

Crystal structures of $\text{Sr}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$, $\text{Sr}(\text{ClO}_4)_2 \cdot 4\text{H}_2\text{O}$ and $\text{Sr}(\text{ClO}_4)_2 \cdot 9\text{H}_2\text{O}$

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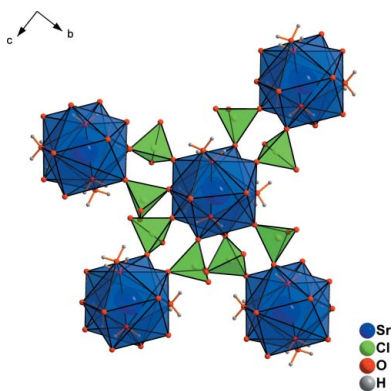
CCDC references: 1033590; 1033589; 1033588

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The title compounds, strontium perchlorate trihydrate {di- μ -aqua-aquadi- μ -perchlorato-strontium, $[\text{Sr}(\text{ClO}_4)_2(\text{H}_2\text{O})_3]_n$ }, strontium perchlorate tetrahydrate {di- μ -aqua-bis(triaquadiperchloratostrontium), $[\text{Sr}_2(\text{ClO}_4)_4(\text{H}_2\text{O})_8]$ } and strontium perchlorate nonahydrate {heptaaquadiperchloratostrontium dihydrate, $[\text{Sr}(\text{ClO}_4)_2(\text{H}_2\text{O})_7] \cdot 2\text{H}_2\text{O}$ }, were crystallized at low temperatures according to the solid–liquid phase diagram. The structures of the tri- and tetrahydrate consist of Sr^{2+} cations coordinated by five water molecules and four O atoms of four perchlorate tetrahedra in a distorted tricapped trigonal–prismatic coordination mode. The asymmetric unit of the trihydrate contains two formula units. Two $[\text{SrO}_9]$ polyhedra in the trihydrate are connected by sharing water molecules and thus forming chains parallel to $[100]$. In the tetrahydrate, dimers of two $[\text{SrO}_9]$ polyhedra connected by two sharing water molecules are formed. The structure of the nonahydrate contains one Sr^{2+} cation coordinated by seven water molecules and by two O atoms of two perchlorate tetrahedra (point group symmetry m), forming a tricapped trigonal prism (point group symmetry $m2m$). The structure contains additional non-coordinating water molecules, which are located on twofold rotation axes. $\text{O}—\text{H} \cdots \text{O}$ hydrogen bonds between the water molecules as donor and ClO_4 tetrahedra and water molecules as acceptor groups lead to the formation of a three-dimensional network in each of the three structures.

1. Chemical context

The amount of research into perchlorates has increased considerably in the last few years, beginning with the Phoenix Mars mission (Kim *et al.*, 2013; Kerr, 2013; Chevrier *et al.*, 2009; Quinn *et al.*, 2013; Davila *et al.*, 2013; Gough *et al.*, 2011; Navarro-González & McKay, 2011; Robertson & Bish, 2011; Schuttlefield *et al.*, 2011; Navarro-González *et al.*, 2010; Marion *et al.*, 2010; Hecht *et al.*, 2009). Important perchlorate salts in the martian regolith are Mg and Ca perchlorates. It seemed worthwhile to complete the chemical systematics in this series of alkaline-earth perchlorates. The solubility diagram of strontium perchlorate has been investigated by several authors (Pestova *et al.*, 2005; Lilich & Djurinskii, 1956; Nicholson & Felsing, 1950; Willard & Smith, 1923) in different temperature and concentration regions. They reported the tetrahydrate and the hexahydrate to be stable phases. While re-investigating the phase diagram, we found at higher temperatures the trihydrate, the tetrahydrate at room temperature and the nonahydrate near the eutectic temperature. The existence of the hexahydrate could not be confirmed.



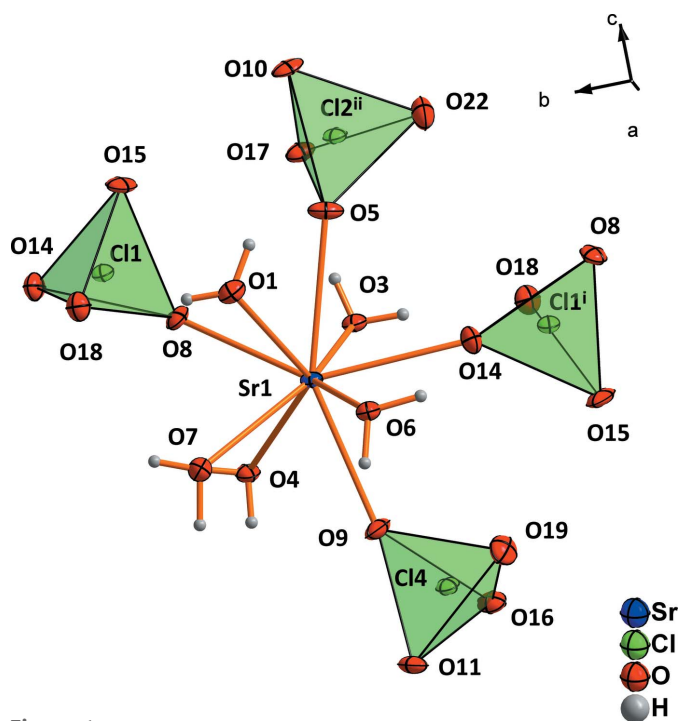


Figure 1
Coordination around the Sr^{2+} cation in $\text{Sr}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$. Atoms O3 and O4 as well as O6 and O1 are shared between two different Sr^{2+} cations. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $\frac{1}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$; (ii) $-\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z$.]

2. Structural commentary

The crystal structure of strontium perchlorate trihydrate contains two crystallographically distinct Sr^{2+} cations. Both are coordinated by five water molecules and four monodentately bonding perchlorate tetrahedra (Fig. 1). Four of the five water molecules (O1, O6 and O3, O4) share edges between two Sr^{2+} cations, resulting in chains with alternating Sr1 and Sr2 cations. The chains extend parallel to $[100]$ (Fig. 2). The crystal

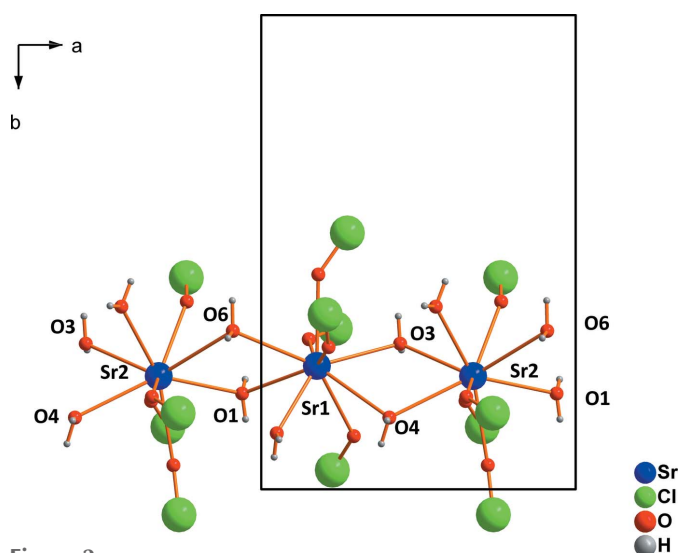


Figure 2
Formation of chains parallel $[100]$ by sharing water molecules in the structure of $\text{Sr}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$.

