2	15.92 (13)	C1—C6—C7—O2	21.03 (19)
Sr1^{ii}—O3—C7—O2	15.92 (13)	C5—C6—C7—Ca1^{ii}	−55.8 (4)
Sr1—O3—C7—C6	47.1 (2)	C1—C6—C7—Ca1^{ii}	124.0 (3)
Ca1^{ii}—O3—C7—C6	−163.03 (10)	C5—C6—C7—Sr1^{ii}	−55.8 (4)
Sr1^{ii}—O3—C7—C6	−163.03 (10)	C1—C6—C7—Sr1^{ii}	124.0 (3)
Sr1—O3—C7—Ca1^{ii}	−149.92 (19)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.87 (2)	1.83 (2)	2.6174 (14)	148 (2)
O1*W*—H1*W*···O1^{iv}	0.89 (3)	1.95 (3)	2.8372 (15)	170 (2)
O1*W*—H2*W*···O2^{v}	0.89 (2)	2.02 (2)	2.8984 (16)	168.7 (19)

Symmetry codes: (iv) −*x*+1/2, −*y*+1/2, −*z*; (v) *x*, *y*, *z*−1.

(CaSr5050)

Crystal data

$C_{14}H_{14}Ca_{0.47}O_8Sr_{0.53}$	*V* = 1479.57 (15) Å^3
M_r = 375.48	*Z* = 4
Monoclinic, *C*2/*c*	*F*(000) = 766
a = 16.5994 (10) Å	D_x = 1.686 Mg m^{-3}
b = 11.4832 (6) Å	Mo *Kα* radiation, *λ* = 0.71073 Å
c = 7.7650 (5) Å	Cell parameters from 4653 reflections
β = 91.555 (5)°	*θ* = 3.4–30.1°

μ = 2.17 mm^{-1}
T = 150 K

Prism, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: sealed tube
ω scans

Absorption correction: multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.847, T_{max} = 1.000
8207 measured reflections
1691 independent reflections
1546 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −21→21
k = −14→14
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.058
S = 1.12
1691 reflections
118 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0194P)^2 + 0.3827P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.5000	0.44561 (2)	−0.2500	0.01158 (11)	0.529 (3)
Ca1	0.5000	0.44561 (2)	−0.2500	0.01158 (11)	0.471 (3)
O1	0.25645 (8)	0.25386 (12)	0.26716 (17)	0.0212 (3)	
O2	0.37738 (7)	0.39876 (10)	0.26651 (17)	0.0198 (3)	
O3	0.45461 (7)	0.39421 (10)	0.03917 (17)	0.0204 (3)	
O1W	0.39635 (9)	0.31743 (13)	−0.3803 (2)	0.0277 (4)	
C1	0.30099 (11)	0.18734 (15)	0.1584 (2)	0.0165 (4)	
C2	0.27182 (12)	0.07802 (15)	0.1141 (2)	0.0209 (4)	
H2	0.2214	0.0522	0.1550	0.025*	
C3	0.31666 (13)	0.00696 (16)	0.0102 (3)	0.0242 (5)	
H3	0.2972	−0.0686	−0.0185	0.029*	
C4	0.38967 (12)	0.04380 (16)	−0.0531 (3)	0.0240 (5)	
H4	0.4204	−0.0065	−0.1229	0.029*	
C5	0.41717 (11)	0.15415 (15)	−0.0138 (2)	0.0200 (4)	
H5	0.4664	0.1805	−0.0595	0.024*	
C6	0.37345 (10)	0.22793 (14)	0.0929 (2)	0.0153 (4)	

C7	0.40331 (10)	0.34674 (15)	0.1335 (2)	0.0153 (4)
H1O	0.2830 (15)	0.322 (2)	0.281 (3)	0.053 (8)*
H1W	0.3526 (17)	0.290 (2)	−0.338 (3)	0.061 (9)*
H2W	0.3873 (16)	0.334 (2)	−0.492 (4)	0.060 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01033 (17)	0.01192 (16)	0.01263 (18)	0.000	0.00294 (11)	0.000
Ca1	0.01033 (17)	0.01192 (16)	0.01263 (18)	0.000	0.00294 (11)	0.000
O1	0.0186 (7)	0.0224 (7)	0.0230 (8)	−0.0039 (6)	0.0078 (6)	−0.0032 (6)
O2	0.0193 (7)	0.0182 (6)	0.0220 (8)	−0.0027 (5)	0.0045 (6)	−0.0042 (5)
O3	0.0173 (7)	0.0180 (6)	0.0264 (8)	−0.0043 (5)	0.0072 (6)	−0.0002 (6)
O1W	0.0216 (8)	0.0379 (9)	0.0239 (9)	−0.0071 (7)	0.0059 (7)	0.0032 (7)
C1	0.0174 (9)	0.0181 (9)	0.0140 (10)	−0.0001 (7)	0.0005 (7)	0.0020 (7)
C2	0.0225 (10)	0.0212 (9)	0.0190 (11)	−0.0082 (8)	−0.0002 (8)	0.0036 (8)
C3	0.0354 (12)	0.0161 (9)	0.0209 (12)	−0.0072 (9)	−0.0020 (9)	−0.0003 (8)
C4	0.0302 (11)	0.0191 (9)	0.0228 (11)	0.0019 (8)	0.0023 (9)	−0.0032 (8)
C5	0.0187 (10)	0.0205 (9)	0.0210 (11)	−0.0002 (8)	0.0033 (8)	−0.0001 (8)
C6	0.0143 (9)	0.0160 (9)	0.0155 (10)	−0.0001 (7)	0.0004 (7)	0.0020 (7)
C7	0.0108 (9)	0.0175 (9)	0.0176 (10)	0.0015 (7)	−0.0005 (7)	0.0018 (7)

Geometric parameters (Å, º)

Sr1—O3^{i}	2.4596 (13)	O3—C7	1.262 (2)
Sr1—O3	2.4597 (13)	O3—Ca1^{ii}	2.5621 (13)
Sr1—O1W^{i}	2.4608 (15)	O3—Sr1^{ii}	2.5621 (13)
Sr1—O1W	2.4608 (15)	O1W—H1W	0.86 (3)
Sr1—O3^{ii}	2.5621 (13)	O1W—H2W	0.90 (3)
Sr1—O3^{iii}	2.5621 (13)	C1—C2	1.385 (2)
Sr1—O2^{ii}	2.7143 (12)	C1—C6	1.398 (2)
Sr1—O2^{iii}	2.7143 (12)	C2—C3	1.380 (3)
Sr1—C7^{ii}	3.0001 (18)	C2—H2	0.9500
Sr1—C7^{iii}	3.0001 (18)	C3—C4	1.386 (3)
Sr1—Sr1^{ii}	4.0785 (3)	C3—H3	0.9500
Sr1—Ca1^{ii}	4.0785 (3)	C4—C5	1.378 (2)
Sr1—H2W	2.92 (3)	C4—H4	0.9500
O1—C1	1.370 (2)	C5—C6	1.401 (2)
O1—H1O	0.90 (3)	C5—H5	0.9500
O2—C7	1.278 (2)	C6—C7	1.483 (2)
O2—Ca1^{ii}	2.7143 (12)	C7—Ca1^{ii}	3.0001 (18)
O2—Sr1^{ii}	2.7143 (12)	C7—Sr1^{ii}	3.0001 (18)
O3^{i}—Sr1—O3	152.23 (6)	O3^{iii}—Sr1—Ca1^{ii}	112.38 (3)
O3^{i}—Sr1—O1W^{i}	90.21 (5)	O2^{ii}—Sr1—Ca1^{ii}	82.11 (3)
O3—Sr1—O1W^{i}	73.10 (5)	O2^{iii}—Sr1—Ca1^{ii}	74.57 (3)
O3^{i}—Sr1—O1W	73.10 (5)	C7^{ii}—Sr1—Ca1^{ii}	58.90 (4)
O3—Sr1—O1W	90.21 (5)	C7^{iii}—Sr1—Ca1^{ii}	91.70 (4)
O1W^{i}—Sr1—O1W	106.53 (7)	Sr1^{ii}—Sr1—Ca1^{ii}	0.000 (8)
O3^{i}—Sr1—O3^{ii}	131.57 (4)	O3^{i}—Sr1—H2W	60.8 (5)
O3—Sr1—O3^{ii}	71.40 (4)	O3—Sr1—H2W	106.1 (5)
O1W^{i}—Sr1—O3^{ii}	88.66 (5)	O1W^{i}—Sr1—H2W	115.5 (5)

O1W—Sr1—O3^{ii}	151.92 (5)	O1W—Sr1—H2W	16.7 (5)
O3^{i}—Sr1—O3^{iii}	71.40 (4)	O3^{ii}—Sr1—H2W	154.3 (5)
O3—Sr1—O3^{iii}	131.57 (4)	O3^{iii}—Sr1—H2W	74.4 (5)
O1W^{i}—Sr1—O3^{iii}	151.92 (5)	O2^{ii}—Sr1—H2W	136.7 (5)
O1W—Sr1—O3^{iii}	88.66 (5)	O2^{iii}—Sr1—H2W	81.5 (5)
O3^{ii}—Sr1—O3^{iii}	88.23 (6)	C7^{ii}—Sr1—H2W	150.8 (5)
O3^{i}—Sr1—O2^{ii}	82.31 (4)	C7^{iii}—Sr1—H2W	80.0 (5)
O3—Sr1—O2^{ii}	116.73 (4)	Sr1^{ii}—Sr1—H2W	137.1 (5)
O1W^{i}—Sr1—O2^{ii}	84.05 (4)	Ca1^{ii}—Sr1—H2W	137.1 (5)
O1W—Sr1—O2^{ii}	153.03 (5)	C1—O1—H1O	106.5 (15)
O3^{ii}—Sr1—O2^{ii}	49.43 (4)	C7—O2—Ca1^{ii}	90.00 (10)
O3^{iii}—Sr1—O2^{ii}	72.84 (4)	C7—O2—Sr1^{ii}	90.00 (10)
O3^{i}—Sr1—O2^{iii}	116.73 (4)	Ca1^{ii}—O2—Sr1^{ii}	0.0
O3—Sr1—O2^{iii}	82.31 (4)	C7—O3—Sr1	149.53 (12)
O1W^{i}—Sr1—O2^{iii}	153.03 (5)	C7—O3—Ca1^{ii}	97.49 (11)
O1W—Sr1—O2^{iii}	84.05 (4)	Sr1—O3—Ca1^{ii}	108.6
O3^{ii}—Sr1—O2^{iii}	72.84 (4)	C7—O3—Sr1^{ii}	97.49 (11)
O3^{iii}—Sr1—O2^{iii}	49.43 (4)	Sr1—O3—Sr1^{ii}	108.60 (4)
O2^{ii}—Sr1—O2^{iii}	97.64 (5)	Ca1^{ii}—O3—Sr1^{ii}	0.0
O3^{i}—Sr1—C7^{ii}	106.94 (4)	Sr1—O1W—H1W	130.5 (18)
O3—Sr1—C7^{ii}	95.17 (5)	Sr1—O1W—H2W	111.7 (17)
O1W^{i}—Sr1—C7^{ii}	89.38 (5)	H1W—O1W—H2W	109 (2)
O1W—Sr1—C7^{ii}	164.08 (5)	O1—C1—C2	117.85 (16)
O3^{ii}—Sr1—C7^{ii}	24.65 (4)	O1—C1—C6	121.47 (16)
O3^{iii}—Sr1—C7^{ii}	76.56 (4)	C2—C1—C6	120.68 (17)
O2^{ii}—Sr1—C7^{ii}	25.21 (4)	C3—C2—C1	119.37 (18)
O2^{iii}—Sr1—C7^{ii}	81.84 (4)	C3—C2—H2	120.3
O3^{i}—Sr1—C7^{iii}	95.17 (5)	C1—C2—H2	120.3
O3—Sr1—C7^{iii}	106.94 (4)	C2—C3—C4	121.17 (18)
O1W^{i}—Sr1—C7^{iii}	164.08 (5)	C2—C3—H3	119.4
O1W—Sr1—C7^{iii}	89.38 (5)	C4—C3—H3	119.4
O3^{ii}—Sr1—C7^{iii}	76.56 (4)	C5—C4—C3	119.30 (18)
O3^{iii}—Sr1—C7^{iii}	24.65 (4)	C5—C4—H4	120.4
O2^{ii}—Sr1—C7^{iii}	81.84 (4)	C3—C4—H4	120.4
O2^{iii}—Sr1—C7^{iii}	25.21 (4)	C4—C5—C6	120.88 (17)
C7^{ii}—Sr1—C7^{iii}	74.73 (7)	C4—C5—H5	119.6
O3^{i}—Sr1—Sr1^{ii}	161.89 (3)	C6—C5—H5	119.6
O3—Sr1—Sr1^{ii}	36.54 (3)	C1—C6—C5	118.54 (16)
O1W^{i}—Sr1—Sr1^{ii}	79.04 (4)	C1—C6—C7	121.03 (16)
O1W—Sr1—Sr1^{ii}	123.81 (4)	C5—C6—C7	120.43 (16)
O3^{ii}—Sr1—Sr1^{ii}	34.86 (3)	O3—C7—O2	120.98 (16)
O3^{iii}—Sr1—Sr1^{ii}	112.38 (3)	O3—C7—C6	120.06 (16)
O2^{ii}—Sr1—Sr1^{ii}	82.11 (3)	O2—C7—C6	118.95 (16)
O2^{iii}—Sr1—Sr1^{ii}	74.57 (3)	O3—C7—Ca1^{ii}	57.86 (9)
C7^{ii}—Sr1—Sr1^{ii}	58.90 (4)	O2—C7—Ca1^{ii}	64.79 (9)
C7^{iii}—Sr1—Sr1^{ii}	91.70 (4)	C6—C7—Ca1^{ii}	165.59 (12)
O3^{i}—Sr1—Ca1^{ii}	161.89 (3)	O3—C7—Sr1^{ii}	57.86 (9)
O3—Sr1—Ca1^{ii}	36.54 (3)	O2—C7—Sr1^{ii}	64.79 (9)
O1W^{i}—Sr1—Ca1^{ii}	79.04 (4)	C6—C7—Sr1^{ii}	165.59 (12)
O1W—Sr1—Ca1^{ii}	123.81 (4)	Ca1^{ii}—C7—Sr1^{ii}	0.0
O3^{ii}—Sr1—Ca1^{ii}	34.86 (3)		

