

Crystal structure of strontium thiosulfate monohydrate

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$\text{SrS}_2\text{O}_3 \cdot \text{H}_2\text{O}$ was obtained from an aqueous solution of $\text{Na}_2\text{S}_2\text{O}_3$ and $\text{Sr}(\text{NO}_3)_2$ and crystallizes in space group $P\bar{1}$ with all atoms at general positions. The Sr^{2+} ion exhibits an $[8 + 1]$ coordination defined by two terminal S and six O atoms of thiosulfate ions, one of the latter at a longer distance, and by one O atom of a water molecule. Two thiosulfate anions act as bidentate, four as monodentate ligands. The structure consists of mainly ionically interacting layers lying parallel to the crystallographic ab plane. The layers are connected by $\text{O} \cdots \text{H} \cdots \text{S}$ and $\text{O} \cdots \text{H} \cdots \text{O}$ hydrogen bonds of moderate strength.

1. Chemical context

Although thiosulfuric acid and its salts are common topics in textbooks of inorganic chemistry, the preparation of the pure acid was achieved just recently by a sophisticated synthesis *via* reaction of $\text{Na}_2\text{S}_2\text{O}_3$ and anhydrous HF (Hopfinger *et al.*, 2018). Its salts are much better explored, as they are naturally and geologically widely spread (Caufield & Raiswell, 1999), and $\text{Na}_2\text{S}_2\text{O}_3$, as well as $(\text{NH}_4)_2\text{S}_2\text{O}_3$, is produced on a large industrial scale (Barberá *et al.*, 2012). To date, thiosulfates of alkaline earth metals are solely known as hydrates. For example, $\text{MgS}_2\text{O}_3 \cdot 6\text{H}_2\text{O}$ has been investigated by Elerman *et al.* (1983) to determine its deformation electron density, and the first example of an S–H hydrogen bond that was confirmed by a single crystal-structure determination was found in $\text{BaS}_2\text{O}_3 \cdot \text{H}_2\text{O}$ (Manojlović-Muir, 1969).

Next to $\text{SrS}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ (Held & Bohatý, 2004), the title compound represents the second known crystal structure of a hydrate of strontium thiosulfate. As one route of preparation, the pentahydrate has been crystallized from aqueous solutions of $\text{Na}_2\text{S}_2\text{O}_3$ and $\text{Sr}(\text{NO}_3)_2$, whereby these solutions were reported to show a tendency to decompose, inhibiting the growth of larger single crystals (Held & Bohatý, 2004). A possible step within the decomposition process, and maybe a competing product in a later stage of crystallization, might be associated with the monohydrate, the crystal structure of which is presented here.

2. Structural commentary

$\text{SrS}_2\text{O}_3 \cdot \text{H}_2\text{O}$ crystallizes in the space group $P\bar{1}$ with one formula unit in the asymmetric unit and all atoms on general positions. Many structural features resemble the closely related pentahydrate of SrS_2O_3 . The thiosulfate anion adopts a slightly distorted tetrahedral shape with a mean bond angle of 109.47° where the average O–S–O angles (110.32°) are

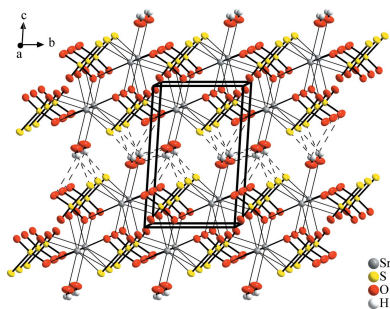


Table 1

S—S and averaged S—O bond lengths (Å) in thiosulfates of divalent cations.

| Cation/solvent molecules | S—S | mean S—O |
|---|-------|----------|
| Ba ²⁺ /1 H ₂ O ^a | 1.979 | 1.477 |
| Sr ²⁺ /5 H ₂ O ^b | 1.995 | 1.472 |
| Sr ²⁺ /1 H ₂ O ^c | 2.004 | 1.474 |
| Ca ²⁺ /6 H ₂ O ^b | 2.008 | 1.468 |
| Mg ²⁺ /6 H ₂ O ^d | 2.019 | 1.471 |
| Ni ²⁺ /6 H ₂ O ^e | 2.015 | 1.459 |
| Cd ²⁺ /2 H ₂ O ^f | 2.056 | 1.454 |
| Pb ²⁺ /0 H ₂ O ^g | 2.11 | 1.455 |