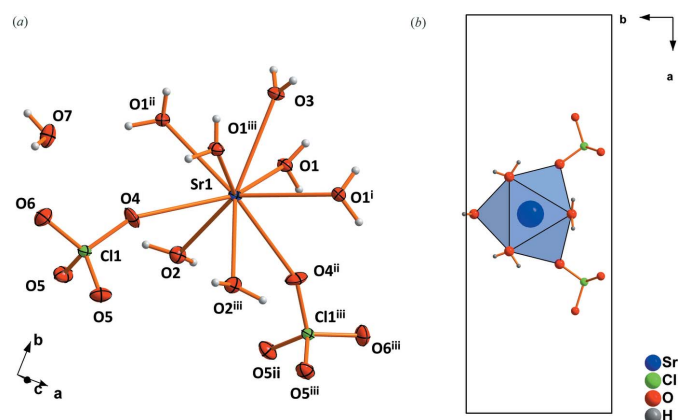


Figure 3
(a) Coordination around the Sr^{2+} cation and (b) the resulting coordination polyhedron in the structure of $\text{Sr}(\text{ClO}_4)_2 \cdot 9\text{H}_2\text{O}$. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $x, y, \frac{3}{2} - z$; (ii) $2 - x, y, z$; (iii) $2 - x, y, \frac{3}{2} - z$.]

structure of strontium perchlorate tetrahydrate is similar to the trihydrate, but different to the magnesium analogue (Robertson & Bish, 2010; Solovyov, 2012) or mercury perchlorate tetrahydrate (Johansson *et al.*, 1966). Two symmetry-related Sr^{2+} cations, both coordinated by five water molecules and four monodentately perchlorate tetrahedra, form dimers by sharing two water molecules. In strontium perchlorate nonahydrate, the Sr^{2+} cation occupies a single crystallographic site with site symmetry $m2m$. It is coordinated by seven water molecules and two monodentately perchlorate tetrahedra (point group symmetry $..m$; Fig. 3a) within a tricapped trigonal-prismatic oxygen coordination environment (Fig. 3b). Thereby, the trigonal base planes are chosen

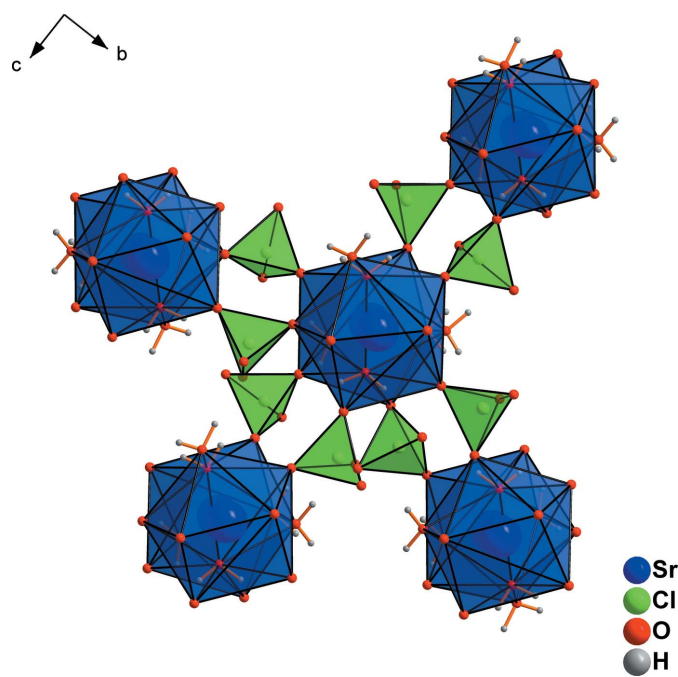


Figure 4
Perchlorate tetrahedra in the structure of $\text{Sr}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$ linking the chains (oriented parallel to $[100]$) into (100) layers.

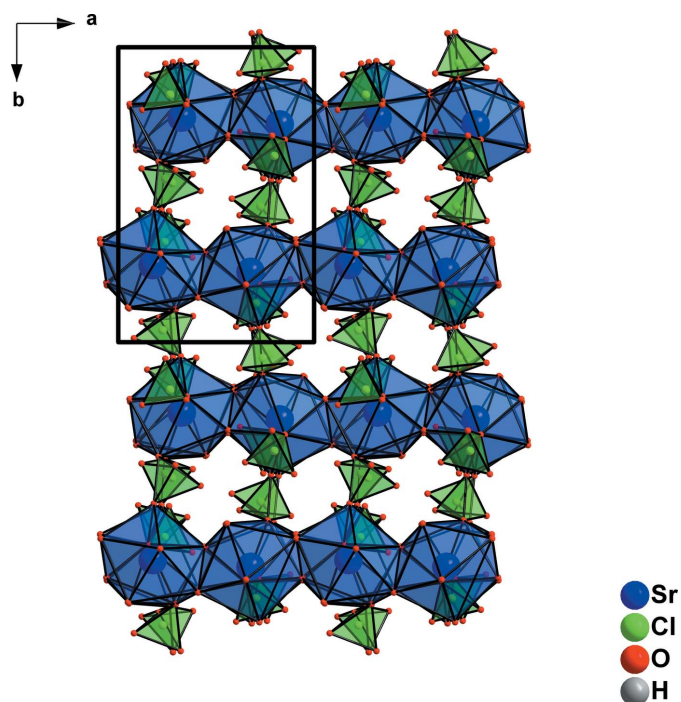


Figure 5
Zigzag chains parallel to [100] in the structure of $\text{Sr}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$, linked by perchlorate tetrahedra into (100) layers, as viewed along [001].

such that each oxygen atom of the perchlorate anions represents a capping atom. The third cap is provided by a water oxygen atom.

3. Supramolecular features

In strontium perchlorate trihydrate, chains are formed with alternating Sr^{2+} cations (Fig. 2). These zigzag chains are oriented parallel to [100] and are linked by edge-sharing with the perchlorate tetrahedra (Fig. 4) into a layered arrangement parallel to (001), as shown in Fig. 5. Within the structure of the tetrahydrate, each perchlorate anion coordinates to the dimeric unit of two Sr^{2+} cations (Fig. 6). At the same time, it also coordinates to another dimeric unit. Thus, each dimeric unit is connected pairwise by perchlorate anions with four others. This yields in (001) layers stacked along [001], as visualized in Fig. 7. The nonahydrate structure contains additional lattice water molecules, which are both donor and acceptor groups, resulting in a tetrahedral arrangement of O—

Table 1
Hydrogen-bond geometry (\AA , $^\circ$) for $\text{Sr}(\text{ClO}_4)_2 \cdot 9\text{H}_2\text{O}$.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O1}-\text{H1B} \cdots \text{O7}^i$	0.84 (1)	2.02 (2)	2.844 (4)	169 (5)
$\text{O1}-\text{H1A} \cdots \text{O4}$	0.84 (1)	1.98 (1)	2.811 (4)	170 (5)
$\text{O2}-\text{H2A} \cdots \text{O1}^{ii}$	0.84 (1)	1.99 (2)	2.780 (4)	156 (5)
$\text{O3}-\text{H3A} \cdots \text{O2}^i$	0.84 (1)	2.05 (3)	2.851 (5)	158 (7)
$\text{O4}-\text{H4A} \cdots \text{O6}^{iii}$	0.84 (1)	2.62 (3)	3.337 (2)	144 (4)
$\text{O4}-\text{H4A} \cdots \text{O7}^{iv}$	0.84 (1)	2.39 (3)	3.041 (4)	135 (4)

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

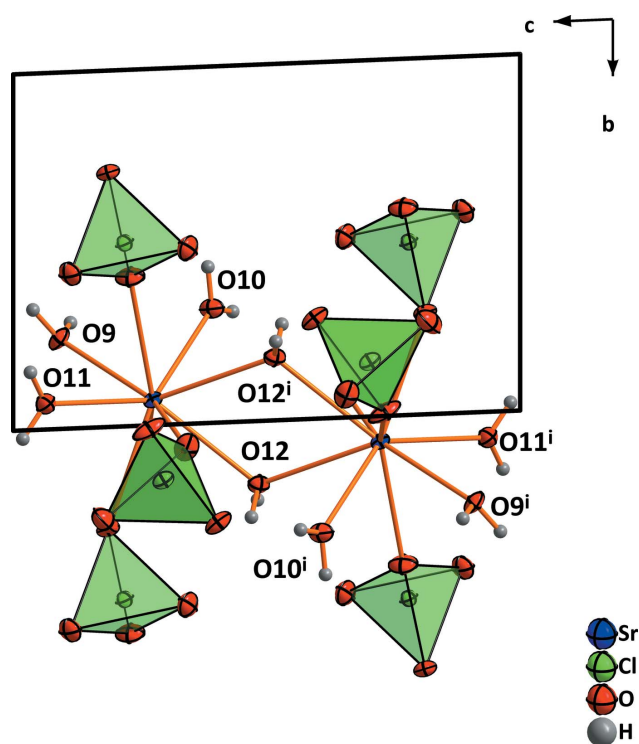


Figure 6
Formation of dimers in the structure of $\text{Sr}(\text{ClO}_4)_2 \cdot 4\text{H}_2\text{O}$ by sharing two water molecules. [Symmetry code: (i) $1-x, 2-y, 1-z$.]