O1—C1—C2—C3	−177.53 (17)	Sr1^{ii}—O3—C7—Ca1^{ii}	0.0
C6—C1—C2—C3	2.7 (3)	Sr1—O3—C7—Sr1^{ii}	−149.1 (2)
C1—C2—C3—C4	−1.1 (3)	Ca1^{ii}—O3—C7—Sr1^{ii}	0.0
C2—C3—C4—C5	−1.1 (3)	Ca1^{ii}—O2—C7—O3	−14.40 (17)
C3—C4—C5—C6	1.8 (3)	Sr1^{ii}—O2—C7—O3	−14.40 (17)
O1—C1—C6—C5	178.20 (16)	Ca1^{ii}—O2—C7—C6	164.36 (14)
C2—C1—C6—C5	−2.1 (3)	Sr1^{ii}—O2—C7—C6	164.36 (14)
O1—C1—C6—C7	−2.4 (3)	Sr1^{ii}—O2—C7—Ca1^{ii}	0.0
C2—C1—C6—C7	177.32 (17)	Ca1^{ii}—O2—C7—Sr1^{ii}	0.0
C4—C5—C6—C1	−0.2 (3)	C1—C6—C7—O3	−160.07 (17)
C4—C5—C6—C7	−179.59 (18)	C5—C6—C7—O3	19.3 (3)
Sr1—O3—C7—O2	−133.67 (19)	C1—C6—C7—O2	21.2 (3)
Ca1^{ii}—O3—C7—O2	15.42 (18)	C5—C6—C7—O2	−159.47 (17)
Sr1^{ii}—O3—C7—O2	15.42 (18)	C1—C6—C7—Ca1^{ii}	122.5 (5)
Sr1—O3—C7—C6	47.6 (3)	C5—C6—C7—Ca1^{ii}	−58.1 (6)
Ca1^{ii}—O3—C7—C6	−163.33 (14)	C1—C6—C7—Sr1^{ii}	122.5 (5)
Sr1^{ii}—O3—C7—C6	−163.33 (14)	C5—C6—C7—Sr1^{ii}	−58.1 (6)
Sr1—O3—C7—Ca1^{ii}	−149.1 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.90 (3)	1.81 (3)	2.6075 (17)	147 (2)
O1*W*—H1*W*···O1^{iv}	0.86 (3)	1.97 (3)	2.8276 (19)	171 (2)
O1*W*—H2*W*···O2^{v}	0.90 (3)	2.02 (3)	2.906 (2)	169 (2)

Symmetry codes: (iv) −*x*+1/2, −*y*+1/2, −*z*; (v) *x*, *y*, *z*−1.

(CaSr3070)

Crystal data

$C_{14}H_{14}Ca_{0.37}O_8Sr_{0.63}$
M_r = 380.38
Monoclinic, *C*2/*c*
a = 16.6319 (6) Å
b = 11.4995 (4) Å
c = 7.7729 (3) Å
β = 91.599 (4)°
V = 1486.05 (9) Å^3
Z = 4
F(000) = 774
D_x = 1.700 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 10979 reflections
θ = 3.4–30.4°
μ = 2.49 mm^{-1}
T = 150 K
Prism, colourless
0.30 × 0.25 × 0.12 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: sealed tube
ω scans
Absorption correction: multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.735, T_{max} = 1.000
16351 measured reflections
1704 independent reflections
1622 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −21→21
k = −14→14
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.052$
$S = 1.06$
1704 reflections
118 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2 + 1.2252P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.5000	0.44518 (2)	−0.2500	0.01297 (8)	0.632 (4)
Ca1	0.5000	0.44518 (2)	−0.2500	0.01297 (8)	0.368 (4)
O1	0.25649 (6)	0.25358 (10)	0.26696 (14)	0.0226 (3)	
O2	0.37727 (6)	0.39842 (9)	0.26602 (13)	0.0206 (2)	
O3	0.45448 (6)	0.39323 (9)	0.03965 (14)	0.0215 (3)	
O1W	0.39587 (7)	0.31632 (11)	−0.38135 (16)	0.0283 (3)	
C1	0.30065 (8)	0.18750 (12)	0.15863 (18)	0.0173 (3)	
C2	0.27135 (9)	0.07781 (13)	0.11396 (19)	0.0220 (3)	
H2	0.2210	0.0523	0.1546	0.026*	
C3	0.31588 (10)	0.00648 (14)	0.0105 (2)	0.0255 (3)	
H3	0.2963	−0.0689	−0.0180	0.031*	
C4	0.38909 (11)	0.04319 (14)	−0.0530 (2)	0.0263 (4)	
H4	0.4197	−0.0070	−0.1229	0.032*	
C5	0.41673 (9)	0.15382 (13)	−0.01308 (19)	0.0217 (3)	
H5	0.4660	0.1800	−0.0584	0.026*	
C6	0.37330 (8)	0.22746 (12)	0.09286 (18)	0.0169 (3)	
C7	0.40328 (8)	0.34645 (12)	0.13462 (18)	0.0167 (3)	
H1O	0.2833 (15)	0.321 (2)	0.284 (3)	0.054 (7)*	
H1W	0.3520 (17)	0.292 (2)	−0.344 (3)	0.064 (8)*	
H2W	0.3891 (13)	0.3347 (19)	−0.487 (3)	0.043 (6)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01299 (12)	0.01185 (12)	0.01419 (12)	0.000	0.00261 (7)	0.000
Ca1	0.01299 (12)	0.01185 (12)	0.01419 (12)	0.000	0.00261 (7)	0.000
O1	0.0202 (5)	0.0221 (6)	0.0258 (6)	−0.0037 (4)	0.0074 (4)	−0.0023 (4)
O2	0.0208 (5)	0.0177 (5)	0.0234 (5)	−0.0025 (4)	0.0042 (4)	−0.0034 (4)
O3	0.0209 (5)	0.0186 (5)	0.0254 (6)	−0.0041 (4)	0.0069 (4)	−0.0001 (4)
O1W	0.0243 (6)	0.0364 (7)	0.0245 (6)	−0.0067 (5)	0.0053 (5)	0.0037 (5)
C1	0.0188 (7)	0.0170 (7)	0.0162 (6)	−0.0010 (5)	−0.0003 (5)	0.0024 (5)
C2	0.0238 (7)	0.0211 (7)	0.0210 (7)	−0.0078 (6)	−0.0001 (6)	0.0034 (6)
C3	0.0373 (9)	0.0163 (7)	0.0226 (8)	−0.0064 (6)	−0.0023 (6)	0.0001 (6)
C4	0.0339 (9)	0.0203 (8)	0.0248 (8)	0.0015 (6)	0.0039 (6)	−0.0039 (6)

C5	0.0220 (7)	0.0200 (7)	0.0231 (7)	−0.0001 (6)	0.0037 (6)	0.0003 (6)
C6	0.0173 (6)	0.0152 (7)	0.0182 (7)	−0.0013 (5)	0.0000 (5)	0.0014 (5)
C7	0.0137 (6)	0.0170 (7)	0.0192 (7)	0.0006 (5)	0.0003 (5)	0.0013 (5)

Geometric parameters (Å, º)