Notes: (a) Manojlović-Muir (1975); (b) Held & Bohatý (2004); (c) this work; (d) Elerman *et al.* (1983); (e) Elerman *et al.* (1978); (f) Baggio *et al.* (1997); (g) Christensen *et al.* (1991).

slightly larger than the S—S—O angles (108.62°). Similar to the S—S bond length found in the pentahydrate (1.995 Å), the S—S bond length of 2.0044 (7) Å in the monohydrate is between those of the Ca (2.008 Å) and the Ba (1.979 Å) salts. The S—O bond lengths are between 1.466 (2) Å and 1.478 (2) Å and are in the same range as those of other alkaline earth thiosulfate hydrates (Table 1).

The Sr²⁺ cation is coordinated by five O and two S atoms, belonging to six neighbouring S₂O₃²⁻ anions, and one additional O atom of an H₂O molecule. One of the anions acts as a bidentate S/O ligand, while the remaining five coordinate only *via* one S or O atom, respectively. These six O ligands are found in narrow Sr—O distances ranging from 2.531 (2) to 2.623 (2) Å, whereas the S atoms exhibit Sr—S distances of 3.1618 (6) and 3.2379 (6) Å. A more remote O atom at a distance of 3.305 (2) Å might also be ascribed to the first

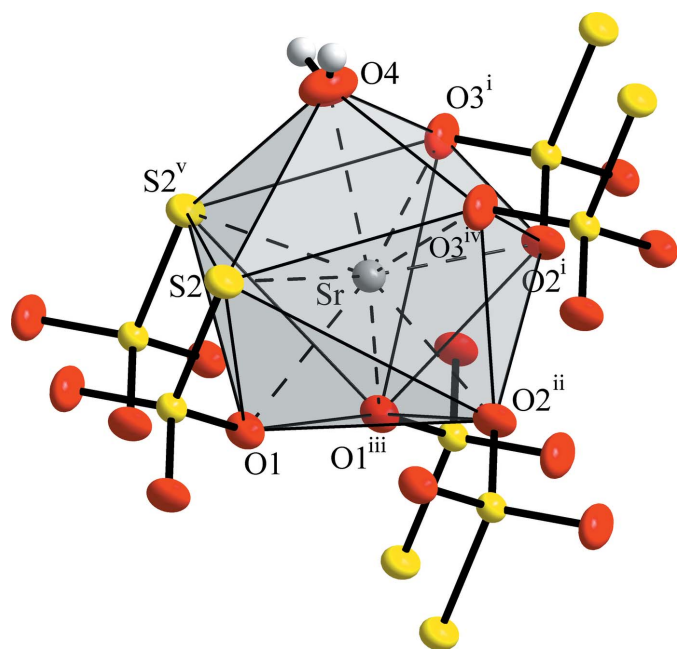


Figure 1

Coordination polyhedron of the Sr²⁺ cation in SrS₂O₃·H₂O. Anisotropic displacement ellipsoids are drawn at the 70% probability level; H atoms are shown with arbitrary radius. [Symmetry codes: (i) $x - 1, y + 1, z$; (ii) $-x + 1, -y + 1, -z$; (iii) $-x, -y + 1, -z$; (iv) $x, y + 1, z$; (v) $x - 1, y, z$.]

Table 2

Hydrogen-bond geometry (Å, °).

| D—H...A | D—H | H...A | D...A | D—H...A |
|---------------------------|----------|----------|-----------|---------|
| O4—H2...S2 ⁱ | 0.76 (3) | 2.62 (4) | 3.344 (2) | 163 (4) |
| O4—H1...O4 ⁱⁱ | 0.78 (4) | 2.42 (4) | 2.962 (4) | 128 (4) |
| O4—H1...S2 ⁱⁱⁱ | 0.78 (4) | 2.84 (4) | 3.458 (2) | 138 (4) |

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

coordination sphere, although exhibiting a larger distance than the neighbouring S atoms. This [8 + 1] coordination of the Sr²⁺ atom (Fig. 1) again resembles the ninefold coordination of the cation in SrS₂O₃·5H₂O, with the difference being that in the pentahydrate no S atoms are found in the first coordination sphere of Sr²⁺, but four water molecules instead. As a consequence of the presence of the larger S atoms close to Sr²⁺, in the title structure one O atom is shifted into an outer region of the coordination shell and thus is found at a considerably longer distance.