$\text{H} \cdots \text{O}$ hydrogen bonds. Two hydrogen bonds are formed towards the $[\text{SrO}_2(\text{OH}_2)_7]$ coordination polyhedra and two towards perchlorate tetrahedra (Fig. 8a, Table 1). The $[\text{SrO}_2(\text{OH}_2)_7]$ polyhedra additionally are linked *via* other O—

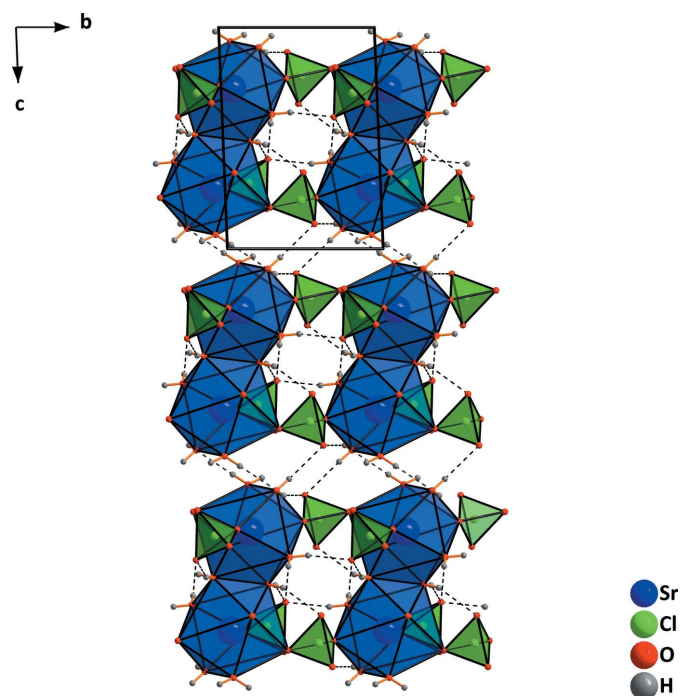


Figure 7
Formation of layers in the structure of $\text{Sr}(\text{ClO}_4)_2 \cdot 4\text{H}_2\text{O}$, viewed along [100].

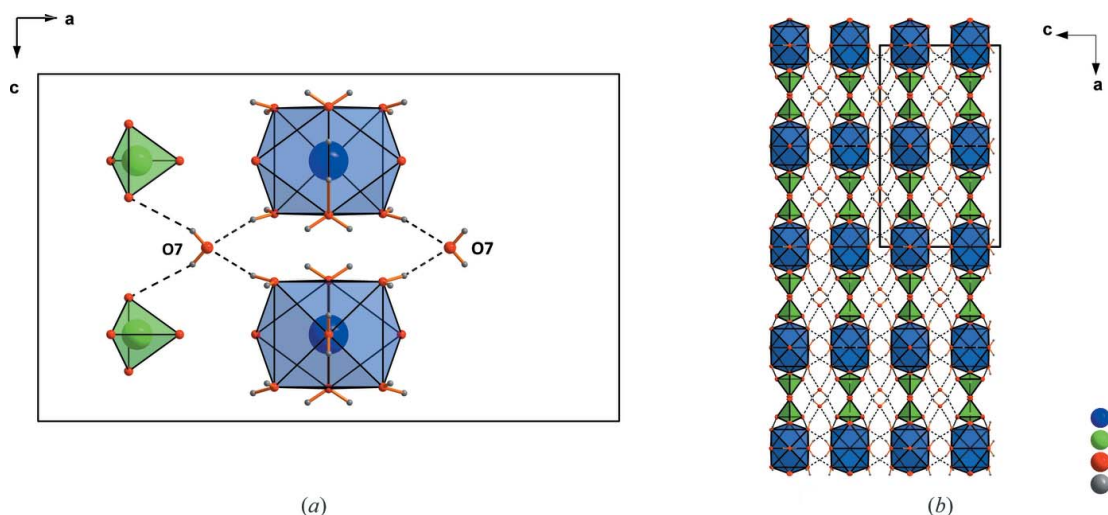


Figure 8
(a) Coordination of the lattice water molecules in the structure of Sr(ClO₄)₂·9H₂O by hydrogen bonds. (b) A larger section of the structure in the viewing direction [010]. Dashed lines indicate hydrogen bonds.

H···O hydrogen bonds. The resulting arrangement can be seen in a larger section of the structure (Fig. 8b). O—H···O hydrogen bonds also dominate the crystal packing in the two other structures, in each case leading to the formation of a three-dimensional network (Tables 2 and 3).

Table 2
Hydrogen-bond geometry (Å, °) for Sr(ClO₄)₂·3H₂O.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O5 ⁱ	0.84 (1)	2.13 (4)	2.683 (4)	123 (4)
O1—H1B···O18 ⁱ	0.84 (1)	2.07 (2)	2.858 (4)	158 (4)
O2—H2B···O16 ⁱⁱ	0.84 (1)	2.10 (1)	2.923 (4)	169 (4)
O2—H2A···O16	0.84 (1)	2.17 (2)	2.992 (4)	167 (7)
O3—H3A···O18 ⁱⁱⁱ	0.84 (1)	1.96 (1)	2.793 (4)	172 (4)
O3—H3B···O17 ^{iv}	0.84 (1)	2.06 (2)	2.857 (4)	159 (4)
O4—H4B···O21 ^v	0.84 (1)	2.15 (2)	2.953 (4)	161 (5)
O4—H4A···O22 ^{vi}	0.84 (1)	2.42 (2)	3.173 (4)	150 (4)
O6—H6A···O14 ⁱⁱⁱ	0.84 (7)	2.56 (7)	3.069 (4)	121 (5)
O6—H6A···O19 ^{vii}	0.84 (7)	2.19 (7)	2.964 (4)	155 (6)
O6—H6B···O17 ^{viii}	0.92 (6)	2.09 (6)	2.920 (4)	150 (5)
O7—H7A···O20 ^{ix}	0.84 (1)	2.31 (4)	3.044 (4)	146 (7)
O7—H7A···O22 ^{vi}	0.84 (1)	2.44 (7)	2.902 (4)	116 (6)
O7—H7B···O17 ^{viii}	0.84 (1)	2.48 (5)	2.916 (4)	114 (4)
O7—H7B···O20 ^v	0.84 (1)	2.25 (2)	3.071 (4)	167 (5)

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

Table 3
Hydrogen-bond geometry (Å, °) for Sr(ClO₄)₂·4H₂O.

D—H···A	D—H	H···A	D···A	D—H···A
O9—H9A···O8 ⁱ	0.84 (1)	2.15 (2)	2.966 (3)	164 (4)
O9—H9B···O8 ⁱⁱ	0.84 (1)	2.18 (2)	2.986 (3)	161 (5)
O10—H10B···O4 ⁱⁱⁱ	0.84 (1)	2.04 (2)	2.858 (3)	165 (6)
O10—H10A···O4 ^{iv}	0.84 (1)	2.17 (2)	2.967 (3)	157 (5)
O11—H11B···O9 ^v	0.84 (1)	1.99 (2)	2.809 (3)	164 (4)
O11—H11A···O8	0.84 (1)	2.38 (3)	3.093 (3)	143 (5)
O12—H12A···O7 ^{vi}	0.84 (1)	2.23 (2)	2.986 (3)	150 (4)
O12—H12A···O10 ^{vii}	0.84 (1)	2.31 (4)	2.820 (3)	120 (3)
O12—H12B···O4	0.84 (1)	2.06 (2)	2.875 (3)	164 (5)

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

4. Database survey

For crystal structures of other $M(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$ phases, see: Gallucci & Gerkin (1988; $M = \text{Ba}$); Hennings *et al.* (2014a; Sn). For crystal structures of other $M(\text{ClO}_4)_2 \cdot 4\text{H}_2\text{O}$ phases, see: Robertson & Bish (2010; Mg); Hennings *et al.* (2014b; Ca); Solovyov (2012; Mg); Johansson *et al.* (1966; Hg).

5. Synthesis and crystallization

Crystals of Sr(ClO₄)₂·3H₂O were used as purchased (ABCR, 98%). The isolated crystals were stored in a freezer separated and embedded in perfluorinated ether to avoid contact with humidity. Sr(ClO₄)₂·4H₂O crystallized from an aqueous solution of 75.08 wt% Sr(ClO₄)₂ at 273 K after two days and Sr(ClO₄)₂·9H₂O from an aqueous solution of 60.12 wt% Sr(ClO₄)₂ at 238 K after one week. For preparing these aqueous solutions, strontium perchlorate trihydrate was used. The Sr²⁺ content was analyzed per complexometric titration with EDTA. The crystals are stable in the saturated aqueous solutions over a range of at least four weeks. The samples were stored in a freezer or a cryostat at low temperatures and were separated and embedded in perfluorinated ether for X-ray analysis.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. The H atoms of each structure were placed in the positions indicated by difference Fourier maps. For Sr(ClO₄)₂·3H₂O and Sr(ClO₄)₂·4H₂O distance restraints were applied for all water molecules, with O—H and H—H distance restraints of 0.84 (1) and 1.4 (1) Å, respectively. For Sr(ClO₄)₂·9H₂O U_{iso} values were set at $1.2U_{\text{eq}}(\text{O})$ using a riding model approximation. Distance restraints were applied for that structure for all water molecules, with O—H and H—H distance restraints of 0.84 (1) and 1.4 (1) Å, respectively.