Sr1—O3^{i}	2.4686 (10)	O3—C7	1.2627 (17)
Sr1—O3	2.4686 (10)	O3—Ca1^{ii}	2.5749 (10)
Sr1—O1W^{i}	2.4777 (12)	O3—Sr1^{ii}	2.5749 (10)
Sr1—O1W	2.4778 (12)	O1W—H1W	0.84 (3)
Sr1—O3^{ii}	2.5749 (10)	O1W—H2W	0.85 (2)
Sr1—O3^{iii}	2.5749 (10)	C1—C2	1.393 (2)
Sr1—O2^{ii}	2.7260 (10)	C1—C6	1.403 (2)
Sr1—O2^{iii}	2.7260 (10)	C2—C3	1.379 (2)
Sr1—C7^{ii}	3.0088 (14)	C2—H2	0.9500
Sr1—C7^{iii}	3.0088 (14)	C3—C4	1.392 (2)
Sr1—Sr1^{ii}	4.0858 (2)	C3—H3	0.9500
Sr1—Ca1^{ii}	4.0858 (2)	C4—C5	1.385 (2)
Sr1—H2W	2.87 (2)	C4—H4	0.9500
O1—C1	1.3639 (18)	C5—C6	1.397 (2)
O1—H1O	0.90 (3)	C5—H5	0.9500
O2—C7	1.2697 (18)	C6—C7	1.4890 (19)
O2—Ca1^{ii}	2.7260 (10)	C7—Ca1^{ii}	3.0088 (14)
O2—Sr1^{ii}	2.7260 (10)	C7—Sr1^{ii}	3.0088 (14)
O3^{i}—Sr1—O3	151.99 (5)	O3^{iii}—Sr1—Ca1^{ii}	111.93 (2)
O3^{i}—Sr1—O1W^{i}	90.14 (4)	O2^{ii}—Sr1—Ca1^{ii}	81.94 (2)
O3—Sr1—O1W^{i}	73.03 (4)	O2^{iii}—Sr1—Ca1^{ii}	74.52 (2)
O3^{i}—Sr1—O1W	73.03 (4)	C7^{ii}—Sr1—Ca1^{ii}	59.00 (3)
O3—Sr1—O1W	90.14 (4)	C7^{iii}—Sr1—Ca1^{ii}	91.35 (3)
O1W^{i}—Sr1—O1W	106.53 (6)	Sr1^{ii}—Sr1—Ca1^{ii}	0.0
O3^{i}—Sr1—O3^{ii}	131.42 (4)	O3^{i}—Sr1—H2W	61.0 (5)
O3—Sr1—O3^{ii}	71.81 (4)	O3—Sr1—H2W	105.7 (5)
O1W^{i}—Sr1—O3^{ii}	88.87 (4)	O1W^{i}—Sr1—H2W	115.4 (5)
O1W—Sr1—O3^{ii}	152.01 (4)	O1W—Sr1—H2W	16.4 (5)
O3^{i}—Sr1—O3^{iii}	71.81 (4)	O3^{ii}—Sr1—H2W	154.2 (4)
O3—Sr1—O3^{iii}	131.42 (4)	O3^{iii}—Sr1—H2W	74.9 (5)
O1W^{i}—Sr1—O3^{iii}	152.01 (4)	O2^{ii}—Sr1—H2W	137.1 (5)
O1W—Sr1—O3^{iii}	88.87 (4)	O2^{iii}—Sr1—H2W	81.5 (4)
O3^{ii}—Sr1—O3^{iii}	87.62 (5)	C7^{ii}—Sr1—H2W	150.9 (5)
O3^{i}—Sr1—O2^{ii}	82.47 (3)	C7^{iii}—Sr1—H2W	80.3 (5)
O3—Sr1—O2^{ii}	116.77 (3)	Sr1^{ii}—Sr1—H2W	137.0 (5)
O1W^{i}—Sr1—O2^{ii}	84.13 (4)	Ca1^{ii}—Sr1—H2W	137.0 (5)
O1W—Sr1—O2^{ii}	153.06 (4)	C1—O1—H1O	107.2 (15)
O3^{ii}—Sr1—O2^{ii}	49.13 (3)	C7—O2—Ca1^{ii}	90.08 (8)
O3^{iii}—Sr1—O2^{ii}	72.67 (3)	C7—O2—Sr1^{ii}	90.08 (8)
O3^{i}—Sr1—O2^{iii}	116.77 (3)	Ca1^{ii}—O2—Sr1^{ii}	0.0
O3—Sr1—O2^{iii}	82.47 (3)	C7—O3—Sr1	149.91 (9)
O1W^{i}—Sr1—O2^{iii}	153.06 (4)	C7—O3—Ca1^{ii}	97.32 (8)
O1W—Sr1—O2^{iii}	84.13 (4)	Sr1—O3—Ca1^{ii}	108.2
O3^{ii}—Sr1—O2^{iii}	72.67 (3)	C7—O3—Sr1^{ii}	97.32 (8)
O3^{iii}—Sr1—O2^{iii}	49.13 (3)	Sr1—O3—Sr1^{ii}	108.19 (4)

O2^{ii}—Sr1—O2^{iii}	97.44 (4)	Ca1^{ii}—O3—Sr1^{ii}	0.0
O3^{i}—Sr1—C7^{ii}	106.83 (4)	Sr1—O1W—H1W	131.2 (18)
O3—Sr1—C7^{ii}	95.50 (4)	Sr1—O1W—H2W	108.7 (15)
O1W^{i}—Sr1—C7^{ii}	89.53 (4)	H1W—O1W—H2W	109 (2)
O1W—Sr1—C7^{ii}	163.92 (4)	O1—C1—C2	117.89 (13)
O3^{ii}—Sr1—C7^{ii}	24.60 (3)	O1—C1—C6	121.78 (13)
O3^{iii}—Sr1—C7^{ii}	76.10 (4)	C2—C1—C6	120.32 (14)
O2^{ii}—Sr1—C7^{ii}	24.96 (3)	C3—C2—C1	119.63 (14)
O2^{iii}—Sr1—C7^{ii}	81.71 (3)	C3—C2—H2	120.2
O3^{i}—Sr1—C7^{iii}	95.50 (4)	C1—C2—H2	120.2
O3—Sr1—C7^{iii}	106.83 (4)	C2—C3—C4	121.05 (14)
O1W^{i}—Sr1—C7^{iii}	163.92 (4)	C2—C3—H3	119.5
O1W—Sr1—C7^{iii}	89.53 (4)	C4—C3—H3	119.5
O3^{ii}—Sr1—C7^{iii}	76.10 (4)	C5—C4—C3	119.16 (15)
O3^{iii}—Sr1—C7^{iii}	24.60 (3)	C5—C4—H4	120.4
O2^{ii}—Sr1—C7^{iii}	81.71 (3)	C3—C4—H4	120.4
O2^{iii}—Sr1—C7^{iii}	24.96 (3)	C4—C5—C6	121.02 (14)
C7^{ii}—Sr1—C7^{iii}	74.43 (5)	C4—C5—H5	119.5
O3^{i}—Sr1—Sr1^{ii}	161.86 (2)	C6—C5—H5	119.5
O3—Sr1—Sr1^{ii}	36.78 (2)	C5—C6—C1	118.77 (13)
O1W^{i}—Sr1—Sr1^{ii}	79.12 (3)	C5—C6—C7	120.68 (13)
O1W—Sr1—Sr1^{ii}	123.91 (3)	C1—C6—C7	120.55 (13)
O3^{ii}—Sr1—Sr1^{ii}	35.03 (2)	O3—C7—O2	121.35 (13)
O3^{iii}—Sr1—Sr1^{ii}	111.93 (2)	O3—C7—C6	119.42 (13)
O2^{ii}—Sr1—Sr1^{ii}	81.94 (2)	O2—C7—C6	119.23 (12)
O2^{iii}—Sr1—Sr1^{ii}	74.52 (2)	O3—C7—Ca1^{ii}	58.08 (7)
C7^{ii}—Sr1—Sr1^{ii}	59.00 (3)	O2—C7—Ca1^{ii}	64.96 (7)
C7^{iii}—Sr1—Sr1^{ii}	91.35 (3)	C6—C7—Ca1^{ii}	165.88 (9)
O3^{i}—Sr1—Ca1^{ii}	161.86 (2)	O3—C7—Sr1^{ii}	58.08 (7)
O3—Sr1—Ca1^{ii}	36.78 (2)	O2—C7—Sr1^{ii}	64.96 (7)
O1W^{i}—Sr1—Ca1^{ii}	79.12 (3)	C6—C7—Sr1^{ii}	165.88 (9)
O1W—Sr1—Ca1^{ii}	123.91 (3)	Ca1^{ii}—C7—Sr1^{ii}	0.0
O3^{ii}—Sr1—Ca1^{ii}	35.03 (2)		

O1—C1—C2—C3	−177.33 (13)	Sr1^{ii}—O3—C7—Ca1^{ii}	0.0
C6—C1—C2—C3	2.8 (2)	Sr1—O3—C7—Sr1^{ii}	−148.2 (2)
C1—C2—C3—C4	−1.3 (2)	Ca1^{ii}—O3—C7—Sr1^{ii}	0.0
C2—C3—C4—C5	−0.9 (2)	Ca1^{ii}—O2—C7—O3	−14.58 (13)
C3—C4—C5—C6	1.6 (2)	Sr1^{ii}—O2—C7—O3	−14.58 (13)
C4—C5—C6—C1	−0.1 (2)	Ca1^{ii}—O2—C7—C6	164.83 (11)
C4—C5—C6—C7	−179.76 (14)	Sr1^{ii}—O2—C7—C6	164.83 (11)
O1—C1—C6—C5	177.99 (13)	Sr1^{ii}—O2—C7—Ca1^{ii}	0.0
C2—C1—C6—C5	−2.1 (2)	Ca1^{ii}—O2—C7—Sr1^{ii}	0.0
O1—C1—C6—C7	−2.3 (2)	C5—C6—C7—O3	19.7 (2)
C2—C1—C6—C7	177.57 (13)	C1—C6—C7—O3	−160.00 (13)
Sr1—O3—C7—O2	−132.57 (16)	C5—C6—C7—O2	−159.73 (14)
Ca1^{ii}—O3—C7—O2	15.58 (14)	C1—C6—C7—O2	20.6 (2)
Sr1^{ii}—O3—C7—O2	15.58 (14)	C5—C6—C7—Ca1^{ii}	−56.1 (5)
Sr1—O3—C7—C6	48.0 (2)	C1—C6—C7—Ca1^{ii}	124.2 (4)
Ca1^{ii}—O3—C7—C6	−163.82 (10)	C5—C6—C7—Sr1^{ii}	−56.1 (5)

Sr1^{ii}—O3—C7—C6	−163.82 (10)	C1—C6—C7—Sr1^{ii}	124.2 (4)
Sr1—O3—C7—Ca1^{ii}	−148.2 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.90 (3)	1.81 (3)	2.6096 (15)	147 (2)
O1*W*—H1*W*···O1^{iv}	0.84 (3)	1.99 (3)	2.8255 (16)	175 (3)
O1*W*—H2*W*···O2^{v}	0.85 (2)	2.06 (2)	2.9074 (17)	173 (2)

Symmetry codes: (iv) −*x*+1/2, −*y*+1/2, −*z*; (v) *x*, *y*, *z*−1.

(CaSr2080)

Crystal data

$C_{14}H_{14}Ca_{0.21}O_8Sr_{0.79}$
M_r = 387.85
Monoclinic, *C*2/*c*
a = 16.6650 (11) Å
b = 11.4816 (7) Å
c = 7.8105 (5) Å
β = 91.576 (6)°
V = 1493.90 (16) Å^3
Z = 4
F(000) = 785
D_x = 1.724 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4057 reflections
θ = 3.4–30.1°
μ = 2.98 mm^{-1}
T = 150 K
Cut prism, colourless
0.26 × 0.25 × 0.15 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: sealed tube
ω scans
Absorption correction: multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.896, T_{max} = 1.000
6802 measured reflections
1716 independent reflections
1594 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −21→21
k = −14→14
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.054
S = 1.06
1716 reflections
118 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0229P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.5000	0.44477 (2)	−0.2500	0.01095 (9)	0.789 (4)
Ca1	0.5000	0.44477 (2)	−0.2500	0.01095 (9)	0.211 (4)
O1	0.25656 (7)	0.25362 (12)	0.26623 (17)	0.0208 (3)	
O2	0.37707 (7)	0.39785 (11)	0.26542 (16)	0.0186 (3)	
O3	0.45435 (7)	0.39201 (11)	0.04011 (16)	0.0187 (3)	
O1W	0.39514 (8)	0.31499 (13)	−0.38344 (19)	0.0262 (4)	
C1	0.30041 (10)	0.18727 (15)	0.1585 (2)	0.0160 (4)	
C2	0.27070 (11)	0.07764 (15)	0.1144 (2)	0.0199 (4)	
H2	0.2205	0.0522	0.1554	0.024*	
C3	0.31486 (12)	0.00625 (16)	0.0105 (2)	0.0239 (4)	
H3	0.2949	−0.0689	−0.0187	0.029*	
C4	0.38783 (12)	0.04244 (16)	−0.0520 (3)	0.0248 (5)	
H4	0.4183	−0.0081	−0.1213	0.030*	
C5	0.41577 (11)	0.15290 (15)	−0.0124 (2)	0.0201 (4)	
H5	0.4650	0.1788	−0.0578	0.024*	
C6	0.37279 (10)	0.22681 (15)	0.0933 (2)	0.0155 (4)	
C7	0.40303 (10)	0.34547 (15)	0.1344 (2)	0.0146 (4)	
H1O	0.2797 (15)	0.323 (2)	0.280 (4)	0.064 (9)*	
H1W	0.3496 (16)	0.288 (2)	−0.344 (4)	0.060 (8)*	
H2W	0.3899 (14)	0.338 (2)	−0.487 (3)	0.047 (8)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01062 (14)	0.01113 (14)	0.01121 (13)	0.000	0.00220 (9)	0.000
Ca1	0.01062 (14)	0.01113 (14)	0.01121 (13)	0.000	0.00220 (9)	0.000
O1	0.0178 (7)	0.0216 (7)	0.0234 (7)	−0.0037 (5)	0.0074 (5)	−0.0023 (6)
O2	0.0183 (7)	0.0181 (7)	0.0197 (7)	−0.0025 (5)	0.0047 (5)	−0.0036 (5)
O3	0.0169 (6)	0.0196 (7)	0.0198 (7)	−0.0055 (5)	0.0052 (5)	0.0007 (5)
O1W	0.0222 (8)	0.0356 (9)	0.0210 (8)	−0.0090 (6)	0.0045 (6)	0.0022 (6)
C1	0.0177 (9)	0.0176 (9)	0.0126 (9)	0.0008 (7)	−0.0001 (7)	0.0026 (7)
C2	0.0211 (10)	0.0204 (10)	0.0181 (9)	−0.0069 (7)	−0.0016 (7)	0.0025 (7)
C3	0.0366 (11)	0.0154 (9)	0.0194 (10)	−0.0079 (8)	−0.0029 (8)	0.0001 (8)
C4	0.0328 (12)	0.0194 (10)	0.0223 (10)	0.0027 (8)	0.0031 (8)	−0.0039 (8)
C5	0.0197 (10)	0.0211 (10)	0.0194 (10)	0.0006 (7)	0.0026 (7)	−0.0001 (8)
C6	0.0165 (9)	0.0159 (9)	0.0142 (9)	−0.0018 (7)	−0.0010 (7)	0.0001 (7)
C7	0.0112 (8)	0.0170 (9)	0.0153 (9)	0.0008 (7)	−0.0012 (6)	0.0020 (7)