As a characteristic feature of the crystal structure, SrS₂O₃·H₂O is made up from layers extending parallel to the crystallographic *ab* plane (Fig. 2). Within the layers, the condensed coordination polyhedra are packed alternately to form double sheets in such a way that the terminal S2 atoms and water molecules are directed towards the layer boundaries (Fig. 3). The layers are linked by hydrogen bonds of medium strength between the water molecules (O4...O4ⁱⁱ) and the water molecules and thiosulfate anions *via* S2 atoms (Table 2). This involves also a bifurcated hydrogen bond O4—H1... (O4ⁱⁱ/S2ⁱⁱⁱ). The O4—H2...S2ⁱ bond as well as the D...A distances are in the same range as in SrS₂O₃·5H₂O (Held & Bohatý, 2004). For the H1 atom, a disorder model similar to that proposed for BaS₂O₃·H₂O (Manojlović-Muir, 1975) was

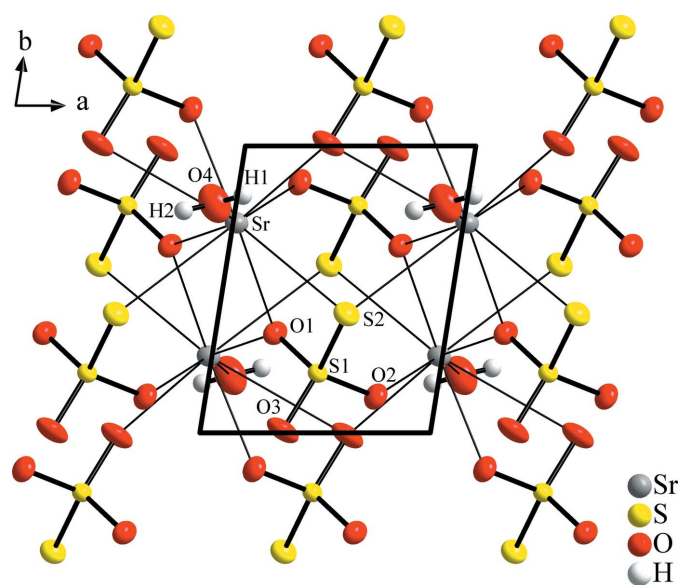


Figure 2

Crystal structure of SrS₂O₃·H₂O, in a view onto (001). Displacement ellipsoids are shown as in Fig. 1.

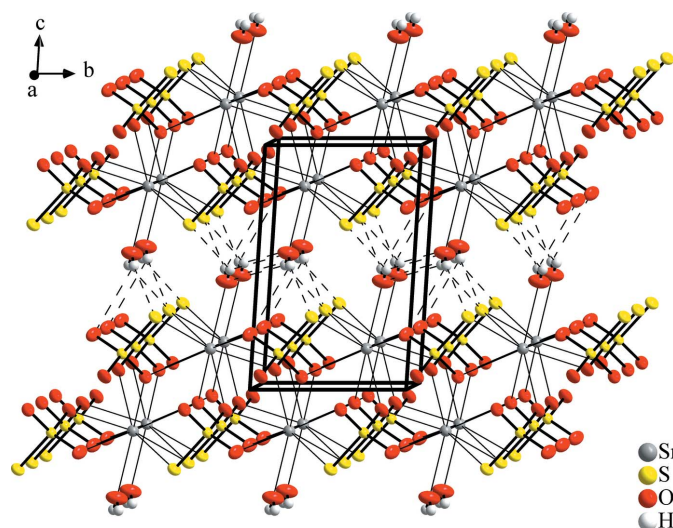


Figure 3
A projection of the crystal structure of $\text{SrS}_2\text{O}_3\cdot\text{H}_2\text{O}$, approximately along $[100]$. Displacement ellipsoids are shown as in Fig. 1.

considered, which would result in shorter and more linear $\text{O4}-\text{H1}\cdots\text{O4}^{\text{ii}}$ and $\text{O4}-\text{H1}\cdots\text{S2}^{\text{iii}}$ bonds. However, a reasonable refinement of these disordered H atoms was not possible.