Table 4
Experimental details.

	Sr(ClO ₄) ₂ ·3H ₂ O	Sr(ClO ₄) ₂ ·4H ₂ O	Sr(ClO ₄) ₂ ·9H ₂ O
Crystal data			
<i>M_r</i>	340.57	358.58	448.66
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>	Triclinic, <i>P</i> $\bar{1}$	Orthorhombic, <i>Cmcm</i>
Temperature (K)	100	150	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.9787 (6), 13.4870 (12), 14.7875 (10)	7.1571 (6), 7.3942 (6), 10.0231 (9)	18.7808 (15), 6.860 (3), 11.1884 (16)
α , β , γ (°)	90, 95.448 (5), 90	86.674 (7), 86.291 (7), 72.027 (6)	90, 90, 90
<i>V</i> (Å ³)	1782.6 (2)	503.09 (8)	1441.5 (7)
<i>Z</i>	8	2	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	6.70	5.94	4.20
Crystal size (mm)	0.45 × 0.34 × 0.23	0.33 × 0.25 × 0.16	0.20 × 0.11 × 0.05
Data collection			
Diffractometer	Stoe IPDS 2T	Stoe IPDS 2T	Stoe IPDS 2T
Absorption correction	Integration (Coppens, 1970)	Integration (Coppens, 1970)	Integration (Coppens, 1970)
<i>T</i> _{min} , <i>T</i> _{max}	0.081, 0.212	0.187, 0.383	0.015, 0.085
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	50555, 4941, 3337	10691, 2818, 2650	6877, 1087, 993
<i>R</i> _{int}	0.125	0.065	0.020
(sin θ / λ) _{max} (Å ⁻¹)	0.650	0.695	0.693
Refinement			
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.024, 0.046, 1.09	0.028, 0.076, 1.10	0.048, 0.134, 1.16
No. of reflections	4087	2795	1087
No. of parameters	297	169	70
No. of restraints	15	12	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	All H-atom parameters refined	Only H-atom coordinates refined
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.56, -0.63	0.83, -1.15	1.27, -2.26

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2009), *SHELXS97* and *SHELXL2012* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 2006) and *pubCIF* (Westrip, 2010).

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supporting information

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Computing details

For all compounds, data collection: *X-AREA* (Stoe & Cie, 2009); cell refinement: *X-AREA* (Stoe & Cie, 2009); data reduction: *X-RED* (Stoe & Cie, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(SrClO4_3H2O_100K) Di- μ -aqua-aquadi- μ -perchlorato-strontium

Crystal data

$[\text{Sr}(\text{ClO}_4)_2(\text{H}_2\text{O})_3]$

$M_r = 340.57$

Monoclinic, $P2_1/n$

$a = 8.9787$ (6) Å

$b = 13.4870$ (12) Å

$c = 14.7875$ (10) Å

$\beta = 95.448$ (5)°

$V = 1782.6$ (2) Å³

$Z = 8$

$F(000) = 1328$

$D_x = 2.538$ Mg m⁻³

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

Cell parameters from 32895 reflections

$\theta = 2.3$ – 29.7 °

$\mu = 6.70$ mm⁻¹

$T = 100$ K

Plate, colourless

$0.45 \times 0.34 \times 0.23$ mm

Data collection

Stoe IPDS 2T

diffractometer

Radiation source: fine-focus sealed tube

Detector resolution: 6.67 pixels mm⁻¹

rotation method scans

Absorption correction: integration

(Coppens, 1970)

$T_{\min} = 0.081$, $T_{\max} = 0.212$

50555 measured reflections

4941 independent reflections

3337 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.125$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 2.7$ °

$h = -12$ → 12

$k = -18$ → 18

$l = -20$ → 20

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.046$

$S = 1.09$

4087 reflections

297 parameters

15 restraints

Hydrogen site location: difference Fourier map

H atoms treated by a mixture of independent

and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.015P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.56$ e Å⁻³

$\Delta\rho_{\min} = -0.63$ e Å⁻³

Special details

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

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.17700 (4)	0.73963 (3)	0.16063 (2)	0.00938 (8)
Sr2	0.67377 (4)	0.76115 (3)	0.16252 (2)	0.00958 (8)
Cl3	0.76166 (10)	0.55363 (6)	0.34594 (6)	0.01186 (17)
Cl4	0.20327 (9)	0.63169 (6)	−0.08358 (6)	0.01123 (17)
O2	0.5554 (3)	0.6148 (2)	0.07663 (19)	0.0157 (6)
H2B	0.584 (5)	0.5569 (14)	0.089 (3)	0.022 (12)*
H2A	0.503 (7)	0.618 (5)	0.027 (3)	0.09 (3)*
O5	0.1514 (3)	0.6834 (2)	0.33230 (18)	0.0173 (6)
O7	0.0494 (3)	0.8819 (2)	0.07657 (19)	0.0169 (6)
H7A	0.040 (8)	0.939 (2)	0.098 (4)	0.09 (3)*
H7B	0.054 (6)	0.891 (4)	0.0208 (11)	0.049 (17)*
O11	0.1497 (3)	0.6863 (2)	−0.16432 (18)	0.0159 (6)
O8	0.2947 (3)	0.8877 (2)	0.26593 (18)	0.0142 (6)
O3	0.4421 (3)	0.6926 (2)	0.23812 (18)	0.0122 (5)
H3A	0.427 (5)	0.6316 (10)	0.232 (3)	0.015*
H3B	0.446 (5)	0.704 (3)	0.2940 (9)	0.015*
O6	−0.0905 (3)	0.6659 (2)	0.0871 (2)	0.0126 (5)
H6A	−0.074 (8)	0.606 (5)	0.096 (4)	0.07 (2)*
H6B	−0.102 (7)	0.682 (4)	0.026 (4)	0.057 (18)*
O1	0.9396 (3)	0.7980 (2)	0.24536 (19)	0.0155 (6)
H1A	0.954 (5)	0.767 (3)	0.2947 (15)	0.019*
H1B	0.958 (5)	0.8588 (10)	0.248 (3)	0.019*
O4	0.4076 (3)	0.8486 (2)	0.09960 (19)	0.0142 (6)
H4B	0.401 (7)	0.852 (4)	0.0427 (8)	0.055 (19)*
H4A	0.385 (5)	0.9070 (13)	0.112 (3)	0.017 (11)*
O9	0.2141 (3)	0.7003 (2)	−0.00724 (17)	0.0166 (6)
O12	0.7632 (4)	0.6041 (2)	0.25968 (19)	0.0223 (7)
O10	0.6522 (3)	0.8049 (2)	−0.00904 (17)	0.0165 (5)
O13	0.7794 (4)	0.4491 (2)	0.3295 (2)	0.0282 (7)
Cl1	0.22615 (10)	0.95938 (6)	0.32252 (5)	0.01093 (16)
Cl2	0.73566 (10)	0.83941 (6)	−0.08210 (6)	0.01110 (17)
O17	0.8781 (3)	0.78723 (18)	−0.07714 (16)	0.0148 (5)
O15	0.2081 (3)	0.91715 (19)	0.40937 (17)	0.0193 (6)
O16	0.3517 (3)	0.59257 (18)	−0.09445 (17)	0.0163 (5)
O14	0.3185 (3)	1.0469 (2)	0.33193 (18)	0.0164 (6)
O18	0.0800 (3)	0.98662 (17)	0.27720 (17)	0.0160 (5)
O20	0.6198 (3)	0.56974 (19)	0.38222 (17)	0.0171 (5)
O19	0.1020 (3)	0.55287 (19)	−0.06828 (18)	0.0209 (6)
O22	0.7597 (3)	0.94455 (18)	−0.07510 (19)	0.0230 (6)