Geometric parameters (Å, º)

Sr1—O3^{i}	2.4849 (12)	O3—C7	1.2623 (19)
Sr1—O3	2.4849 (12)	O3—Ca1^{ii}	2.5903 (12)
Sr1—O1W^{i}	2.5020 (14)	O3—Sr1^{ii}	2.5903 (12)

Sr1—O1W	2.5020 (14)	O1W—H1W	0.88 (3)
Sr1—O3^{ii}	2.5902 (12)	O1W—H2W	0.85 (3)
Sr1—O3^{iii}	2.5902 (12)	C1—C2	1.393 (2)
Sr1—O2^{ii}	2.7368 (12)	C1—C6	1.398 (2)
Sr1—O2^{iii}	2.7368 (12)	C2—C3	1.380 (3)
Sr1—C7^{ii}	3.0245 (17)	C2—H2	0.9500
Sr1—C7^{iii}	3.0245 (17)	C3—C4	1.387 (3)
Sr1—Sr1^{ii}	4.1061 (3)	C3—H3	0.9500
Sr1—Ca1^{ii}	4.1061 (3)	C4—C5	1.383 (2)
Sr1—H2W	2.85 (3)	C4—H4	0.9500
O1—C1	1.362 (2)	C5—C6	1.395 (2)
O1—H1O	0.89 (3)	C5—H5	0.9500
O2—C7	1.273 (2)	C6—C7	1.485 (2)
O2—Ca1^{ii}	2.7368 (12)	C7—Ca1^{ii}	3.0245 (17)
O2—Sr1^{ii}	2.7368 (12)	C7—Sr1^{ii}	3.0245 (17)

O3^{i}—Sr1—O3	151.79 (6)	O3^{iii}—Sr1—Ca1^{ii}	111.76 (3)
O3^{i}—Sr1—O1W^{i}	90.39 (4)	O2^{ii}—Sr1—Ca1^{ii}	81.81 (3)
O3—Sr1—O1W^{i}	72.71 (4)	O2^{iii}—Sr1—Ca1^{ii}	74.61 (3)
O3^{i}—Sr1—O1W	72.71 (4)	C7^{ii}—Sr1—Ca1^{ii}	58.93 (3)
O3—Sr1—O1W	90.39 (4)	C7^{iii}—Sr1—Ca1^{ii}	91.38 (3)
O1W^{i}—Sr1—O1W	106.90 (7)	Sr1^{ii}—Sr1—Ca1^{ii}	0.0
O3^{i}—Sr1—O3^{ii}	131.42 (4)	O3^{i}—Sr1—H2W	60.7 (5)
O3—Sr1—O3^{ii}	72.01 (4)	O3—Sr1—H2W	106.2 (5)
O1W^{i}—Sr1—O3^{ii}	88.72 (5)	O1W^{i}—Sr1—H2W	116.3 (5)
O1W—Sr1—O3^{ii}	152.14 (4)	O1W—Sr1—H2W	16.7 (5)
O3^{i}—Sr1—O3^{iii}	72.01 (4)	O3^{ii}—Sr1—H2W	153.7 (5)
O3—Sr1—O3^{iii}	131.42 (4)	O3^{iii}—Sr1—H2W	74.3 (5)
O1W^{i}—Sr1—O3^{iii}	152.14 (4)	O2^{ii}—Sr1—H2W	136.6 (5)
O1W—Sr1—O3^{iii}	88.72 (5)	O2^{iii}—Sr1—H2W	81.1 (5)
O3^{ii}—Sr1—O3^{iii}	87.32 (6)	C7^{ii}—Sr1—H2W	150.2 (5)
O3^{i}—Sr1—O2^{ii}	82.68 (4)	C7^{iii}—Sr1—H2W	79.7 (5)
O3—Sr1—O2^{ii}	116.70 (4)	Sr1^{ii}—Sr1—H2W	137.2 (5)
O1W^{i}—Sr1—O2^{ii}	84.06 (4)	Ca1^{ii}—Sr1—H2W	137.2 (5)
O1W—Sr1—O2^{ii}	152.87 (4)	C1—O1—H1O	109.9 (16)
O3^{ii}—Sr1—O2^{ii}	48.93 (3)	C7—O2—Ca1^{ii}	90.30 (9)
O3^{iii}—Sr1—O2^{ii}	72.64 (4)	C7—O2—Sr1^{ii}	90.30 (9)
O3^{i}—Sr1—O2^{iii}	116.70 (4)	Ca1^{ii}—O2—Sr1^{ii}	0.0
O3—Sr1—O2^{iii}	82.68 (4)	C7—O3—Sr1	149.79 (11)
O1W^{i}—Sr1—O2^{iii}	152.87 (4)	C7—O3—Ca1^{ii}	97.42 (10)
O1W—Sr1—O2^{iii}	84.06 (4)	Sr1—O3—Ca1^{ii}	108.0
O3^{ii}—Sr1—O2^{iii}	72.64 (4)	C7—O3—Sr1^{ii}	97.42 (10)
O3^{iii}—Sr1—O2^{iii}	48.93 (3)	Sr1—O3—Sr1^{ii}	107.99 (4)
O2^{ii}—Sr1—O2^{iii}	97.36 (5)	Ca1^{ii}—O3—Sr1^{ii}	0.0
O3^{i}—Sr1—C7^{ii}	106.98 (4)	Sr1—O1W—H1W	131.3 (17)
O3—Sr1—C7^{ii}	95.52 (4)	Sr1—O1W—H2W	105.4 (17)
O1W^{i}—Sr1—C7^{ii}	89.34 (5)	H1W—O1W—H2W	112 (2)
O1W—Sr1—C7^{ii}	163.73 (5)	O1—C1—C2	117.73 (15)
O3^{ii}—Sr1—C7^{ii}	24.45 (4)	O1—C1—C6	121.76 (15)
O3^{iii}—Sr1—C7^{ii}	76.00 (4)	C2—C1—C6	120.51 (16)
O2^{ii}—Sr1—C7^{ii}	24.90 (4)	C3—C2—C1	119.39 (17)
O2^{iii}—Sr1—C7^{ii}	81.69 (4)	C3—C2—H2	120.3

O3^{i}—Sr1—C7^{iii}	95.52 (4)	C1—C2—H2	120.3
O3—Sr1—C7^{iii}	106.98 (4)	C2—C3—C4	121.07 (17)
O1W^{i}—Sr1—C7^{iii}	163.73 (5)	C2—C3—H3	119.5
O1W—Sr1—C7^{iii}	89.34 (5)	C4—C3—H3	119.5
O3^{ii}—Sr1—C7^{iii}	76.00 (4)	C5—C4—C3	119.28 (18)
O3^{iii}—Sr1—C7^{iii}	24.45 (4)	C5—C4—H4	120.4
O2^{ii}—Sr1—C7^{iii}	81.69 (4)	C3—C4—H4	120.4
O2^{iii}—Sr1—C7^{iii}	24.90 (4)	C4—C5—C6	120.99 (16)
C7^{ii}—Sr1—C7^{iii}	74.44 (6)	C4—C5—H5	119.5
O3^{i}—Sr1—Sr1^{ii}	161.91 (3)	C6—C5—H5	119.5
O3—Sr1—Sr1^{ii}	36.87 (3)	C5—C6—C1	118.70 (16)
O1W^{i}—Sr1—Sr1^{ii}	78.82 (4)	C5—C6—C7	120.60 (15)
O1W—Sr1—Sr1^{ii}	124.19 (3)	C1—C6—C7	120.69 (15)
O3^{ii}—Sr1—Sr1^{ii}	35.14 (3)	O3—C7—O2	121.30 (15)
O3^{iii}—Sr1—Sr1^{ii}	111.76 (3)	O3—C7—C6	119.60 (15)
O2^{ii}—Sr1—Sr1^{ii}	81.81 (3)	O2—C7—C6	119.10 (15)
O2^{iii}—Sr1—Sr1^{ii}	74.61 (3)	O3—C7—Ca1^{ii}	58.13 (9)
C7^{ii}—Sr1—Sr1^{ii}	58.93 (3)	O2—C7—Ca1^{ii}	64.81 (9)
C7^{iii}—Sr1—Sr1^{ii}	91.38 (3)	C6—C7—Ca1^{ii}	166.10 (12)
O3^{i}—Sr1—Ca1^{ii}	161.91 (3)	O3—C7—Sr1^{ii}	58.13 (9)
O3—Sr1—Ca1^{ii}	36.87 (3)	O2—C7—Sr1^{ii}	64.81 (9)
O1W^{i}—Sr1—Ca1^{ii}	78.82 (4)	C6—C7—Sr1^{ii}	166.10 (12)
O1W—Sr1—Ca1^{ii}	124.19 (3)	Ca1^{ii}—C7—Sr1^{ii}	0.0
O3^{ii}—Sr1—Ca1^{ii}	35.14 (3)		

