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# Crystal structure of $\mathrm{Sr}_{5} \mathrm{Te}_{4} \mathrm{O}_{12}(\mathrm{OH})_{2}$, the first basic strontium oxotellurate(IV) 

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The asymmetric unit of the title basic strontium oxotellurate(IV), $\mathrm{Sr}_{5} \mathrm{Te}_{4} \mathrm{O}_{12}(\mathrm{OH})_{2}$ \{systematic name pentastrontium tetrakis[oxotellurate(IV)] dihydroxide\}, comprises three $\mathrm{Sr}^{\mathrm{II}}$ cations (one with site symmetry 2) and two $\mathrm{Te}^{\mathrm{IV}}$ atoms, as well as seven O atoms. The coordination numbers of the alkaline earth cations to nearby O atoms range from seven $(2 \times)$ to eight, and the $\mathrm{Te}^{\mathrm{IV}}$ atoms are surrounded by three oxygen partners in the form of trigonal pyramids. The $\mathrm{SrO}_{x}$ polyhedra share corners and edges to build up a three-dimensional framework structure encapsulating channels propagating along [010]. The $\mathrm{Te}^{\mathrm{IV}}$ atoms flank the framework O atoms and are situated at the outer array of the channels with the $5 s^{2}$ lone electron pairs protruding into the empty space of the channels (diameter $\simeq 4 \AA$ ). Although the H atom of the OH group could not be located, bond-valence-sum calculations and typical $\mathrm{O} \cdots \mathrm{O}$ distances (range 2.81-3.06 $\AA$ ) clearly indicate hydrogen bonding of medium to weak strengths.

## 1. Chemical context

The peculiar feature of the crystal chemistry of oxotellurates(IV) (Christy et al., 2016) is the presence of the $5 s^{2}$ lone electron pair, denoted $E$. In the majority of cases, the lone electron pair $E$ is stereochemically active, making oxotellurates(IV) interesting for crystal engineering, e.g. in terms of the synthesis of compounds with non-centrosymmetric structures or structures with polar directions. Next to the influence of the (metal) cation on the physico-chemical characteristics of oxotellurates(IV), physical and underlying structural properties of such compounds can also be varied by incorporation of other oxoanions into the oxotellurate(IV) framework, e.g. by p-block oxoanions such as nitrate (Stöger \& Weil, 2013) or selenate (Weil \& Shirkanlou, 2015), or by $d$-block oxoanions such as vanadate (Weil, 2015).

In this context we attempted the hydrothermal synthesis of new oxotellurate phases in the system $\mathrm{Sr}-\mathrm{Te}-\mathrm{Se}-\mathrm{O}-(\mathrm{H})$. In comparison with typical solid-state reactions using open crucibles under atmospheric conditions, this method is more feasible because $\mathrm{Te}^{\mathrm{IV}}$ then tends not to be oxidized or to be evaporated during the reaction process. However, a clear disadvantage of the hydrothermal method is the high(er) number of adjustable parameters (pressure, concentration, temperature, time, filling degree, solvent etc), which often makes the products of these experiments difficult to predict or even to reproduce, accompanied by formation of several solid phases in one batch. This was also the case for the present study. Instead of a strontium oxoselenatotellurate, several oxotellurate phases were obtained without incorporation of selenium. Amongst these phases, the title compound,

Table 1
Selected geometric parameters $\left(\AA{ }^{\circ}{ }^{\circ}\right)$.