O21 0.8810 (3) 0.5889 (3) 0.4073 (2) 0.0371 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.00941 (16)	0.01189 (17)	0.00731 (16)	0.00047 (14)	0.00327 (12)	0.00006 (14)
Sr2	0.00977 (16)	0.01221 (17)	0.00729 (16)	-0.00071 (14)	0.00355 (12)	0.00017 (14)
Cl3	0.0138 (4)	0.0126 (4)	0.0097 (4)	-0.0003 (3)	0.0036 (3)	0.0002 (3)
Cl4	0.0124 (4)	0.0140 (4)	0.0079 (3)	0.0004 (3)	0.0043 (3)	-0.0001 (3)
O2	0.0220 (15)	0.0140 (14)	0.0112 (15)	-0.0028 (12)	0.0031 (12)	-0.0009 (12)
O5	0.0159 (14)	0.0286 (17)	0.0078 (14)	-0.0028 (12)	0.0024 (11)	0.0044 (12)
O7	0.0231 (15)	0.0150 (14)	0.0125 (15)	0.0029 (12)	0.0016 (12)	-0.0007 (12)
O11	0.0184 (15)	0.0220 (16)	0.0077 (13)	0.0056 (12)	0.0040 (11)	0.0054 (11)
O8	0.0170 (13)	0.0140 (13)	0.0125 (13)	0.0020 (10)	0.0056 (10)	-0.0052 (10)
O3	0.0140 (13)	0.0154 (13)	0.0077 (13)	0.0002 (11)	0.0032 (10)	-0.0005 (11)
O6	0.0143 (13)	0.0126 (12)	0.0112 (14)	-0.0004 (10)	0.0030 (10)	0.0003 (11)
O1	0.0141 (14)	0.0190 (13)	0.0135 (14)	0.0015 (11)	0.0012 (11)	-0.0027 (11)
O4	0.0180 (14)	0.0163 (14)	0.0094 (13)	0.0024 (11)	0.0069 (10)	0.0014 (10)
O9	0.0213 (14)	0.0182 (12)	0.0110 (12)	-0.0017 (11)	0.0057 (11)	-0.0055 (10)
O12	0.0307 (16)	0.0240 (16)	0.0140 (14)	0.0088 (13)	0.0119 (12)	0.0093 (12)
O10	0.0161 (13)	0.0255 (13)	0.0094 (12)	0.0004 (11)	0.0094 (10)	0.0040 (10)
O13	0.0450 (19)	0.0104 (14)	0.0319 (17)	0.0083 (12)	0.0183 (14)	0.0030 (12)
Cl1	0.0134 (4)	0.0117 (4)	0.0082 (3)	-0.0002 (3)	0.0036 (3)	-0.0006 (3)
Cl2	0.0129 (4)	0.0142 (4)	0.0068 (4)	-0.0004 (3)	0.0042 (3)	0.0000 (3)
O17	0.0122 (11)	0.0201 (13)	0.0128 (12)	0.0017 (9)	0.0045 (9)	0.0016 (9)
O15	0.0282 (16)	0.0224 (13)	0.0090 (12)	0.0012 (11)	0.0101 (11)	0.0059 (10)
O16	0.0133 (13)	0.0214 (13)	0.0150 (13)	0.0061 (10)	0.0055 (10)	0.0007 (10)
O14	0.0192 (13)	0.0108 (12)	0.0195 (13)	-0.0051 (11)	0.0021 (10)	-0.0023 (11)
O18	0.0139 (12)	0.0146 (12)	0.0191 (13)	0.0032 (9)	0.0003 (10)	-0.0003 (10)
O20	0.0124 (12)	0.0249 (13)	0.0156 (13)	0.0010 (11)	0.0085 (10)	0.0009 (10)
O19	0.0212 (14)	0.0172 (13)	0.0255 (14)	-0.0074 (11)	0.0089 (11)	0.0013 (11)
O22	0.0280 (15)	0.0118 (12)	0.0294 (15)	-0.0044 (11)	0.0041 (12)	0.0002 (11)
O21	0.0178 (15)	0.077 (2)	0.0173 (15)	-0.0198 (15)	0.0059 (12)	-0.0202 (15)

Geometric parameters (Å, °)

Sr1—O7	2.504 (3)	Sr2—O6 ^v	2.797 (3)
Sr1—O9	2.591 (3)	Cl3—O21	1.419 (3)
Sr1—O14 ⁱ	2.602 (3)	Cl3—O13	1.442 (3)
Sr1—O3	2.619 (3)	Cl3—O20	1.445 (2)
Sr1—O5	2.680 (3)	Cl3—O12	1.447 (3)
Sr1—O8	2.686 (3)	Cl4—O19	1.430 (3)
Sr1—O1 ⁱⁱ	2.691 (3)	Cl4—O11	1.446 (3)
Sr1—O6	2.729 (3)	Cl4—O9	1.456 (3)
Sr1—O4	2.760 (3)	Cl4—O16	1.456 (3)
Sr2—O2	2.527 (3)	Cl1—O15	1.428 (2)
Sr2—O13 ⁱⁱⁱ	2.571 (3)	Cl1—O14	1.441 (3)
Sr2—O10	2.594 (2)	Cl1—O18	1.463 (3)

Sr2—O3	2.622 (3)	O8—C11	1.453 (3)
Sr2—O1	2.625 (3)	C12—O22	1.437 (3)
Sr2—O12	2.641 (3)	C12—O5 ^{vi}	1.445 (3)
Sr2—O11 ^{iv}	2.685 (3)	C12—O17	1.456 (3)
Sr2—O4	2.747 (3)	O10—C12	1.449 (2)
O7—Sr1—O9	77.04 (9)	O3—Sr2—O11 ^{iv}	63.08 (8)
O7—Sr1—O14 ⁱ	142.31 (9)	O1—Sr2—O11 ^{iv}	69.95 (9)
O9—Sr1—O14 ⁱ	80.39 (9)	O12—Sr2—O11 ^{iv}	74.97 (9)
O7—Sr1—O3	139.15 (9)	O2—Sr2—O4	81.63 (9)
O9—Sr1—O3	100.11 (9)	O13 ⁱⁱⁱ —Sr2—O4	74.05 (9)
O14 ⁱ —Sr1—O3	74.33 (9)	O10—Sr2—O4	65.74 (8)
O7—Sr1—O5	127.65 (10)	O3—Sr2—O4	66.16 (8)
O9—Sr1—O5	151.64 (9)	O1—Sr2—O4	143.12 (9)
O14 ⁱ —Sr1—O5	71.31 (9)	O12—Sr2—O4	137.59 (9)
O3—Sr1—O5	70.93 (8)	O11 ^{iv} —Sr2—O4	93.63 (9)
O7—Sr1—O8	81.62 (9)	O2—Sr2—O6 ^v	74.85 (9)
O9—Sr1—O8	128.93 (8)	O13 ⁱⁱⁱ —Sr2—O6 ^v	110.16 (10)
O14 ⁱ —Sr1—O8	135.59 (9)	O10—Sr2—O6 ^v	72.76 (9)
O3—Sr1—O8	68.60 (8)	O3—Sr2—O6 ^v	132.01 (9)
O5—Sr1—O8	74.09 (9)	O1—Sr2—O6 ^v	65.43 (8)
O7—Sr1—O1 ⁱⁱ	70.21 (9)	O12—Sr2—O6 ^v	69.26 (9)
O9—Sr1—O1 ⁱⁱ	133.29 (9)	O11 ^{iv} —Sr2—O6 ^v	129.34 (9)
O14 ⁱ —Sr1—O1 ⁱⁱ	106.42 (9)	O4—Sr2—O6 ^v	136.82 (8)
O3—Sr1—O1 ⁱⁱ	126.45 (8)	O21—C13—O13	110.3 (2)
O5—Sr1—O1 ⁱⁱ	59.93 (9)	O21—C13—O20	110.54 (17)
O8—Sr1—O1 ⁱⁱ	78.34 (8)	O13—C13—O20	108.95 (17)
O7—Sr1—O6	74.80 (10)	O21—C13—O12	109.65 (19)
O9—Sr1—O6	74.45 (8)	O13—C13—O12	107.51 (18)
O14 ⁱ —Sr1—O6	70.26 (9)	O20—C13—O12	109.82 (17)
O3—Sr1—O6	144.59 (9)	O19—C14—O11	110.03 (17)
O5—Sr1—O6	97.05 (9)	O19—C14—O9	110.27 (16)
O8—Sr1—O6	141.72 (8)	O11—C14—O9	107.98 (16)
O1 ⁱⁱ —Sr1—O6	65.54 (9)	O19—C14—O16	110.49 (16)
O7—Sr1—O4	75.61 (9)	O11—C14—O16	109.26 (16)
O9—Sr1—O4	68.10 (8)	O9—C14—O16	108.76 (16)
O14 ⁱ —Sr1—O4	122.46 (9)	C12 ^{vii} —O5—Sr1	143.63 (17)
O3—Sr1—O4	66.00 (8)	C14—O11—Sr2 ^{viii}	150.58 (17)
O5—Sr1—O4	126.51 (9)	C11—O8—Sr1	131.56 (15)
O8—Sr1—O4	61.80 (8)	Sr1—O3—Sr2	116.94 (10)
O1 ⁱⁱ —Sr1—O4	130.41 (9)	Sr1—O6—Sr2 ⁱⁱ	110.15 (10)
O6—Sr1—O4	136.33 (8)	Sr2—O1—Sr1 ^v	116.91 (10)
O2—Sr2—O13 ⁱⁱⁱ	148.51 (10)	Sr2—O4—Sr1	108.42 (9)
O2—Sr2—O10	72.37 (9)	C14—O9—Sr1	150.23 (16)
O13 ⁱⁱⁱ —Sr2—O10	79.47 (9)	C13—O12—Sr2	145.98 (17)
O2—Sr2—O3	68.04 (9)	C12—O10—Sr2	143.74 (16)
O13 ⁱⁱⁱ —Sr2—O3	117.46 (9)	C13—O13—Sr2 ^{ix}	167.61 (19)
O10—Sr2—O3	120.57 (8)	O15—C11—O14	110.68 (16)