O1—C1—C2—C3	−177.70 (17)	Sr1^{ii}—O3—C7—Ca1^{ii}	0.0
C6—C1—C2—C3	2.4 (3)	Sr1—O3—C7—Sr1^{ii}	−147.4 (2)
C1—C2—C3—C4	−0.7 (3)	Ca1^{ii}—O3—C7—Sr1^{ii}	0.0
C2—C3—C4—C5	−1.4 (3)	Ca1^{ii}—O2—C7—O3	−14.34 (17)
C3—C4—C5—C6	1.9 (3)	Sr1^{ii}—O2—C7—O3	−14.34 (17)
C4—C5—C6—C1	−0.2 (3)	Ca1^{ii}—O2—C7—C6	164.99 (14)
C4—C5—C6—C7	−179.67 (17)	Sr1^{ii}—O2—C7—C6	164.99 (14)
O1—C1—C6—C5	178.14 (16)	Sr1^{ii}—O2—C7—Ca1^{ii}	0.0
C2—C1—C6—C5	−2.0 (3)	Ca1^{ii}—O2—C7—Sr1^{ii}	0.0
O1—C1—C6—C7	−2.4 (3)	C5—C6—C7—O3	19.4 (3)
C2—C1—C6—C7	177.50 (16)	C1—C6—C7—O3	−160.11 (16)
Sr1—O3—C7—O2	−132.13 (19)	C5—C6—C7—O2	−159.97 (17)
Ca1^{ii}—O3—C7—O2	15.30 (18)	C1—C6—C7—O2	20.6 (3)
Sr1^{ii}—O3—C7—O2	15.30 (18)	C5—C6—C7—Ca1^{ii}	−57.2 (6)
Sr1—O3—C7—C6	48.5 (3)	C1—C6—C7—Ca1^{ii}	123.3 (4)
Ca1^{ii}—O3—C7—C6	−164.02 (13)	C5—C6—C7—Sr1^{ii}	−57.2 (6)
Sr1^{ii}—O3—C7—C6	−164.02 (13)	C1—C6—C7—Sr1^{ii}	123.3 (4)
Sr1—O3—C7—Ca1^{ii}	−147.4 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.89 (3)	1.84 (3)	2.6031 (17)	142 (2)

O1*W*—H1*W*···O1^{iv}	0.88 (3)	1.94 (3)	2.8244 (18)	173 (2)
O1*W*—H2*W*···O2^{v}	0.85 (3)	2.06 (3)	2.911 (2)	178 (2)

Symmetry codes: (iv) −*x*+1/2, −*y*+1/2, −*z*; (v) *x*, *y*, *z*−1.

(CaSr1090)

Crystal data

$C_{14}H_{14}Ca_{0.17}O_8Sr_{0.83}$
M_r = 390.00
Monoclinic, *C*2/*c*
a = 16.6693 (9) Å
b = 11.4865 (7) Å
c = 7.8446 (4) Å
β = 91.510 (5)°
V = 1501.50 (14) Å^3
Z = 4

F(000) = 788
D_x = 1.725 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5187 reflections
θ = 3.3–29.8°
μ = 3.11 mm^{-1}
T = 150 K
Prism, colourless
0.30 × 0.15 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: sealed tube
ω scans

Absorption correction: multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.462, T_{max} = 1.000
8538 measured reflections
1720 independent reflections
1589 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −21→21
k = −14→14
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.065
S = 1.08
1720 reflections
118 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.5000	0.44477 (2)	−0.2500	0.01276 (11)	0.835 (5)
Ca1	0.5000	0.44477 (2)	−0.2500	0.01276 (11)	0.165 (5)
O1	0.25676 (9)	0.25384 (14)	0.26678 (18)	0.0233 (4)	

O2	0.37708 (9)	0.39750 (13)	0.26522 (17)	0.0209 (4)
O3	0.45424 (9)	0.39167 (13)	0.04016 (17)	0.0210 (4)
O1W	0.39510 (10)	0.31466 (16)	−0.3837 (2)	0.0290 (4)
C1	0.30050 (12)	0.18684 (18)	0.1590 (2)	0.0181 (4)
C2	0.27068 (14)	0.07795 (19)	0.1142 (3)	0.0234 (5)
H2	0.2203	0.0529	0.1544	0.028*
C3	0.31465 (15)	0.0064 (2)	0.0112 (3)	0.0267 (5)
H3	0.2947	−0.0688	−0.0172	0.032*
C4	0.38764 (15)	0.04259 (19)	−0.0520 (3)	0.0279 (5)
H4	0.4178	−0.0079	−0.1217	0.033*
C5	0.41582 (13)	0.15248 (19)	−0.0125 (3)	0.0229 (5)
H5	0.4651	0.1783	−0.0577	0.027*
C6	0.37269 (12)	0.22650 (18)	0.0935 (2)	0.0170 (4)
C7	0.40300 (12)	0.34517 (17)	0.1347 (2)	0.0164 (4)
H1O	0.2833 (18)	0.321 (3)	0.279 (4)	0.050 (9)*
H1W	0.353 (2)	0.289 (3)	−0.350 (4)	0.053 (10)*
H2W	0.3914 (19)	0.335 (2)	−0.497 (4)	0.054 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01047 (16)	0.01452 (17)	0.01349 (14)	0.000	0.00403 (10)	0.000
Ca1	0.01047 (16)	0.01452 (17)	0.01349 (14)	0.000	0.00403 (10)	0.000
O1	0.0175 (8)	0.0256 (9)	0.0273 (8)	−0.0046 (7)	0.0095 (6)	−0.0026 (6)
O2	0.0187 (8)	0.0225 (8)	0.0219 (7)	−0.0029 (6)	0.0066 (6)	−0.0042 (6)
O3	0.0181 (8)	0.0221 (8)	0.0231 (7)	−0.0045 (6)	0.0076 (6)	0.0001 (6)
O1W	0.0221 (9)	0.0409 (11)	0.0243 (8)	−0.0111 (8)	0.0060 (7)	0.0012 (7)
C1	0.0156 (10)	0.0221 (11)	0.0168 (9)	−0.0007 (8)	0.0019 (8)	0.0018 (8)
C2	0.0218 (11)	0.0256 (12)	0.0227 (10)	−0.0082 (9)	−0.0003 (9)	0.0034 (8)
C3	0.0368 (14)	0.0190 (12)	0.0244 (11)	−0.0084 (10)	−0.0004 (10)	−0.0012 (9)
C4	0.0338 (14)	0.0223 (13)	0.0278 (11)	0.0014 (10)	0.0045 (10)	−0.0061 (9)
C5	0.0202 (11)	0.0243 (12)	0.0244 (10)	−0.0004 (9)	0.0061 (9)	−0.0002 (8)
C6	0.0159 (10)	0.0183 (11)	0.0169 (9)	−0.0014 (8)	0.0008 (8)	0.0024 (8)
C7	0.0116 (9)	0.0194 (11)	0.0183 (9)	0.0006 (8)	0.0010 (8)	0.0029 (7)

Geometric parameters (Å, º)

Sr1—O3^{i}	2.4953 (13)	O3—C7	1.264 (2)
Sr1—O3	2.4953 (13)	O3—Ca1^{ii}	2.5990 (14)
Sr1—O1W^{i}	2.5091 (17)	O3—Sr1^{ii}	2.5990 (14)
Sr1—O1W	2.5091 (17)	O1W—H1W	0.81 (3)
Sr1—O3^{ii}	2.5990 (14)	O1W—H2W	0.92 (3)
Sr1—O3^{iii}	2.5990 (14)	C1—C2	1.388 (3)
Sr1—O2^{ii}	2.7400 (15)	C1—C6	1.397 (3)
Sr1—O2^{iii}	2.7400 (15)	C2—C3	1.377 (3)
Sr1—C7^{ii}	3.029 (2)	C2—H2	0.9500
Sr1—C7^{iii}	3.029 (2)	C3—C4	1.389 (3)
Sr1—Sr1^{ii}	4.1224 (2)	C3—H3	0.9500
Sr1—Ca1^{ii}	4.1224 (2)	C4—C5	1.379 (3)
Sr1—H2W	2.90 (3)	C4—H4	0.9500
O1—C1	1.368 (2)	C5—C6	1.401 (3)
O1—H1O	0.90 (3)	C5—H5	0.9500

O2—C7	1.273 (2)	C6—C7	1.486 (3)
O2—Ca1^{ii}	2.7400 (15)	C7—Ca1^{ii}	3.029 (2)
O2—Sr1^{ii}	2.7400 (15)	C7—Sr1^{ii}	3.029 (2)
O3^{i}—Sr1—O3	151.70 (7)	O3^{iii}—Sr1—Ca1^{ii}	111.89 (3)
O3^{i}—Sr1—O1W^{i}	90.54 (5)	O2^{ii}—Sr1—Ca1^{ii}	81.76 (3)
O3—Sr1—O1W^{i}	72.51 (5)	O2^{iii}—Sr1—Ca1^{ii}	74.71 (3)
O3^{i}—Sr1—O1W	72.51 (5)	C7^{ii}—Sr1—Ca1^{ii}	58.94 (4)
O3—Sr1—O1W	90.54 (5)	C7^{iii}—Sr1—Ca1^{ii}	91.47 (4)
O1W^{i}—Sr1—O1W	106.88 (8)	Sr1^{ii}—Sr1—Ca1^{ii}	0.0
O3^{i}—Sr1—O3^{ii}	131.51 (5)	O3^{i}—Sr1—H2W	59.1 (6)
O3—Sr1—O3^{ii}	71.98 (5)	O3—Sr1—H2W	107.5 (6)
O1W^{i}—Sr1—O3^{ii}	88.62 (5)	O1W^{i}—Sr1—H2W	115.8 (6)
O1W—Sr1—O3^{ii}	152.26 (5)	O1W—Sr1—H2W	17.6 (6)
O3^{i}—Sr1—O3^{iii}	71.98 (5)	O3^{ii}—Sr1—H2W	154.7 (6)
O3—Sr1—O3^{iii}	131.51 (5)	O3^{iii}—Sr1—H2W	74.1 (6)
O1W^{i}—Sr1—O3^{iii}	152.26 (5)	O2^{ii}—Sr1—H2W	135.4 (6)
O1W—Sr1—O3^{iii}	88.63 (5)	O2^{iii}—Sr1—H2W	82.1 (6)
O3^{ii}—Sr1—O3^{iii}	87.42 (7)	C7^{ii}—Sr1—H2W	149.8 (6)
O3^{i}—Sr1—O2^{ii}	82.82 (5)	C7^{iii}—Sr1—H2W	80.2 (6)
O3—Sr1—O2^{ii}	116.64 (4)	Sr1^{ii}—Sr1—H2W	138.8 (6)
O1W^{i}—Sr1—O2^{ii}	84.17 (5)	Ca1^{ii}—Sr1—H2W	138.8 (6)
O1W—Sr1—O2^{ii}	152.79 (5)	C1—O1—H1O	106.4 (19)
O3^{ii}—Sr1—O2^{ii}	48.88 (4)	C7—O2—Ca1^{ii}	90.41 (12)
O3^{iii}—Sr1—O2^{ii}	72.65 (5)	C7—O2—Sr1^{ii}	90.41 (12)
O3^{i}—Sr1—O2^{iii}	116.64 (4)	Ca1^{ii}—O2—Sr1^{ii}	0.0
O3—Sr1—O2^{iii}	82.82 (5)	C7—O3—Sr1	149.97 (13)
O1W^{i}—Sr1—O2^{iii}	152.79 (5)	C7—O3—Ca1^{ii}	97.22 (11)
O1W—Sr1—O2^{iii}	84.17 (5)	Sr1—O3—Ca1^{ii}	108.0
O3^{ii}—Sr1—O2^{iii}	72.65 (5)	C7—O3—Sr1^{ii}	97.22 (11)
O3^{iii}—Sr1—O2^{iii}	48.88 (4)	Sr1—O3—Sr1^{ii}	108.02 (5)
O2^{ii}—Sr1—O2^{iii}	97.22 (6)	Ca1^{ii}—O3—Sr1^{ii}	0.0
O3^{i}—Sr1—C7^{ii}	107.07 (5)	Sr1—O1W—H1W	133 (2)
O3—Sr1—C7^{ii}	95.50 (5)	Sr1—O1W—H2W	106.5 (19)
O1W^{i}—Sr1—C7^{ii}	89.36 (5)	H1W—O1W—H2W	112 (3)
O1W—Sr1—C7^{ii}	163.72 (6)	O1—C1—C2	118.05 (19)
O3^{ii}—Sr1—C7^{ii}	24.45 (4)	O1—C1—C6	121.47 (18)
O3^{iii}—Sr1—C7^{ii}	76.05 (5)	C2—C1—C6	120.5 (2)
O2^{ii}—Sr1—C7^{ii}	24.85 (5)	C3—C2—C1	119.6 (2)
O2^{iii}—Sr1—C7^{ii}	81.62 (5)	C3—C2—H2	120.2
O3^{i}—Sr1—C7^{iii}	95.50 (5)	C1—C2—H2	120.2
O3—Sr1—C7^{iii}	107.07 (5)	C2—C3—C4	121.1 (2)
O1W^{i}—Sr1—C7^{iii}	163.72 (6)	C2—C3—H3	119.5
O1W—Sr1—C7^{iii}	89.36 (5)	C4—C3—H3	119.5
O3^{ii}—Sr1—C7^{iii}	76.05 (5)	C5—C4—C3	119.3 (2)
O3^{iii}—Sr1—C7^{iii}	24.45 (4)	C5—C4—H4	120.3
O2^{ii}—Sr1—C7^{iii}	81.62 (5)	C3—C4—H4	120.3
O2^{iii}—Sr1—C7^{iii}	24.85 (5)	C4—C5—C6	120.8 (2)
C7^{ii}—Sr1—C7^{iii}	74.42 (7)	C4—C5—H5	119.6
O3^{i}—Sr1—Sr1^{ii}	161.96 (3)	C6—C5—H5	119.6
O3—Sr1—Sr1^{ii}	36.84 (3)	C1—C6—C5	118.74 (19)
O1W^{i}—Sr1—Sr1^{ii}	78.63 (4)	C1—C6—C7	120.69 (18)