| Sr1-O7 | 2.430 (12) | Sr3-O2 | 2.507 (11) |
| :---: | :---: | :---: | :---: |
| $\mathrm{Sr} 1-\mathrm{O} 5^{\mathrm{i}}$ | 2.476 (12) | $\mathrm{Sr} 3-\mathrm{O} 4^{\text {v }}$ | 2.517 (11) |
| $\mathrm{Sr} 1-\mathrm{O} 1^{\text {ii }}$ | 2.593 (12) | $\mathrm{Sr} 3-\mathrm{O} 6^{\text {i }}$ | 2.536 (11) |
| $\mathrm{Sr} 1-\mathrm{O} 3$ | 2.596 (11) | Sr3-O6 ${ }^{\text {vi }}$ | 2.590 (12) |
| $\mathrm{Sr} 1-\mathrm{O} 2^{\mathrm{iii}}$ | 2.616 (12) | Sr3-O4 ${ }^{\text {vii }}$ | 2.644 (11) |
| $\mathrm{Sr} 1-\mathrm{O} 7^{\text {iii }}$ | 2.700 (11) | $\mathrm{Sr} 3-\mathrm{O}{ }^{\text {viii }}$ | 2.666 (11) |
| $\mathrm{Sr} 1-\mathrm{O} 2$ | 2.852 (12) | Te1-O6 | 1.865 (11) |
| Sr2-O3 | 2.510 (11) | Te1-O2 | 1.871 (11) |
| $\mathrm{Sr} 2-\mathrm{O} 1^{\text {iv }}$ | 2.624 (12) | Te1-O5 | 1.890 (12) |
| Sr2-O5 | 2.633 (12) | Te2-O4 | 1.858 (11) |
| Sr2-O7 | 2.960 (11) | Te2-O3 | 1.882 (11) |
| Sr3-O7 ${ }^{\text {iii }}$ | 2.393 (11) | Te2-O1 | 1.886 (11) |
| $\mathrm{O} 6-\mathrm{Te} 1-\mathrm{O} 2$ | 99.4 (4) | $\mathrm{O} 4-\mathrm{Te} 2-\mathrm{O} 3$ | 101.1 (5) |
| O6-Te1-O5 | 100.3 (5) | $\mathrm{O} 4-\mathrm{Te} 2-\mathrm{O} 1$ | 100.3 (5) |
| $\mathrm{O} 2-\mathrm{Te} 1-\mathrm{O} 5$ | 98.0 (5) | $\mathrm{O} 3-\mathrm{Te} 2-\mathrm{O} 1$ | 98.8 (5) |

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, y,-z+1$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2},-z+1$; (iv) $-x, y+1,-z+1$; (v) $x+\frac{1}{2}, y-\frac{1}{2}, z$; (vi) $-x+\frac{1}{2}, y-\frac{1}{2},-z$; (vii) $-x, y,-z$; (viii) $x+\frac{1}{2}, y+\frac{1}{2}, z$.
$\mathrm{Sr}_{5} \mathrm{Te}_{4} \mathrm{O}_{12}(\mathrm{OH})_{2}$, a hitherto unknown strontium oxotellurate, was isolated and structurally determined by single crystal X-ray diffraction.

## 2. Structural commentary

The asymmetric unit of $\mathrm{Sr}_{5} \mathrm{Te}_{4} \mathrm{O}_{12}(\mathrm{OH})_{2}$ comprises three Sr , two Te and seven O atoms ( H atoms were not included in the final model, see Section 5 and discussion below). Except one Sr atom (Sr2) that is located on a twofold rotation axis, all atoms are in general positions.

The coordination numbers of the Sr atoms are 7 (for Sr 1 and Sr 3 ) and 8 (for Sr 2 ) if $\mathrm{Sr}-\mathrm{O}$ distances $<3.0 \AA$ are considered as relevant for the first coordination sphere. The

Table 2
Results of the bond-valance-sum (BVS) analysis.

| Atom | BVS | $\Delta$ to expected value |
| :--- | :--- | :--- |
| Sr1 | 2.07 | 0.07 |
| Sr2 | 1.91 | 0.09 |
| Sr3 | 2.23 | 0.23 |
| Te1 | 3.94 | 0.06 |
| Te2 | 3.93 | 0.07 |
| O1 | 2.04 | 0.04 |
| O2 | 2.08 | 0.08 |
| O3 | 1.91 | 0.09 |
| O4 | 1.96 | 0.04 |
| O5 | 1.89 | 0.11 |
| O6 | 1.95 | 0.05 |
| O7 | 1.21 | 0.79 |