A striking analogy to the packing of the pentahydrate structure (Fig. 4a) is apparent. With the presence of five water molecules instead of one, the main packing of ions in $\text{SrS}_2\text{O}_3\cdot 5\text{H}_2\text{O}$ is only slightly changed as a result of the coordination of additional water molecules to the Sr^{2+} cation and widened by two non-coordinating and hydrogen-bonded water molecules situated between the layers. The S—S bond is nearly orthogonal to the layer plane; however, the layer boundaries are also formed by S atoms and water molecules, both forming hydrogen bonds. The very close relationship between the two crystal structures suggests a topotactical degradation of the pentahydrate. Because both hydrates were crystallized at room temperature, a temperature dependence of the crystallization does not seem to be the only possible driving force. An ageing process triggered by concentration or thermodynamic stability must be taken into account as well. The degradation process, possibly running *via* another so far unknown trihydrate after removal of the free water molecules, was not investigated up to now, and in addition a thermal analysis of the title compound could not be carried out because of the presence of large amounts of indistinguishable crystalline by-products, *viz.* NaNO_3 and $\text{Sr}(\text{NO}_3)_2$.

The orthorhombic structure of $\text{BaS}_2\text{O}_3\cdot\text{H}_2\text{O}$ is likewise found to form layers, which are separated by water molecules (Fig. 4b; Nardelli & Fava, 1962; Manojlović-Muir, 1975). Similar to the Sr homologue, two terminal S atoms are part of the first coordination sphere of the Ba^{2+} cation which has, caused by the larger ion radius, a different environment, namely by five thiosulfate anions as bidentate ligands and one additional water molecule. Interestingly, while the number of atoms forming the first coordination sphere is higher in the Ba

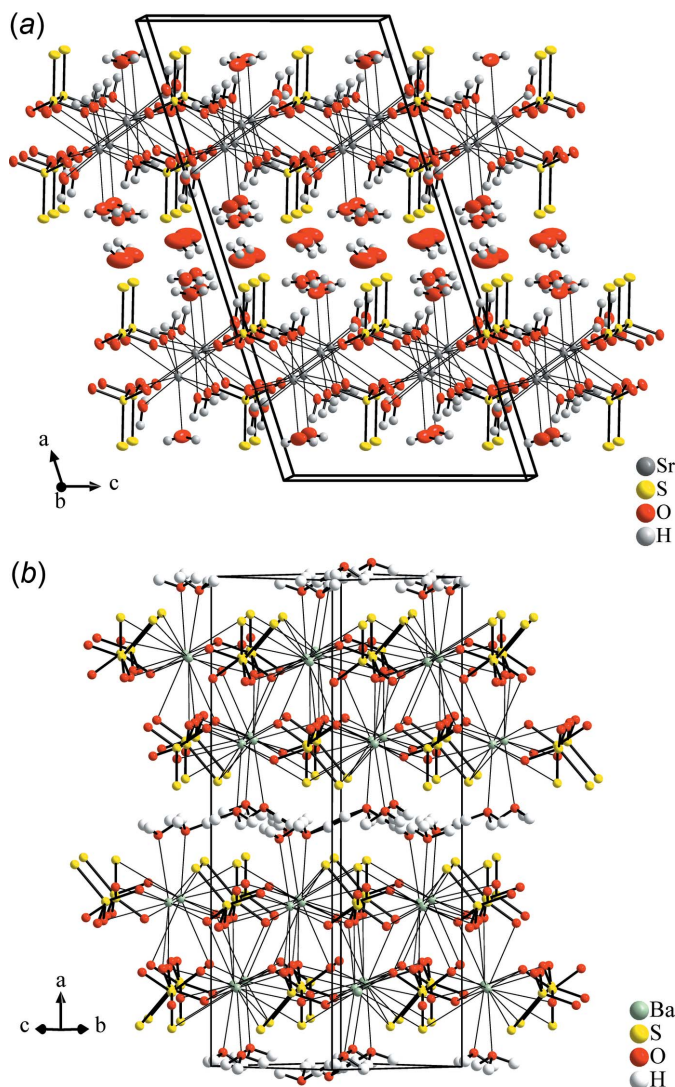


Figure 4
Illustration of the structural relationship between the title compound, $\text{SrS}_2\text{O}_3\cdot\text{H}_2\text{O}$, and (a) $\text{SrS}_2\text{O}_3\cdot 5\text{H}_2\text{O}$ (view approximately along $[0\bar{1}0]$) and (b) $\text{BaS}_2\text{O}_3\cdot\text{H}_2\text{O}$ (view approximately along $[011]$).

compound, the number of directly coordinating anions is smaller.