O1W—Sr1—Sr1^{ii}	124.31 (4)	C5—C6—C7	120.58 (18)
O3^{ii}—Sr1—Sr1^{ii}	35.14 (3)	O3—C7—O2	121.42 (19)
O3^{iii}—Sr1—Sr1^{ii}	111.89 (3)	O3—C7—C6	119.43 (17)
O2^{ii}—Sr1—Sr1^{ii}	81.76 (3)	O2—C7—C6	119.16 (17)
O2^{iii}—Sr1—Sr1^{ii}	74.71 (3)	O3—C7—Ca1^{ii}	58.33 (10)
C7^{ii}—Sr1—Sr1^{ii}	58.94 (4)	O2—C7—Ca1^{ii}	64.75 (11)
C7^{iii}—Sr1—Sr1^{ii}	91.47 (4)	C6—C7—Ca1^{ii}	166.17 (14)
O3^{i}—Sr1—Ca1^{ii}	161.96 (3)	O3—C7—Sr1^{ii}	58.33 (10)
O3—Sr1—Ca1^{ii}	36.84 (3)	O2—C7—Sr1^{ii}	64.75 (11)
O1W^{i}—Sr1—Ca1^{ii}	78.63 (4)	C6—C7—Sr1^{ii}	166.17 (14)
O1W—Sr1—Ca1^{ii}	124.31 (4)	Ca1^{ii}—C7—Sr1^{ii}	0.0
O3^{ii}—Sr1—Ca1^{ii}	35.14 (3)		
O1—C1—C2—C3	−177.54 (19)	Sr1^{ii}—O3—C7—Ca1^{ii}	0.000 (1)
C6—C1—C2—C3	3.2 (3)	Sr1—O3—C7—Sr1^{ii}	−147.4 (3)
C1—C2—C3—C4	−1.5 (3)	Ca1^{ii}—O3—C7—Sr1^{ii}	0.000 (1)
C2—C3—C4—C5	−0.9 (3)	Ca1^{ii}—O2—C7—O3	−14.47 (19)
C3—C4—C5—C6	1.5 (3)	Sr1^{ii}—O2—C7—O3	−14.47 (19)
O1—C1—C6—C5	178.24 (18)	Ca1^{ii}—O2—C7—C6	165.07 (16)
C2—C1—C6—C5	−2.5 (3)	Sr1^{ii}—O2—C7—C6	165.07 (16)
O1—C1—C6—C7	−2.1 (3)	Sr1^{ii}—O2—C7—Ca1^{ii}	0.0
C2—C1—C6—C7	177.16 (18)	Ca1^{ii}—O2—C7—Sr1^{ii}	0.0
C4—C5—C6—C1	0.1 (3)	C1—C6—C7—O3	−160.15 (18)
C4—C5—C6—C7	−179.5 (2)	C5—C6—C7—O3	19.5 (3)
Sr1—O3—C7—O2	−132.0 (2)	C1—C6—C7—O2	20.3 (3)
Ca1^{ii}—O3—C7—O2	15.4 (2)	C5—C6—C7—O2	−160.04 (19)
Sr1^{ii}—O3—C7—O2	15.4 (2)	C1—C6—C7—Ca1^{ii}	123.2 (5)
Sr1—O3—C7—C6	48.5 (4)	C5—C6—C7—Ca1^{ii}	−57.2 (6)
Ca1^{ii}—O3—C7—C6	−164.14 (15)	C1—C6—C7—Sr1^{ii}	123.2 (5)
Sr1^{ii}—O3—C7—C6	−164.14 (15)	C5—C6—C7—Sr1^{ii}	−57.2 (6)
Sr1—O3—C7—Ca1^{ii}	−147.4 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.90 (3)	1.80 (3)	2.597 (2)	147 (3)
O1*W*—H1*W*···O1^{iv}	0.81 (3)	2.03 (3)	2.827 (2)	173 (3)
O1*W*—H2*W*···O2^{v}	0.92 (3)	2.01 (3)	2.921 (2)	173 (3)

Symmetry codes: (iv) −*x*+1/2, −*y*+1/2, −*z*; (v) *x*, *y*, *z*−1.

(Sr100)

Crystal data

$C_{14}H_{14}O_8Sr$
M_r = 397.87
Monoclinic, *C*2/*c*
a = 16.7182 (6) Å
b = 11.4644 (4) Å
c = 7.8627 (3) Å
β = 91.660 (3)°
V = 1506.37 (9) Å^3
Z = 4
F(000) = 800
D_x = 1.754 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.5418 Å
Cell parameters from 1700 reflections
θ = 5.3–65.9°

μ = 5.36 mm^{-1}
T = 150 K

Prism, colourless
0.6 × 0.5 × 0.2 mm

Data collection

Oxford Diffraction Gemini S diffractometer
Radiation source: sealed tube
ω scans

Absorption correction: analytical *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.120, T_{max} = 0.461
2454 measured reflections
1272 independent reflections
1259 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 65.6°, θ_{min} = 5.3°
h = −19→19
k = −11→13
l = −5→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.073
S = 1.17
1272 reflections
118 parameters
3 restraints
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 2.8711P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Extinction correction: *SHELXL2014*/7 (Sheldrick 2015, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0030 (2)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sr1	0.5000	0.44431 (2)	−0.2500	0.00935 (19)
O1	0.25630 (11)	0.25371 (16)	0.2660 (2)	0.0170 (4)
O2	0.37709 (10)	0.39712 (15)	0.2644 (2)	0.0140 (4)
O3	0.45408 (10)	0.39012 (16)	0.0409 (2)	0.0143 (4)
O1W	0.39465 (12)	0.31301 (18)	−0.3853 (3)	0.0200 (4)
C1	0.29980 (15)	0.1867 (2)	0.1585 (3)	0.0130 (5)
C2	0.26953 (17)	0.0777 (2)	0.1141 (4)	0.0173 (6)
H2	0.2193	0.0529	0.1544	0.021*
C3	0.31329 (18)	0.0055 (2)	0.0107 (4)	0.0198 (6)
H3	0.2932	−0.0696	−0.0182	0.024*
C4	0.3864 (2)	0.0415 (2)	−0.0518 (4)	0.0212 (6)
H4	0.4165	−0.0092	−0.1211	0.025*

C5	0.41481 (17)	0.1514 (2)	−0.0121 (3)	0.0166 (6)
H5	0.4639	0.1770	−0.0569	0.020*
C6	0.37212 (15)	0.2254 (2)	0.0934 (3)	0.0124 (5)
C7	0.40301 (15)	0.3448 (2)	0.1348 (3)	0.0114 (5)
H1O	0.279 (2)	0.317 (2)	0.279 (5)	0.031 (10)*
H1W	0.3533 (15)	0.289 (3)	−0.344 (4)	0.029 (10)*
H2W	0.391 (2)	0.336 (3)	−0.487 (3)	0.030 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0106 (2)	0.0095 (2)	0.0081 (2)	0.000	0.00290 (13)	0.000
O1	0.0162 (9)	0.0165 (10)	0.0185 (10)	−0.0050 (8)	0.0071 (7)	−0.0010 (8)
O2	0.0150 (9)	0.0141 (9)	0.0132 (9)	−0.0021 (7)	0.0054 (7)	−0.0024 (7)
O3	0.0149 (9)	0.0148 (9)	0.0134 (9)	−0.0040 (7)	0.0049 (7)	−0.0007 (7)
O1W	0.0181 (10)	0.0281 (11)	0.0140 (10)	−0.0080 (8)	0.0040 (8)	0.0006 (8)
C1	0.0150 (12)	0.0150 (12)	0.0089 (12)	−0.0001 (10)	−0.0001 (10)	0.0025 (10)
C2	0.0193 (14)	0.0179 (12)	0.0145 (13)	−0.0069 (11)	−0.0004 (11)	0.0040 (11)
C3	0.0317 (16)	0.0112 (13)	0.0164 (13)	−0.0058 (11)	−0.0022 (12)	−0.0009 (10)
C4	0.0302 (17)	0.0157 (13)	0.0179 (15)	0.0015 (11)	0.0036 (13)	−0.0038 (11)
C5	0.0185 (13)	0.0172 (13)	0.0141 (13)	0.0002 (11)	0.0038 (10)	0.0003 (10)
C6	0.0141 (12)	0.0126 (12)	0.0106 (12)	0.0002 (10)	−0.0006 (10)	0.0021 (10)
C7	0.0103 (12)	0.0128 (12)	0.0111 (12)	−0.0001 (9)	−0.0010 (10)	0.0028 (10)

Geometric parameters (Å, º)

Sr1—O3	2.5116 (17)	O3—C7	1.257 (3)
Sr1—O3^{i}	2.5116 (17)	O3—Sr1^{ii}	2.6121 (17)
Sr1—O1W	2.528 (2)	O1W—H1W	0.819 (19)
Sr1—O1W^{i}	2.528 (2)	O1W—H2W	0.841 (19)
Sr1—O3^{ii}	2.6120 (17)	C1—C2	1.389 (4)
Sr1—O3^{iii}	2.6120 (17)	C1—C6	1.399 (4)
Sr1—O2^{ii}	2.7484 (17)	C2—C3	1.384 (4)
Sr1—O2^{iii}	2.7484 (17)	C2—H2	0.9500
Sr1—C7^{ii}	3.035 (3)	C3—C4	1.393 (4)
Sr1—C7^{iii}	3.035 (3)	C3—H3	0.9500
Sr1—Sr1^{ii}	4.1335 (2)	C4—C5	1.379 (4)
Sr1—Sr1^{iv}	4.1335 (2)	C4—H4	0.9500
Sr1—H2W	2.86 (3)	C5—C6	1.397 (4)
O1—C1	1.367 (3)	C5—H5	0.9500
O1—H1O	0.825 (19)	C6—C7	1.496 (4)
O2—C7	1.270 (3)	C7—Sr1^{ii}	3.035 (3)
O2—Sr1^{ii}	2.7484 (17)		
O3—Sr1—O3^{i}	151.36 (8)	O3—Sr1—Sr1^{iv}	161.98 (4)
O3—Sr1—O1W	90.48 (6)	O3^{i}—Sr1—Sr1^{iv}	37.05 (4)
O3^{i}—Sr1—O1W	72.37 (6)	O1W—Sr1—Sr1^{iv}	78.63 (5)
O3—Sr1—O1W^{i}	72.37 (6)	O1W^{i}—Sr1—Sr1^{iv}	124.40 (4)
O3^{i}—Sr1—O1W^{i}	90.48 (6)	O3^{ii}—Sr1—Sr1^{iv}	111.47 (4)
O1W—Sr1—O1W^{i}	106.92 (10)	O3^{iii}—Sr1—Sr1^{iv}	35.40 (4)
O3—Sr1—O3^{ii}	72.46 (6)	O2^{ii}—Sr1—Sr1^{iv}	74.68 (4)
O3^{i}—Sr1—O3^{ii}	131.37 (6)	O2^{iii}—Sr1—Sr1^{iv}	81.70 (4)