O2—Sr2—O1	134.68 (9)	O15—C11—O8	110.06 (16)
O13 ⁱⁱⁱ —Sr2—O1	69.76 (10)	O14—C11—O8	109.22 (16)
O10—Sr2—O1	113.18 (9)	O15—C11—O18	109.78 (16)
O3—Sr2—O1	126.23 (8)	O14—C11—O18	108.74 (16)
O2—Sr2—O12	74.83 (10)	O8—C11—O18	108.31 (15)
O13 ⁱⁱⁱ —Sr2—O12	136.56 (10)	O22—C12—O5 ^{vi}	109.62 (18)
O10—Sr2—O12	134.83 (9)	O22—C12—O10	110.39 (17)
O3—Sr2—O12	72.42 (9)	O5 ^{vi} —C12—O10	108.66 (16)
O1—Sr2—O12	71.48 (10)	O22—C12—O17	110.36 (16)
O2—Sr2—O11 ^{iv}	128.12 (9)	O5 ^{vi} —C12—O17	109.02 (16)
O13 ⁱⁱⁱ —Sr2—O11 ^{iv}	73.98 (9)	O10—C12—O17	108.75 (15)
O10—Sr2—O11 ^{iv}	150.15 (9)	C11—O14—Sr1 ^x	145.97 (17)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots O5 ^v	0.84 (1)	2.13 (4)	2.683 (4)	123 (4)
O1—H1B \cdots O18 ^v	0.84 (1)	2.07 (2)	2.858 (4)	158 (4)
O2—H2B \cdots O16 ^{xi}	0.84 (1)	2.10 (1)	2.923 (4)	169 (4)
O2—H2A \cdots O16	0.84 (1)	2.17 (2)	2.992 (4)	167 (7)
O3—H3A \cdots O18 ⁱ	0.84 (1)	1.96 (1)	2.793 (4)	172 (4)
O3—H3B \cdots O17 ^{vii}	0.84 (1)	2.06 (2)	2.857 (4)	159 (4)
O4—H4B \cdots O21 ^{viii}	0.84 (1)	2.15 (2)	2.953 (4)	161 (5)
O4—H4A \cdots O22 ^{xii}	0.84 (1)	2.42 (2)	3.173 (4)	150 (4)
O6—H6A \cdots O14 ⁱ	0.84 (7)	2.56 (7)	3.069 (4)	121 (5)
O6—H6A \cdots O19 ^{xiii}	0.84 (7)	2.19 (7)	2.964 (4)	155 (6)
O6—H6B \cdots O17 ⁱⁱ	0.92 (6)	2.09 (6)	2.920 (4)	150 (5)
O7—H7A \cdots O20 ^x	0.84 (1)	2.31 (4)	3.044 (4)	146 (7)
O7—H7A \cdots O22 ^{xii}	0.84 (1)	2.44 (7)	2.902 (4)	116 (6)
O7—H7B \cdots O17 ⁱⁱ	0.84 (1)	2.48 (5)	2.916 (4)	114 (4)
O7—H7B \cdots O20 ^{viii}	0.84 (1)	2.25 (2)	3.071 (4)	167 (5)

Symmetry codes: (i) $-x+1/2, y-1/2, -z+1/2$; (ii) $x-1, y, z$; (v) $x+1, y, z$; (vii) $x-1/2, -y+3/2, z+1/2$; (viii) $x-1/2, -y+3/2, z-1/2$; (x) $-x+1/2, y+1/2, -z+1/2$; (xi) $-x+1, -y+1, -z$; (xii) $-x+1, -y+2, -z$; (xiii) $-x, -y+1, -z$.

(SrClO₄·4H₂O)_{150K} Di- μ -aqua-bis(triaquadiperchloratostrontium)

Crystal data

[Sr(ClO₄)₂(H₂O)₄]

$M_r = 358.58$

Triclinic, $P\bar{1}$

$a = 7.1571$ (6) \AA

$b = 7.3942$ (6) \AA

$c = 10.0231$ (9) \AA

$\alpha = 86.674$ (7) $^\circ$

$\beta = 86.291$ (7) $^\circ$

$\gamma = 72.027$ (6) $^\circ$

$V = 503.09$ (8) \AA^3

$Z = 2$

$F(000) = 352$

$D_x = 2.367$ Mg m⁻³

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

Cell parameters from 16929 reflections

$\theta = 2.1\text{--}29.6^\circ$

$\mu = 5.94$ mm⁻¹

$T = 150$ K

Prism, colourless

$0.33 \times 0.25 \times 0.16$ mm

Data collection

Stoe IPDS 2T
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 6.67 pixels mm⁻¹
 rotation method scans
 Absorption correction: integration
 (Coppens, 1970)
 $T_{\min} = 0.187$, $T_{\max} = 0.383$

10691 measured reflections
 2818 independent reflections
 2650 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.065$
 $\theta_{\max} = 29.6^\circ$, $\theta_{\min} = 2.9^\circ$
 $h = -9 \rightarrow 9$
 $k = -10 \rightarrow 10$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.076$
 $S = 1.10$
 2795 reflections
 169 parameters
 12 restraints
 Hydrogen site location: difference Fourier map

All H-atom parameters refined
 $w = 1/[\sigma^2(F_o^2) + (0.0332P)^2 + 1.7614P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.83 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.15 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL*,
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.034 (2)

Special details

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

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.53930 (4)	0.92911 (3)	0.72424 (2)	0.01180 (9)
Cl1	0.97143 (9)	1.15488 (9)	0.70369 (6)	0.01360 (14)
Cl2	0.35731 (9)	0.48563 (9)	0.78026 (6)	0.01327 (14)
O11	0.3252 (4)	0.9281 (3)	0.9363 (2)	0.0214 (4)
O9	0.7828 (3)	0.7469 (3)	0.9095 (2)	0.0179 (4)
O12	0.5409 (3)	1.1774 (3)	0.5157 (2)	0.0153 (4)
O10	0.8215 (3)	0.6788 (3)	0.6077 (2)	0.0184 (4)
O4	0.8716 (3)	1.2814 (3)	0.5953 (2)	0.0196 (4)
O8	0.2149 (3)	0.5654 (3)	0.8872 (2)	0.0225 (5)
O6	0.4501 (3)	0.2861 (3)	0.8128 (2)	0.0194 (4)
O5	0.5058 (3)	0.5815 (3)	0.7694 (2)	0.0218 (5)
O2	1.1720 (3)	1.0650 (3)	0.6579 (2)	0.0223 (5)
O3	0.8764 (4)	1.0108 (3)	0.7327 (3)	0.0264 (5)
O1	0.9628 (4)	1.2609 (4)	0.8192 (3)	0.0306 (6)
O7	0.2630 (4)	0.5075 (4)	0.6555 (2)	0.0254 (5)
H11A	0.287 (7)	0.835 (5)	0.962 (5)	0.044 (15)*
H11B	0.271 (6)	1.025 (4)	0.981 (4)	0.029 (11)*
H12B	0.637 (4)	1.218 (6)	0.524 (5)	0.031 (12)*
H12A	0.437 (4)	1.267 (4)	0.531 (4)	0.025 (11)*
H10A	0.926 (4)	0.690 (8)	0.570 (5)	0.044 (14)*