3. Database survey

Besides SrS_2O_3 , crystal structure determinations for three further alkaline-earth thiosulfates have been reported, all of them as hydrates: $\text{BaS}_2\text{O}_3\cdot\text{H}_2\text{O}$ (Nardelli & Fava, 1962; Manojlović-Muir, 1975), $\text{CaS}_2\text{O}_3\cdot 6\text{H}_2\text{O}$ (Held & Bohatý, 2004), and $\text{MgS}_2\text{O}_3\cdot 6\text{H}_2\text{O}$ (Nardelli *et al.*, 1962; Baggio *et al.*, 1969; Elerman *et al.*, 1982, 1983). Together with the known Sr compounds, $\text{SrS}_2\text{O}_3\cdot 5\text{H}_2\text{O}$ (Held & Bohatý, 2004) and the new monohydrate, the trend of incorporating smaller amounts of water into stable crystal structures with increasing cation radius is obvious for alkaline-earth metal thiosulfates. With the exception of two of the five water molecules in $\text{SrS}_2\text{O}_3\cdot 5\text{H}_2\text{O}$, all water molecules in these compounds coordinate to the divalent cations. This trend is confirmed by

divalent transition-metal thiosulfates, as there are those of Ni as the hexahydrate (Elerman *et al.*, 1978; isostructural with the Mg salt) and of Cd as the dihydrate (Baggio *et al.*, 1997). The only crystal structure of a hydrate-free thiosulfate of a divalent cation is reported for Pb (Christensen *et al.*, 1991). Table 1 collates S—S and averaged S—O bond lengths in the corresponding structures of these thiosulfates.

4. Synthesis and crystallization

Crystals of $\text{SrS}_2\text{O}_3 \cdot \text{H}_2\text{O}$ were grown from an aqueous solution of $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ and $\text{Sr}(\text{NO}_3)_2$. The solution was stored at room temperature and the solvent was evaporated very slowly over several months. Single crystals were isolated from highly concentrated solutions where only a little of the mother liquor remained. Besides the title compound, crystals of NaNO_3 and surplus $\text{Sr}(\text{NO}_3)_2$ were also found, and all of these compounds were identified in the X-ray powder pattern of the reaction mixture after drying at room temperature. From all these experiments, no hints of the presence of the pentahydrate were found.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms were refined with a restrained O—H distance of 0.85 (5) Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. A free refinement of H-atom positions resulted in a reliable shape for the water molecule and orientation with respect to possible hydrogen bonds, but included one short O—H distance of only 0.5 Å.

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Table 3

Experimental details.

| | |
|--|--|
| Crystal data | |
| Chemical formula | $\text{SrS}_2\text{O}_3 \cdot \text{H}_2\text{O}$ |
| M_r | 217.76 |
| Crystal system, space group | Triclinic, $P\bar{1}$ |
| Temperature (K) | 297 |
| a, b, c (Å) | 4.6858 (2), 5.9178 (3), 9.0167 (4) |
| α, β, γ (°) | 84.889 (2), 87.284 (2), 80.785 (2) |
| V (Å ³) | 245.68 (2) |
| Z | 2 |
| Radiation type | Mo $K\alpha$ |
| μ (mm ⁻¹) | 11.72 |
| Crystal size (mm) | 0.42 × 0.30 × 0.16 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Numerical (<i>SADABS</i> ; Krause <i>et al.</i> , 2015) |
| $T_{\text{min}}, T_{\text{max}}$ | 0.037, 0.264 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 8011, 1504, 1481 |
| R_{int} | 0.054 |
| $(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹) | 0.715 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$ | 0.024, 0.061, 1.10 |
| No. of reflections | 1504 |
| No. of parameters | 71 |
| No. of restraints | 2 |
| H-atom treatment | Only H-atom coordinates refined |
| $\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³) | 0.97, -0.86 |

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg & Putz, 2012) and *pubCIF* (Westrip, 2010).