BVS parameters of Brown \& Altermatt (1985) were used for all bonds.
corresponding polyhedra are considerably distorted, with $\mathrm{Sr}-$ O bond lengths ranging from 2.393 (11) to 2.960 (11) $\AA$ (Table 1) and might be described as monocapped octahedra for Sr 1 and Sr 3 , and as a bicapped trigonal prism for Sr 2 . The $\mathrm{SrO}_{8}$ and the two $\mathrm{SrO}_{7}$ polyhedra share corners and edges, thereby constructing a three-dimensional framework structure encapsulating channels that propagate along [010]. Each of the two Te atoms connect to the outer oxygen atoms of the framework in a very similar trigonal-prismatic configuration (Table 1), with the $5 s^{2}$ lone electron pair $E$ being stereochemically active, i.e. pointing towards the empty space of the channels (Fig. 1). The channel diameter (without contribution of the lone pairs) is $\simeq 4 \AA$. Te-O bond lengths [1.865 (11)1.890 (12) $\AA$ for Te 1 and 1.858 (11)-1.886 (11) $\AA$ for Te 2$]$ and $\mathrm{O}-\mathrm{Te}-\mathrm{O}$ angles [98.0 (5)-100.3 (5) ${ }^{\circ}$ for Te 1 and 98.8 (5)101.1 (5) ${ }^{\circ}$ for Te 2 ] are typical for oxotellurate(IV) anions with three oxygen partners (Christy et al., 2016).


Figure 1
Projection of the crystal structure of $\mathrm{Sr}_{5} \mathrm{Te}_{4} \mathrm{O}_{12}(\mathrm{OH})_{2}$ along [010], with displacement ellipsoids drawn at the $74 \%$ probability level. The trigonalpyramidal $\mathrm{TeO}_{3}$ groups are given in red; the O atom representing the OH group is given in yellow, all other O atoms are colourless.

Table 3
Hydrogen-bond geometry ( $\AA$ ).

| $D-\mathrm{H} \cdots A$ | $D \cdots A$ |
| :--- | :--- |
| O7 $\cdots$ O5 | $2.808(12)$ |
| O7 $\cdots$ O2 | $2.893(12)$ |
| O7 $\cdots 2^{\text {ix }}$ | $2.991(11)$ |
| O7 $\cdots$ O1 $^{\text {iv }}$ | $3.063(11)$ |

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

Bond-valence calculations (Brown, 2002) clearly reveal the presence of an OH group for atom O 7 (Table 2), also required by charge neutrality. Atom O 7 is bonded to four Sr atoms (Table 1, Fig. 1) and has also four possible oxygen acceptor atoms for hydrogen bonding of medium to weak strength (Table 3). The situation of four possible acceptor atoms is displayed in Fig. 2 and makes it appear likely that the corresponding H atom of the OH group is positionally disordered and thus could not be located during the present study.

In the sense of a crystal-chemically more detailed formula, the title compound may alternatively be formulated as $4 \mathrm{SrTeO}_{3} \cdot \mathrm{Sr}(\mathrm{OH})_{2}$ and represents the first basic strontium oxotellurate(IV), viz. with the presence of an OH functionality. In comparison with the other strontium oxotellurates(IV) compiled in Section 3, all $\mathrm{Sr}-\mathrm{O}$ and $\mathrm{Te}-\mathrm{O}$ lengths are in similar ranges.

## 3. Database survey

In the Inorganic Crystal Structure Database (ICSD, 2016) structural data for the following hydrous or anhydrous


Figure 2
The vicinity of the OH group emphasizing the different possibilities for $\mathrm{O} \cdots \mathrm{O}$ hydrogen bonding (green lines). $\mathrm{Sr}-(\mathrm{OH})$ bonds have been omitted for clarity. Symmetry operators refer to those of Table 3; displacement ellipsoids are the same as in Fig. 1.