O1W—Sr1—O3^{ii}	152.38 (6)	C7^{ii}—Sr1—Sr1^{iv}	91.32 (5)
O1W^{i}—Sr1—O3^{ii}	88.82 (6)	C7^{iii}—Sr1—Sr1^{iv}	58.98 (5)
O3—Sr1—O3^{iii}	131.37 (6)	Sr1^{ii}—Sr1—Sr1^{iv}	144.010 (14)
O3^{i}—Sr1—O3^{iii}	72.46 (6)	O3—Sr1—H2W	106.2 (5)
O1W—Sr1—O3^{iii}	88.82 (6)	O3^{i}—Sr1—H2W	60.4 (6)
O1W^{i}—Sr1—O3^{iii}	152.38 (6)	O1W—Sr1—H2W	16.6 (5)
O3^{ii}—Sr1—O3^{iii}	86.78 (8)	O1W^{i}—Sr1—H2W	116.2 (7)
O3—Sr1—O2^{ii}	116.73 (5)	O3^{ii}—Sr1—H2W	153.8 (7)
O3^{i}—Sr1—O2^{ii}	82.96 (5)	O3^{iii}—Sr1—H2W	74.6 (6)
O1W—Sr1—O2^{ii}	152.75 (6)	O2^{ii}—Sr1—H2W	136.6 (5)
O1W^{i}—Sr1—O2^{ii}	84.18 (6)	O2^{iii}—Sr1—H2W	81.3 (7)
O3^{ii}—Sr1—O2^{ii}	48.61 (5)	C7^{ii}—Sr1—H2W	150.2 (6)
O3^{iii}—Sr1—O2^{ii}	72.53 (5)	C7^{iii}—Sr1—H2W	79.9 (7)
O3—Sr1—O2^{iii}	82.96 (5)	Sr1^{ii}—Sr1—H2W	137.4 (6)
O3^{i}—Sr1—O2^{iii}	116.73 (5)	Sr1^{iv}—Sr1—H2W	62.1 (5)
O1W—Sr1—O2^{iii}	84.18 (6)	C1—O1—H1O	109 (3)
O1W^{i}—Sr1—O2^{iii}	152.75 (6)	C7—O2—Sr1^{ii}	90.36 (14)
O3^{ii}—Sr1—O2^{iii}	72.53 (5)	C7—O3—Sr1	150.19 (16)
O3^{iii}—Sr1—O2^{iii}	48.61 (5)	C7—O3—Sr1^{ii}	97.06 (15)
O2^{ii}—Sr1—O2^{iii}	97.18 (7)	Sr1—O3—Sr1^{ii}	107.54 (6)
O3—Sr1—C7^{ii}	95.74 (6)	Sr1—O1W—H1W	128 (3)
O3^{i}—Sr1—C7^{ii}	107.11 (6)	Sr1—O1W—H2W	104 (2)
O1W—Sr1—C7^{ii}	163.67 (7)	H1W—O1W—H2W	116 (4)
O1W^{i}—Sr1—C7^{ii}	89.37 (6)	O1—C1—C2	117.7 (2)
O3^{ii}—Sr1—C7^{ii}	24.27 (6)	O1—C1—C6	121.9 (2)
O3^{iii}—Sr1—C7^{ii}	75.74 (6)	C2—C1—C6	120.4 (2)
O2^{ii}—Sr1—C7^{ii}	24.74 (6)	C3—C2—C1	119.4 (3)
O2^{iii}—Sr1—C7^{ii}	81.62 (6)	C3—C2—H2	120.3
O3—Sr1—C7^{iii}	107.11 (6)	C1—C2—H2	120.3
O3^{i}—Sr1—C7^{iii}	95.74 (6)	C2—C3—C4	121.0 (3)
O1W—Sr1—C7^{iii}	89.37 (6)	C2—C3—H3	119.5
O1W^{i}—Sr1—C7^{iii}	163.67 (7)	C4—C3—H3	119.5
O3^{ii}—Sr1—C7^{iii}	75.74 (6)	C5—C4—C3	119.4 (3)
O3^{iii}—Sr1—C7^{iii}	24.27 (6)	C5—C4—H4	120.3
O2^{ii}—Sr1—C7^{iii}	81.62 (6)	C3—C4—H4	120.3
O2^{iii}—Sr1—C7^{iii}	24.74 (6)	C4—C5—C6	120.7 (3)
C7^{ii}—Sr1—C7^{iii}	74.37 (9)	C4—C5—H5	119.6
O3—Sr1—Sr1^{ii}	37.05 (4)	C6—C5—H5	119.6
O3^{i}—Sr1—Sr1^{ii}	161.98 (4)	C5—C6—C1	119.1 (2)
O1W—Sr1—Sr1^{ii}	124.40 (4)	C5—C6—C7	120.4 (2)
O1W^{i}—Sr1—Sr1^{ii}	78.63 (5)	C1—C6—C7	120.5 (2)
O3^{ii}—Sr1—Sr1^{ii}	35.40 (4)	O3—C7—O2	122.0 (2)
O3^{iii}—Sr1—Sr1^{ii}	111.47 (4)	O3—C7—C6	119.1 (2)
O2^{ii}—Sr1—Sr1^{ii}	81.70 (4)	O2—C7—C6	118.9 (2)
O2^{iii}—Sr1—Sr1^{ii}	74.68 (4)	O3—C7—Sr1^{ii}	58.66 (13)
C7^{ii}—Sr1—Sr1^{ii}	58.98 (5)	O2—C7—Sr1^{ii}	64.90 (13)
C7^{iii}—Sr1—Sr1^{ii}	91.32 (5)	C6—C7—Sr1^{ii}	166.48 (17)
O1—C1—C2—C3	−177.6 (2)	Sr1^{ii}—O3—C7—O2	15.1 (3)
C6—C1—C2—C3	2.8 (4)	Sr1—O3—C7—C6	49.6 (4)
C1—C2—C3—C4	−1.1 (4)	Sr1^{ii}—O3—C7—C6	−164.54 (19)
C2—C3—C4—C5	−1.1 (4)	Sr1—O3—C7—Sr1^{ii}	−145.8 (3)

C3—C4—C5—C6	1.7 (4)	Sr1^{ii}—O2—C7—O3	−14.2 (2)
C4—C5—C6—C1	−0.1 (4)	Sr1^{ii}—O2—C7—C6	165.4 (2)
C4—C5—C6—C7	−179.5 (3)	C5—C6—C7—O3	19.3 (4)
O1—C1—C6—C5	178.2 (2)	C1—C6—C7—O3	−160.1 (2)
C2—C1—C6—C5	−2.2 (4)	C5—C6—C7—O2	−160.3 (2)
O1—C1—C6—C7	−2.3 (4)	C1—C6—C7—O2	20.2 (4)
C2—C1—C6—C7	177.3 (2)	C5—C6—C7—Sr1^{ii}	−57.5 (8)
Sr1—O3—C7—O2	−130.7 (3)	C1—C6—C7—Sr1^{ii}	123.1 (7)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2	0.83 (2)	1.89 (3)	2.604 (2)	145 (4)
O1*W*—H1*W*···O1^{v}	0.82 (2)	2.01 (2)	2.823 (3)	172 (4)
O1*W*—H2*W*···O2^{vi}	0.84 (2)	2.08 (2)	2.925 (3)	178 (4)

Symmetry codes: (v) −*x*+1/2, −*y*+1/2, −*z*; (vi) *x*, *y*, *z*−1.

(SrBa)

Crystal data

$C_{14}H_{14}Ba_{0.27}O_8Sr_{0.73}$
M_r = 411.35
Monoclinic, *C*2/*c*
a = 16.8381 (7) Å
b = 11.4349 (5) Å
c = 7.9433 (3) Å
β = 91.280 (4)°
V = 1529.04 (11) Å^3
Z = 4

F(000) = 820
D_x = 1.787 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 7047 reflections
θ = 3.3–29.8°
μ = 3.31 mm^{-1}
T = 150 K
Cut prism, colourless
0.28 × 0.25 × 0.15 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: sealed tube
ω scans

Absorption correction: multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.728, T_{max} = 1.000
10452 measured reflections
1754 independent reflections
1685 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −21→21
k = −14→14
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.044
S = 1.17

1754 reflections
118 parameters
0 restraints
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0132P)^2 + 1.6161P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.5000	0.43902 (2)	−0.2500	0.01477 (7)	0.729 (4)
Ba1	0.5000	0.43902 (2)	−0.2500	0.01477 (7)	0.271 (4)
O1	0.25640 (8)	0.25403 (12)	0.26510 (18)	0.0233 (3)	
O2	0.37639 (8)	0.39626 (11)	0.26415 (17)	0.0215 (3)	
O1W	0.39280 (9)	0.31015 (15)	−0.3903 (2)	0.0335 (4)	
O3	0.45452 (8)	0.38793 (11)	0.04491 (18)	0.0233 (3)	
C1	0.29899 (10)	0.18637 (16)	0.1589 (2)	0.0175 (4)	
C2	0.26877 (12)	0.07775 (16)	0.1138 (2)	0.0226 (4)	
H2	0.2188	0.0530	0.1541	0.027*	
C3	0.31155 (13)	0.00609 (18)	0.0105 (3)	0.0267 (5)	
H3	0.2908	−0.0685	−0.0195	0.032*	
C4	0.38438 (13)	0.04069 (17)	−0.0508 (3)	0.0276 (5)	
H4	0.4139	−0.0103	−0.1201	0.033*	
C5	0.41326 (11)	0.14997 (17)	−0.0100 (2)	0.0223 (4)	
H5	0.4625	0.1748	−0.0539	0.027*	
C6	0.37156 (11)	0.22479 (15)	0.0947 (2)	0.0172 (4)	
C7	0.40255 (10)	0.34315 (16)	0.1364 (2)	0.0176 (4)	
H1W	0.3492 (17)	0.287 (2)	−0.361 (3)	0.048 (8)*	
H2W	0.3864 (16)	0.326 (2)	−0.495 (4)	0.048 (8)*	
H7	0.2843 (16)	0.319 (2)	0.285 (3)	0.052 (8)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01305 (10)	0.01757 (11)	0.01383 (11)	0.000	0.00353 (7)	0.000
Ba1	0.01305 (10)	0.01757 (11)	0.01383 (11)	0.000	0.00353 (7)	0.000
O1	0.0196 (7)	0.0219 (7)	0.0288 (8)	−0.0043 (6)	0.0080 (6)	−0.0023 (6)
O2	0.0198 (7)	0.0189 (6)	0.0261 (8)	−0.0030 (5)	0.0063 (6)	−0.0051 (6)
O1W	0.0254 (8)	0.0447 (10)	0.0307 (9)	−0.0075 (7)	0.0081 (7)	0.0061 (8)
O3	0.0209 (7)	0.0200 (7)	0.0293 (8)	−0.0053 (5)	0.0095 (6)	−0.0022 (6)
C1	0.0179 (9)	0.0187 (9)	0.0159 (9)	−0.0006 (7)	0.0001 (7)	0.0037 (7)
C2	0.0255 (10)	0.0219 (10)	0.0204 (10)	−0.0077 (8)	−0.0009 (8)	0.0037 (8)
C3	0.0384 (12)	0.0184 (10)	0.0231 (11)	−0.0072 (9)	−0.0016 (9)	0.0001 (8)
C4	0.0357 (11)	0.0196 (10)	0.0276 (11)	0.0012 (8)	0.0044 (9)	−0.0041 (8)
C5	0.0227 (9)	0.0207 (9)	0.0238 (10)	−0.0001 (8)	0.0055 (8)	0.0002 (8)
C6	0.0173 (8)	0.0161 (9)	0.0183 (9)	−0.0018 (7)	−0.0006 (7)	0.0007 (7)
C7	0.0132 (8)	0.0177 (9)	0.0219 (10)	0.0003 (7)	0.0001 (7)	0.0009 (7)