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Crystal structure of strontium thiosulfate monohydrate

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Computing details

Data collection: *APEX3* (Bruker, 2015); cell refinement: *SAINT* (Bruker, 2015); data reduction: *SAINT* (Bruker, 2015); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2012); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

Strontium thiosulfate monohydrate

Crystal data

SrS₂O₃·H₂O

$M_r = 217.76$

Triclinic, $P\bar{1}$

$a = 4.6858$ (2) Å

$b = 5.9178$ (3) Å

$c = 9.0167$ (4) Å

$\alpha = 84.889$ (2)°

$\beta = 87.284$ (2)°

$\gamma = 80.785$ (2)°

$V = 245.68$ (2) Å³

$Z = 2$

$F(000) = 208$

$D_x = 2.944$ Mg m⁻³

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

Cell parameters from 7034 reflections

$\theta = 2.3$ – 30.6 °

$\mu = 11.72$ mm⁻¹

$T = 297$ K

Block, colourless

$0.42 \times 0.30 \times 0.16$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: rotating anode FR591

MONTELOptic monochromator

Detector resolution: 16 pixels mm⁻¹

φ - and ω -rotation scans

Absorption correction: numerical

(*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.037$, $T_{\max} = 0.264$

8011 measured reflections

1504 independent reflections

1481 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.054$

$\theta_{\max} = 30.6$ °, $\theta_{\min} = 2.3$ °

$h = -6 \rightarrow 6$

$k = -8 \rightarrow 8$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.061$

$S = 1.10$

1504 reflections

71 parameters

2 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: difference Fourier map

Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + (0.0324P)^2 + 0.2036P]$

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

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

$\Delta\rho_{\max} = 0.97$ e Å⁻³

$\Delta\rho_{\min} = -0.86$ e Å⁻³

Extinction correction: SHELXL2014
(Sheldrick, 2015),
 $F_c^* = k F_c [1 + 0.001 x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.085 (5)

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> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|--------------|-------------|--------------|----------------------------------|
| Sr | 0.01493 (4) | 0.73223 (3) | 0.16811 (2) | 0.01372 (10) |
| S1 | 0.47043 (11) | 0.20793 (8) | 0.16097 (5) | 0.01113 (12) |
| S2 | 0.55500 (12) | 0.41404 (9) | 0.31260 (6) | 0.01678 (13) |
| O1 | 0.2582 (3) | 0.3477 (3) | 0.06042 (17) | 0.0163 (3) |
| O2 | 0.7385 (3) | 0.1265 (3) | 0.07573 (19) | 0.0178 (3) |
| O3 | 0.3580 (4) | 0.0090 (3) | 0.23659 (19) | 0.0221 (3) |
| O4 | -0.0933 (5) | 0.7998 (4) | 0.4397 (2) | 0.0309 (4) |
| H1 | 0.024 (9) | 0.827 (8) | 0.491 (5) | 0.046* |
| H2 | -0.223 (8) | 0.774 (7) | 0.487 (4) | 0.046* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|--------------|--------------|--------------|---------------|---------------|---------------|
| Sr | 0.01592 (13) | 0.01292 (12) | 0.01266 (13) | -0.00269 (7) | -0.00130 (7) | -0.00167 (7) |
| S1 | 0.0116 (2) | 0.0105 (2) | 0.0117 (2) | -0.00225 (16) | -0.00057 (16) | -0.00182 (16) |
| S2 | 0.0202 (3) | 0.0170 (2) | 0.0145 (2) | -0.00505 (19) | -0.00235 (19) | -0.00465 (18) |
| O1 | 0.0159 (7) | 0.0160 (7) | 0.0168 (7) | 0.0000 (6) | -0.0053 (6) | -0.0030 (6) |
| O2 | 0.0145 (7) | 0.0194 (7) | 0.0188 (7) | 0.0006 (6) | 0.0027 (6) | -0.0057 (6) |
| O3 | 0.0316 (9) | 0.0187 (7) | 0.0191 (8) | -0.0146 (7) | -0.0033 (7) | 0.0023 (6) |
| O4 | 0.0339 (11) | 0.0433 (11) | 0.0187 (9) | -0.0151 (9) | 0.0037 (8) | -0.0071 (8) |