H10B	0.841 (9)	0.561 (2)	0.619 (6)	0.065 (19)*
H9B	0.757 (8)	0.662 (6)	0.960 (4)	0.048 (15)*
H9A	0.903 (2)	0.707 (6)	0.888 (5)	0.031 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01137 (13)	0.00999 (13)	0.01328 (13)	-0.00231 (8)	-0.00157 (8)	0.00154 (8)
Cl1	0.0113 (3)	0.0126 (3)	0.0167 (3)	-0.0036 (2)	-0.0019 (2)	0.0024 (2)
Cl2	0.0148 (3)	0.0106 (3)	0.0139 (3)	-0.0037 (2)	0.0001 (2)	0.0009 (2)
O11	0.0271 (11)	0.0163 (10)	0.0184 (10)	-0.0045 (9)	0.0045 (9)	-0.0003 (8)
O9	0.0161 (10)	0.0197 (10)	0.0172 (10)	-0.0057 (8)	0.0004 (8)	0.0057 (8)
O12	0.0142 (9)	0.0156 (9)	0.0162 (9)	-0.0041 (8)	-0.0031 (7)	-0.0010 (7)
O10	0.0151 (10)	0.0141 (9)	0.0240 (11)	-0.0030 (8)	0.0037 (8)	0.0009 (8)
O4	0.0157 (10)	0.0183 (10)	0.0239 (11)	-0.0050 (8)	-0.0053 (8)	0.0099 (8)
O8	0.0222 (11)	0.0207 (10)	0.0226 (11)	-0.0050 (9)	0.0071 (9)	-0.0028 (8)
O6	0.0271 (11)	0.0103 (9)	0.0198 (10)	-0.0045 (8)	-0.0020 (8)	0.0015 (7)
O5	0.0196 (10)	0.0149 (10)	0.0326 (12)	-0.0088 (8)	0.0040 (9)	-0.0002 (9)
O2	0.0113 (9)	0.0278 (11)	0.0233 (11)	-0.0001 (8)	-0.0012 (8)	0.0032 (9)
O3	0.0218 (11)	0.0207 (11)	0.0400 (14)	-0.0130 (9)	-0.0091 (10)	0.0148 (10)
O1	0.0314 (13)	0.0299 (13)	0.0271 (13)	-0.0009 (10)	-0.0077 (10)	-0.0120 (10)
O7	0.0273 (12)	0.0262 (12)	0.0197 (11)	-0.0024 (9)	-0.0098 (9)	0.0013 (9)

Geometric parameters (Å, °)

Sr1—O11	2.540 (2)	Cl1—O3	1.438 (2)
Sr1—O10	2.551 (2)	Cl1—O2	1.441 (2)
Sr1—O2 ⁱ	2.623 (2)	Cl1—O4	1.461 (2)
Sr1—O9	2.642 (2)	Cl2—O7	1.437 (2)
Sr1—O5	2.665 (2)	Cl2—O5	1.444 (2)
Sr1—O3	2.669 (2)	Cl2—O6	1.446 (2)
Sr1—O12	2.703 (2)	Cl2—O8	1.448 (2)
Sr1—O6 ⁱⁱ	2.706 (2)	O12—Sr1 ⁱⁱⁱ	2.723 (2)
Sr1—O12 ⁱⁱⁱ	2.723 (2)	O6—Sr1 ^{iv}	2.706 (2)
Sr1—Sr1 ⁱⁱⁱ	4.5867 (6)	O2—Sr1 ^v	2.623 (2)
Cl1—O1	1.423 (2)		
O11—Sr1—O10	134.33 (7)	O9—Sr1—O12 ⁱⁱⁱ	132.16 (7)
O11—Sr1—O2 ⁱ	72.84 (8)	O5—Sr1—O12 ⁱⁱⁱ	74.43 (7)
O10—Sr1—O2 ⁱ	128.32 (8)	O3—Sr1—O12 ⁱⁱⁱ	116.35 (8)
O11—Sr1—O9	74.35 (7)	O12—Sr1—O12 ⁱⁱⁱ	64.57 (7)
O10—Sr1—O9	72.64 (7)	O6 ⁱⁱ —Sr1—O12 ⁱⁱⁱ	127.67 (7)
O2 ⁱ —Sr1—O9	146.33 (7)	O11—Sr1—Sr1 ⁱⁱⁱ	138.29 (6)
O11—Sr1—O5	71.31 (7)	O10—Sr1—Sr1 ⁱⁱⁱ	75.06 (5)
O10—Sr1—O5	68.57 (7)	O2 ⁱ —Sr1—Sr1 ⁱⁱⁱ	65.53 (5)
O2 ⁱ —Sr1—O5	91.52 (8)	O9—Sr1—Sr1 ⁱⁱⁱ	146.06 (5)
O9—Sr1—O5	70.82 (7)	O5—Sr1—Sr1 ⁱⁱⁱ	106.51 (5)
O11—Sr1—O3	120.25 (8)	O3—Sr1—Sr1 ⁱⁱⁱ	96.03 (6)

O10—Sr1—O3	69.06 (8)	O12—Sr1—Sr1 ⁱⁱⁱ	32.42 (4)
O2 ⁱ —Sr1—O3	144.07 (7)	O6 ⁱⁱ —Sr1—Sr1 ⁱⁱⁱ	99.31 (5)
O9—Sr1—O3	62.77 (7)	O12 ⁱⁱⁱ —Sr1—Sr1 ⁱⁱⁱ	32.15 (4)
O5—Sr1—O3	124.01 (7)	O1—Cl1—O3	110.34 (17)
O11—Sr1—O12	135.63 (7)	O1—Cl1—O2	111.09 (16)
O10—Sr1—O12	89.75 (7)	O3—Cl1—O2	108.88 (15)
O2 ⁱ —Sr1—O12	74.61 (7)	O1—Cl1—O4	109.88 (15)
O9—Sr1—O12	137.04 (7)	O3—Cl1—O4	108.60 (14)
O5—Sr1—O12	138.82 (7)	O2—Cl1—O4	107.99 (13)
O3—Sr1—O12	74.40 (7)	O7—Cl2—O5	109.56 (15)
O11—Sr1—O6 ⁱⁱ	75.27 (7)	O7—Cl2—O6	110.02 (14)
O10—Sr1—O6 ⁱⁱ	140.31 (7)	O5—Cl2—O6	108.81 (14)
O2 ⁱ —Sr1—O6 ⁱⁱ	80.03 (8)	O7—Cl2—O8	110.49 (15)
O9—Sr1—O6 ⁱⁱ	98.83 (7)	O5—Cl2—O8	109.30 (14)
O5—Sr1—O6 ⁱⁱ	146.54 (7)	O6—Cl2—O8	108.63 (14)
O3—Sr1—O6 ⁱⁱ	72.64 (8)	Sr1—O12—Sr1 ⁱⁱⁱ	115.43 (7)
O12—Sr1—O6 ⁱⁱ	70.06 (6)	Cl2—O6—Sr1 ^{iv}	144.85 (13)
O11—Sr1—O12 ⁱⁱⁱ	123.23 (7)	Cl2—O5—Sr1	140.13 (14)
O10—Sr1—O12 ⁱⁱⁱ	64.54 (7)	Cl1—O2—Sr1 ^v	146.10 (14)
O2 ⁱ —Sr1—O12 ⁱⁱⁱ	64.25 (7)	Cl1—O3—Sr1	144.73 (14)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O9—H9A \cdots O8 ^v	0.84 (1)	2.15 (2)	2.966 (3)	164 (4)
O9—H9B \cdots O8 ^{vi}	0.84 (1)	2.18 (2)	2.986 (3)	161 (5)
O10—H10B \cdots O4 ^{iv}	0.84 (1)	2.04 (2)	2.858 (3)	165 (6)
O10—H10A \cdots O4 ^{vii}	0.84 (1)	2.17 (2)	2.967 (3)	157 (5)
O11—H11B \cdots O9 ^{viii}	0.84 (1)	1.99 (2)	2.809 (3)	164 (4)
O11—H11A \cdots O8	0.84 (1)	2.38 (3)	3.093 (3)	143 (5)
O12—H12A \cdots O7 ⁱⁱ	0.84 (1)	2.23 (2)	2.986 (3)	150 (4)
O12—H12A \cdots O10 ⁱⁱⁱ	0.84 (1)	2.31 (4)	2.820 (3)	120 (3)
O12—H12B \cdots O4	0.84 (1)	2.06 (2)	2.875 (3)	164 (5)