Geometric parameters (Å, º)

Sr1—O3^{i}	2.5486 (13)	O1W—H2W	0.86 (3)
Sr1—O3	2.5486 (13)	O3—C7	1.259 (2)
Sr1—O1W^{i}	2.5654 (17)	O3—Ba1^{ii}	2.6646 (13)
Sr1—O1W	2.5655 (17)	O3—Sr1^{ii}	2.6646 (13)
Sr1—O3^{ii}	2.6647 (13)	C1—C2	1.386 (3)
Sr1—O3^{iii}	2.6647 (13)	C1—C6	1.405 (2)
Sr1—O2^{ii}	2.8113 (13)	C2—C3	1.375 (3)
Sr1—O2^{iii}	2.8113 (13)	C2—H2	0.9500
Sr1—C7^{ii}	3.1056 (18)	C3—C4	1.387 (3)
Sr1—C7^{iii}	3.1056 (18)	C3—H3	0.9500
Sr1—Ba1^{ii}	4.2094 (2)	C4—C5	1.377 (3)
Sr1—Sr1^{ii}	4.2094 (2)	C4—H4	0.9500
O1—C1	1.361 (2)	C5—C6	1.394 (3)
O1—H7	0.89 (3)	C5—H5	0.9500
O2—C7	1.270 (2)	C6—C7	1.485 (2)
O2—Ba1^{ii}	2.8112 (13)	C7—Ba1^{ii}	3.1056 (18)
O2—Sr1^{ii}	2.8112 (13)	C7—Sr1^{ii}	3.1056 (18)
O1W—H1W	0.82 (3)		

O3^{i}—Sr1—O3	153.49 (6)	C7^{iii}—Sr1—Ba1^{ii}	89.85 (4)
O3^{i}—Sr1—O1W^{i}	92.55 (5)	O3^{i}—Sr1—Sr1^{ii}	161.72 (3)
O3—Sr1—O1W^{i}	72.06 (5)	O3—Sr1—Sr1^{ii}	37.10 (3)
O3^{i}—Sr1—O1W	72.06 (5)	O1W^{i}—Sr1—Sr1^{ii}	78.19 (4)
O3—Sr1—O1W	92.56 (5)	O1W—Sr1—Sr1^{ii}	125.82 (4)
O1W^{i}—Sr1—O1W	109.88 (8)	O3^{ii}—Sr1—Sr1^{ii}	35.23 (3)
O3^{i}—Sr1—O3^{ii}	130.09 (4)	O3^{iii}—Sr1—Sr1^{ii}	108.95 (3)
O3—Sr1—O3^{ii}	72.33 (4)	O2^{ii}—Sr1—Sr1^{ii}	80.29 (3)
O1W^{i}—Sr1—O3^{ii}	88.35 (5)	O2^{iii}—Sr1—Sr1^{ii}	74.02 (3)
O1W—Sr1—O3^{ii}	151.87 (5)	C7^{ii}—Sr1—Sr1^{ii}	58.08 (3)
O3^{i}—Sr1—O3^{iii}	72.33 (4)	C7^{iii}—Sr1—Sr1^{ii}	89.85 (4)
O3—Sr1—O3^{iii}	130.09 (4)	Ba1^{ii}—Sr1—Sr1^{ii}	0.0
O1W^{i}—Sr1—O3^{iii}	151.87 (5)	C1—O1—H7	107.6 (18)
O1W—Sr1—O3^{iii}	88.35 (5)	C7—O2—Ba1^{ii}	91.03 (10)
O3^{ii}—Sr1—O3^{iii}	84.09 (6)	C7—O2—Sr1^{ii}	91.03 (10)
O3^{i}—Sr1—O2^{ii}	83.05 (4)	Ba1^{ii}—O2—Sr1^{ii}	0.0
O3—Sr1—O2^{ii}	115.36 (4)	Sr1—O1W—H1W	133.7 (19)
O1W^{i}—Sr1—O2^{ii}	83.56 (5)	Sr1—O1W—H2W	111.9 (18)
O1W—Sr1—O2^{ii}	151.87 (5)	H1W—O1W—H2W	104 (3)
O3^{ii}—Sr1—O2^{ii}	47.47 (4)	C7—O3—Sr1	148.31 (13)
O3^{iii}—Sr1—O2^{ii}	71.39 (4)	C7—O3—Ba1^{ii}	98.23 (11)
O3^{i}—Sr1—O2^{iii}	115.36 (4)	Sr1—O3—Ba1^{ii}	107.7
O3—Sr1—O2^{iii}	83.05 (4)	C7—O3—Sr1^{ii}	98.23 (11)
O1W^{i}—Sr1—O2^{iii}	151.87 (5)	Sr1—O3—Sr1^{ii}	107.67 (4)
O1W—Sr1—O2^{iii}	83.56 (5)	Ba1^{ii}—O3—Sr1^{ii}	0.0
O3^{ii}—Sr1—O2^{iii}	71.39 (4)	O1—C1—C2	118.31 (16)
O3^{iii}—Sr1—O2^{iii}	47.47 (4)	O1—C1—C6	121.46 (16)
O2^{ii}—Sr1—O2^{iii}	95.86 (5)	C2—C1—C6	120.24 (17)
O3^{i}—Sr1—C7^{ii}	106.46 (5)	C3—C2—C1	119.61 (18)
O3—Sr1—C7^{ii}	94.84 (5)	C3—C2—H2	120.2
O1W^{i}—Sr1—C7^{ii}	88.42 (5)	C1—C2—H2	120.2
O1W—Sr1—C7^{ii}	161.62 (5)	C2—C3—C4	121.24 (18)

O3^{ii}—Sr1—C7^{ii}	23.65 (4)	C2—C3—H3	119.4
O3^{iii}—Sr1—C7^{ii}	74.03 (5)	C4—C3—H3	119.4
O2^{ii}—Sr1—C7^{ii}	24.14 (4)	C5—C4—C3	119.10 (19)
O2^{iii}—Sr1—C7^{ii}	80.67 (4)	C5—C4—H4	120.4
O3^{i}—Sr1—C7^{iii}	94.84 (5)	C3—C4—H4	120.4
O3—Sr1—C7^{iii}	106.46 (5)	C4—C5—C6	121.18 (18)
O1W^{i}—Sr1—C7^{iii}	161.62 (5)	C4—C5—H5	119.4
O1W—Sr1—C7^{iii}	88.42 (5)	C6—C5—H5	119.4
O3^{ii}—Sr1—C7^{iii}	74.03 (5)	C5—C6—C1	118.58 (17)
O3^{iii}—Sr1—C7^{iii}	23.65 (4)	C5—C6—C7	120.86 (16)
O2^{ii}—Sr1—C7^{iii}	80.67 (4)	C1—C6—C7	120.55 (16)
O2^{iii}—Sr1—C7^{iii}	24.14 (4)	O3—C7—O2	121.66 (17)
C7^{ii}—Sr1—C7^{iii}	73.35 (7)	O3—C7—C6	119.18 (16)
O3^{i}—Sr1—Ba1^{ii}	161.72 (3)	O2—C7—C6	119.16 (16)
O3—Sr1—Ba1^{ii}	37.10 (3)	O3—C7—Ba1^{ii}	58.12 (9)
O1W^{i}—Sr1—Ba1^{ii}	78.19 (4)	O2—C7—Ba1^{ii}	64.83 (9)
O1W—Sr1—Ba1^{ii}	125.82 (4)	C6—C7—Ba1^{ii}	167.51 (12)
O3^{ii}—Sr1—Ba1^{ii}	35.23 (3)	O3—C7—Sr1^{ii}	58.12 (9)
O3^{iii}—Sr1—Ba1^{ii}	108.95 (3)	O2—C7—Sr1^{ii}	64.83 (9)
O2^{ii}—Sr1—Ba1^{ii}	80.29 (3)	C6—C7—Sr1^{ii}	167.51 (12)
O2^{iii}—Sr1—Ba1^{ii}	74.02 (3)	Ba1^{ii}—C7—Sr1^{ii}	0.0
C7^{ii}—Sr1—Ba1^{ii}	58.08 (3)		
O1—C1—C2—C3	−178.19 (18)	Sr1^{ii}—O3—C7—Ba1^{ii}	0.0
C6—C1—C2—C3	2.2 (3)	Sr1—O3—C7—Sr1^{ii}	−144.9 (2)
C1—C2—C3—C4	−0.5 (3)	Ba1^{ii}—O3—C7—Sr1^{ii}	0.0
C2—C3—C4—C5	−1.4 (3)	Ba1^{ii}—O2—C7—O3	−12.76 (18)
C3—C4—C5—C6	1.6 (3)	Sr1^{ii}—O2—C7—O3	−12.76 (18)
C4—C5—C6—C1	0.2 (3)	Ba1^{ii}—O2—C7—C6	166.69 (15)
C4—C5—C6—C7	−179.17 (19)	Sr1^{ii}—O2—C7—C6	166.69 (15)
O1—C1—C6—C5	178.34 (17)	Sr1^{ii}—O2—C7—Ba1^{ii}	0.0
C2—C1—C6—C5	−2.1 (3)	Ba1^{ii}—O2—C7—Sr1^{ii}	0.0
O1—C1—C6—C7	−2.3 (3)	C5—C6—C7—O3	18.5 (3)
C2—C1—C6—C7	177.26 (17)	C1—C6—C7—O3	−160.87 (18)
Sr1—O3—C7—O2	−131.29 (19)	C5—C6—C7—O2	−161.00 (18)
Ba1^{ii}—O3—C7—O2	13.61 (19)	C1—C6—C7—O2	19.7 (3)
Sr1^{ii}—O3—C7—O2	13.61 (19)	C5—C6—C7—Ba1^{ii}	−55.5 (7)
Sr1—O3—C7—C6	49.3 (3)	C1—C6—C7—Ba1^{ii}	125.1 (5)
Ba1^{ii}—O3—C7—C6	−165.83 (14)	C5—C6—C7—Sr1^{ii}	−55.5 (7)
Sr1^{ii}—O3—C7—C6	−165.83 (14)	C1—C6—C7—Sr1^{ii}	125.1 (5)
Sr1—O3—C7—Ba1^{ii}	−144.9 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H7···O2	0.89 (3)	1.80 (3)	2.5938 (18)	148 (3)
O1*W*—H1*W*···O1^{iv}	0.82 (3)	2.00 (3)	2.820 (2)	172 (3)
O1*W*—H2*W*···O2^{v}	0.86 (3)	2.08 (3)	2.923 (2)	169 (3)

Symmetry codes: (iv) −*x*+1/2, −*y*+1/2, −*z*; (v) *x*, *y*, *z*−1.