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

| | | | |
|----------------------|-------------|-----------------------|-------------|
| Sr—O4 | 2.531 (2) | S1—O2 | 1.4768 (16) |
| Sr—O2 ⁱ | 2.5698 (16) | S1—O1 | 1.4776 (15) |
| Sr—O2 ⁱⁱ | 2.5708 (17) | S1—S2 | 2.0044 (7) |
| Sr—O1 ⁱⁱⁱ | 2.5934 (15) | S1—Sr ^{vii} | 3.4816 (5) |
| Sr—O3 ^{iv} | 2.6010 (17) | S2—Sr ^{viii} | 3.2379 (6) |
| Sr—O1 | 2.6226 (15) | O1—Sr ⁱⁱⁱ | 2.5934 (15) |
| Sr—S2 | 3.1618 (6) | O2—Sr ^{vii} | 2.5698 (16) |
| Sr—S2 ^v | 3.2379 (6) | O2—Sr ⁱⁱ | 2.5708 (16) |
| Sr—O3 ⁱ | 3.305 (2) | O3—Sr ^{ix} | 2.6010 (17) |
| Sr—S1 | 3.4768 (5) | O3—Sr ^{vii} | 3.305 (2) |
| Sr—S1 ⁱ | 3.4816 (5) | O4—H1 | 0.78 (4) |
| Sr—Sr ^{vi} | 4.1762 (4) | O4—H2 | 0.76 (3) |