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

(SrClO₄·9H₂O) Heptaquadiperchloratostrontium dihydrate

Crystal data

[Sr(ClO₄)₂(H₂O)₇] \cdot 2H₂O

$M_r = 448.66$

Orthorhombic, $Cmcm$

$a = 18.7808$ (15) \AA

$b = 6.860$ (3) \AA

$c = 11.1884$ (16) \AA

$V = 1441.5$ (7) \AA^3

$Z = 4$

$F(000) = 904$

$D_x = 2.067$ Mg m⁻³

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

Cell parameters from 5894 reflections

$\theta = 8.3\text{--}29.6^\circ$

$\mu = 4.20$ mm⁻¹

$T = 100$ K

Prism, colourless

$0.2 \times 0.11 \times 0.05$ mm

Data collection

Stoe IPDS 2T diffractometer	6877 measured reflections 1087 independent reflections
Radiation source: fine-focus sealed tube	993 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm ⁻¹	$R_{\text{int}} = 0.020$
rotation method scans	$\theta_{\text{max}} = 29.5^\circ$, $\theta_{\text{min}} = 3.2^\circ$
Absorption correction: integration (Coppens, 1970)	$h = -26 \rightarrow 26$
$T_{\text{min}} = 0.015$, $T_{\text{max}} = 0.085$	$k = -9 \rightarrow 9$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	Only H-atom coordinates refined
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$
$wR(F^2) = 0.134$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.16$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1087 reflections	$\Delta\rho_{\text{max}} = 1.27 \text{ e } \text{Å}^{-3}$
70 parameters	$\Delta\rho_{\text{min}} = -2.25 \text{ e } \text{Å}^{-3}$
6 restraints	

Special details

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

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.5000	0.05870 (8)	0.2500	0.0096 (2)
Cl1	0.32953 (5)	-0.30996 (15)	0.2500	0.0113 (3)
O7	0.34391 (14)	-0.4247 (4)	0.3560 (2)	0.0177 (5)
O4	0.29063 (18)	0.0000	0.5000	0.0203 (7)
H4A	0.263 (2)	0.041 (7)	0.553 (3)	0.024*
O2	0.5000	-0.2257 (5)	0.4061 (3)	0.0156 (7)
H2A	0.5369 (16)	-0.215 (6)	0.448 (4)	0.019*
O1	0.40632 (13)	0.2050 (4)	0.4020 (2)	0.0147 (5)
H1A	0.3693 (15)	0.146 (6)	0.424 (4)	0.018*
H1B	0.392 (2)	0.315 (3)	0.380 (5)	0.018*
O5	0.3748 (2)	-0.1397 (5)	0.2500	0.0211 (8)
O6	0.2561 (2)	-0.2480 (6)	0.2500	0.0209 (8)
O3	0.5000	0.4459 (6)	0.2500	0.0141 (9)
H3A	0.5000	0.519 (9)	0.310 (4)	0.017*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0111 (3)	0.0142 (3)	0.0035 (3)	0.000	0.000	0.000
Cl1	0.0105 (5)	0.0152 (5)	0.0083 (5)	-0.0003 (3)	0.000	0.000
O7	0.0221 (11)	0.0230 (11)	0.0079 (11)	0.0032 (10)	0.0004 (9)	0.0033 (8)
O4	0.0117 (15)	0.0346 (18)	0.0147 (17)	0.000	0.000	0.0023 (16)

O2	0.0144 (14)	0.0219 (15)	0.0106 (16)	0.000	0.000	0.0009 (13)
O1	0.0143 (10)	0.0202 (10)	0.0095 (10)	-0.0006 (9)	0.0009 (8)	-0.0001 (9)
O5	0.0208 (17)	0.0181 (16)	0.0243 (19)	-0.0067 (14)	0.000	0.000
O6	0.0096 (15)	0.0243 (17)	0.029 (2)	0.0032 (12)	0.000	0.000
O3	0.021 (2)	0.0122 (19)	0.009 (2)	0.000	0.000	0.000

Geometric parameters (Å, °)

Sr1—O2	2.619 (4)	Sr1—O5	2.716 (4)
Sr1—O2 ⁱ	2.619 (4)	Sr1—O5 ⁱⁱ	2.716 (4)
Sr1—O1 ⁱⁱ	2.645 (2)	Cl1—O6	1.443 (4)
Sr1—O1 ⁱ	2.645 (2)	Cl1—O5	1.445 (4)
Sr1—O1 ⁱⁱⁱ	2.645 (2)	Cl1—O7	1.449 (3)
Sr1—O1	2.645 (2)	Cl1—O7 ⁱ	1.449 (3)
Sr1—O3	2.656 (5)		
O2—Sr1—O2 ⁱ	83.68 (16)	O2 ⁱ —Sr1—O5	68.08 (7)
O2—Sr1—O1 ⁱⁱ	81.60 (8)	O1 ⁱⁱ —Sr1—O5	139.99 (5)
O2 ⁱ —Sr1—O1 ⁱⁱ	135.37 (6)	O1 ⁱ —Sr1—O5	67.32 (8)
O2—Sr1—O1 ⁱ	135.37 (6)	O1 ⁱⁱⁱ —Sr1—O5	139.99 (5)
O2 ⁱ —Sr1—O1 ⁱ	81.60 (8)	O1—Sr1—O5	67.33 (8)
O1 ⁱⁱ —Sr1—O1 ⁱ	135.38 (11)	O3—Sr1—O5	120.07 (8)
O2—Sr1—O1 ⁱⁱⁱ	135.37 (6)	O2—Sr1—O5 ⁱⁱ	68.08 (7)
O2 ⁱ —Sr1—O1 ⁱⁱⁱ	81.60 (8)	O2 ⁱ —Sr1—O5 ⁱⁱ	68.08 (7)
O1 ⁱⁱ —Sr1—O1 ⁱⁱⁱ	80.01 (11)	O1 ⁱⁱ —Sr1—O5 ⁱⁱ	67.32 (8)
O1 ⁱ —Sr1—O1 ⁱⁱⁱ	83.41 (11)	O1 ⁱ —Sr1—O5 ⁱⁱ	139.99 (5)
O2—Sr1—O1	81.60 (8)	O1 ⁱⁱⁱ —Sr1—O5 ⁱⁱ	67.32 (8)
O2 ⁱ —Sr1—O1	135.37 (6)	O1—Sr1—O5 ⁱⁱ	139.99 (5)
O1 ⁱⁱ —Sr1—O1	83.41 (11)	O3—Sr1—O5 ⁱⁱ	120.07 (8)
O1 ⁱ —Sr1—O1	80.01 (11)	O5—Sr1—O5 ⁱⁱ	119.85 (17)
O1 ⁱⁱⁱ —Sr1—O1	135.38 (11)	O6—Cl1—O5	108.9 (2)
O2—Sr1—O3	138.16 (8)	O6—Cl1—O7	109.77 (14)
O2 ⁱ —Sr1—O3	138.16 (8)	O5—Cl1—O7	109.23 (14)
O1 ⁱⁱ —Sr1—O3	67.69 (6)	O6—Cl1—O7 ⁱ	109.77 (14)
O1 ⁱ —Sr1—O3	67.69 (6)	O5—Cl1—O7 ⁱ	109.24 (14)
O1 ⁱⁱⁱ —Sr1—O3	67.69 (6)	O7—Cl1—O7 ⁱ	109.9 (2)
O1—Sr1—O3	67.69 (6)	Cl1—O5—Sr1	156.2 (2)
O2—Sr1—O5	68.08 (7)		

Symmetry codes: (i) $x, y, -z+1/2$; (ii) $-x+1, y, z$; (iii) $-x+1, y, -z+1/2$.*Hydrogen-bond geometry (Å, °)*

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1B \cdots O7 ^{iv}	0.84 (1)	2.02 (2)	2.844 (4)	169 (5)
O1—H1A \cdots O4	0.84 (1)	1.98 (1)	2.811 (4)	170 (5)
O2—H2A \cdots O1 ^v	0.84 (1)	1.99 (2)	2.780 (4)	156 (5)
O3—H3A \cdots O2 ^{iv}	0.84 (1)	2.05 (3)	2.851 (5)	158 (7)

O4—H4A···O6 ^{vi}	0.84 (1)	2.62 (3)	3.337 (2)	144 (4)
O4—H4A···O7 ^{vii}	0.84 (1)	2.39 (3)	3.041 (4)	135 (4)

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