| | | | |
|--|-------------|--|--------------|
| S1—O3 | 1.4663 (16) | | |
| O4—Sr—O2 ⁱ | 93.29 (7) | O1 ⁱⁱⁱ —Sr—S1 ⁱ | 80.94 (3) |
| O4—Sr—O2 ⁱⁱ | 145.14 (6) | O3 ^{iv} —Sr—S1 ⁱ | 86.26 (4) |
| O2 ⁱ —Sr—O2 ⁱⁱ | 71.34 (6) | O1—Sr—S1 ⁱ | 150.22 (3) |
| O4—Sr—O1 ⁱⁱⁱ | 138.36 (6) | S2—Sr—S1 ⁱ | 152.443 (14) |
| O2 ⁱ —Sr—O1 ⁱⁱⁱ | 75.45 (5) | S2 ^v —Sr—S1 ⁱ | 89.500 (14) |
| O2 ⁱⁱ —Sr—O1 ⁱⁱⁱ | 69.30 (5) | O3 ⁱ —Sr—S1 ⁱ | 24.78 (3) |
| O4—Sr—O3 ^{iv} | 73.47 (6) | S1—Sr—S1 ⁱ | 170.625 (18) |
| O2 ⁱ —Sr—O3 ^{iv} | 77.99 (6) | O4—Sr—Sr ^{vi} | 122.71 (6) |
| O2 ⁱⁱ —Sr—O3 ^{iv} | 72.79 (5) | O2 ⁱ —Sr—Sr ^{vi} | 35.68 (4) |
| O1 ⁱⁱⁱ —Sr—O3 ^{iv} | 138.90 (5) | O2 ⁱⁱ —Sr—Sr ^{vi} | 35.66 (4) |
| O4—Sr—O1 | 126.88 (7) | O1 ⁱⁱⁱ —Sr—Sr ^{vi} | 68.15 (3) |
| O2 ⁱ —Sr—O1 | 139.15 (5) | O3 ^{iv} —Sr—Sr ^{vi} | 71.93 (4) |
| O2 ⁱⁱ —Sr—O1 | 77.29 (5) | O1—Sr—Sr ^{vi} | 109.27 (4) |
| O1 ⁱⁱⁱ —Sr—O1 | 69.30 (5) | S2—Sr—Sr ^{vi} | 129.735 (12) |
| O3 ^{iv} —Sr—O1 | 116.91 (6) | S2 ^v —Sr—Sr ^{vi} | 134.574 (12) |
| O4—Sr—S2 | 80.16 (6) | O3 ⁱ —Sr—Sr ^{vi} | 80.32 (3) |
| O2 ⁱ —Sr—S2 | 152.24 (4) | S1—Sr—Sr ^{vi} | 124.721 (11) |
| O2 ⁱⁱ —Sr—S2 | 98.85 (4) | S1 ⁱ —Sr—Sr ^{vi} | 58.002 (9) |
| O1 ⁱⁱⁱ —Sr—S2 | 126.47 (3) | O3—S1—O2 | 108.96 (11) |
| O3 ^{iv} —Sr—S2 | 74.28 (4) | O3—S1—O1 | 112.09 (10) |
| O1—Sr—S2 | 57.20 (3) | O2—S1—O1 | 109.91 (9) |
| O4—Sr—S2 ^v | 69.28 (5) | O3—S1—S2 | 109.49 (7) |
| O2 ⁱ —Sr—S2 ^v | 108.83 (4) | O2—S1—S2 | 109.77 (7) |
| O2 ⁱⁱ —Sr—S2 ^v | 144.82 (4) | O1—S1—S2 | 106.59 (7) |
| O1 ⁱⁱⁱ —Sr—S2 ^v | 76.67 (4) | O3—S1—Sr | 115.97 (8) |
| O3 ^{iv} —Sr—S2 ^v | 142.38 (4) | O2—S1—Sr | 134.05 (7) |
| O1—Sr—S2 ^v | 82.74 (4) | O1—S1—Sr | 43.98 (6) |
| S2—Sr—S2 ^v | 94.134 (15) | S2—S1—Sr | 64.00 (2) |
| O4—Sr—O3 ⁱ | 65.98 (6) | O3—S1—Sr ^{vii} | 70.87 (8) |
| O2 ⁱ —Sr—O3 ⁱ | 46.05 (5) | O2—S1—Sr ^{vii} | 41.53 (7) |
| O2 ⁱⁱ —Sr—O3 ⁱ | 114.88 (5) | O1—S1—Sr ^{vii} | 141.36 (6) |
| O1 ⁱⁱⁱ —Sr—O3 ⁱ | 78.38 (4) | S2—S1—Sr ^{vii} | 108.24 (2) |
| O3 ^{iv} —Sr—O3 ⁱ | 104.37 (6) | Sr—S1—Sr ^{vii} | 170.625 (18) |
| O1—Sr—O3 ⁱ | 138.65 (4) | S1—S2—Sr | 81.26 (2) |
| S2—Sr—O3 ⁱ | 144.49 (3) | S1—S2—Sr ^{viii} | 109.00 (2) |
| S2 ^v —Sr—O3 ⁱ | 64.83 (3) | Sr—S2—Sr ^{viii} | 94.134 (15) |
| O4—Sr—S1 | 106.66 (6) | S1—O1—Sr ⁱⁱⁱ | 134.66 (9) |
| O2 ⁱ —Sr—S1 | 159.58 (4) | S1—O1—Sr | 112.99 (8) |
| O2 ⁱⁱ —Sr—S1 | 89.34 (4) | Sr ⁱⁱⁱ —O1—Sr | 110.70 (5) |
| O1 ⁱⁱⁱ —Sr—S1 | 91.84 (3) | S1—O2—Sr ^{vii} | 116.07 (9) |
| O3 ^{iv} —Sr—S1 | 103.11 (4) | S1—O2—Sr ⁱⁱ | 134.93 (10) |
| O1—Sr—S1 | 23.03 (3) | Sr ^{vii} —O2—Sr ⁱⁱ | 108.66 (6) |
| S2—Sr—S1 | 34.737 (12) | S1—O3—Sr ^{ix} | 135.58 (10) |
| S2 ^v —Sr—S1 | 82.985 (14) | S1—O3—Sr ^{vii} | 84.35 (8) |
| O3 ⁱ —Sr—S1 | 147.67 (3) | Sr ^{ix} —O3—Sr ^{vii} | 104.37 (6) |
| O4—Sr—S1 ⁱ | 75.63 (6) | Sr—O4—H1 | 122 (3) |

| | | | |
|--------------------------------------|-----------|----------|---------|
| O2 ⁱ —Sr—S1 ⁱ | 22.40 (4) | Sr—O4—H2 | 128 (3) |
| O2 ⁱⁱ —Sr—S1 ⁱ | 93.64 (4) | H1—O4—H2 | 109 (4) |

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

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O4—H2 \cdots S2 ^x | 0.76 (3) | 2.62 (4) | 3.344 (2) | 163 (4) |
| O4—H1 \cdots O4 ^{xi} | 0.78 (4) | 2.42 (4) | 2.962 (4) | 128 (4) |
| O4—H1 \cdots S2 ^{xii} | 0.78 (4) | 2.84 (4) | 3.458 (2) | 138 (4) |

Symmetry codes: (x) $-x, -y+1, -z+1$; (xi) $-x, -y+2, -z+1$; (xii) $-x+1, -y+1, -z+1$.