Table 4
Experimental details.
Crystal data
Chemical formula
$M_{\mathrm{r}}$
Crystal system, space group
Temperature (K)
$a, b, c(\AA)$
$\beta\left({ }^{\circ}\right)$
$V\left(\mathrm{~A}^{3}\right)$
Z
Radiation type
$\mu\left(\mathrm{mm}^{-1}\right)$
Crystal size (mm)
Data collection
Diffractometer
Absorption correction
$T_{\text {min }}, T_{\text {max }}$
No. of measured, independent and observed $[I>2 \sigma(I)]$ reflections
$R_{\text {int }}$
$(\sin \theta / \lambda)_{\max }\left(\AA^{-1}\right)$
Refinement
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right], w R\left(F^{2}\right), S$
No. of reflections
No. of parameters
No. of restraints H -atom treatment
$\Delta \rho_{\text {max }}, \Delta \rho_{\text {min }}\left(\mathrm{e} \AA^{-3}\right)$
Absolute structure
Absolute structure parameter
$\mathrm{Sr}_{5} \mathrm{Te}_{4} \mathrm{O}_{12}(\mathrm{OH})_{2}$
1174.52

Monoclinic, C2
295
16.0785 (10), 5.7927 (5), 8.9262 (7)
107.542 (4)
792.71 (11)

2
Mo $K \alpha$
23.99
$0.18 \times 0.06 \times 0.01$

Bruker APEXII CCD
Multi-scan (SADABS; Bruker, 2012)
0.099, 0.795

12913, 1914, 1319
0.088
0.660
$0.042,0.085,1.02$
1914
71
1
H -atom parameters not defined
2.31, -1.78

Refined as an inversion twin 0.058 (18)

Computer programs: APEX2 and SAINT (Bruker, 2012), SHELXS97 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015), ATOMS (Dowty, 2006) and publCIF (Westrip, 2010).
strontium oxotellurate(IV) phases have been deposited: $\mathrm{SrTe}_{5} \mathrm{O}_{11}$ (Burckhardt \& Trömel, 1983), $\mathrm{Sr}_{3} \mathrm{Te}_{4} \mathrm{O}_{11}$ (Dytyatyev \& Dolgikh, 1999), various polymorphs of $\mathrm{SrTeO}_{3}$ (Dityatiev et al., 2006; Zavodnik et al., 2007a,b,c, 2008; Stöger et al., 2011), $\mathrm{SrTe}_{3} \mathrm{O}_{8}$ (Barrier et al., 2006; Weil \& Stöger, 2007) and $\mathrm{SrTeO}_{3}\left(\mathrm{H}_{2} \mathrm{O}\right)$ (Stöger et al., 2011). Additionally, in the International Centre for Diffraction Data PDF-4 database (ICDD, 2015) diffraction data for the following phases are compiled: $\mathrm{Sr}_{2} \mathrm{Te}_{3} \mathrm{O}_{8}$ (Elerman \& Koçak, 1986), $\mathrm{SrTe}_{2} \mathrm{O}_{5}$ (Redman et al., 1970; Gorbenko et al., 1983) and a high-temperature phase of the latter (Külcü et al., 1984).

## 4. Synthesis and crystallization

For the hydrothermal experiment, a Teflon container was filled with 0.0733 g of strontium oxide, 0.1529 g of tellurium dioxide and 0.032 ml of selenic acid (conc.; $96 \mathrm{wt} \%$ ), corresponding to the stoichiometric ratio 3:2:1. To this mixture 10 ml water were added to about three-fourth of the container volume. The container was then sealed with a Teflon lid and loaded into a stainless steel autoclave and then heated at autogenous pressure in an oven at 403 K for one week. After the reaction time, the autoclave was allowed to cool down to room temperature over six h. The formed solid product was filtered off and washed with water and ethanol. Inspection under a polarizing microscope revealed a phase mixture with different
crystal forms clearly discernible. According to X-ray powder diffraction of the bulk material, the following phases could be identified: $\alpha-\mathrm{TeO}_{2}$ (Lindqvist, 1968), $\mathrm{SrTe}_{2} \mathrm{O}_{5}$ (Redman et al., 1970), $\mathrm{SrTe}_{3} \mathrm{O}_{8}$ (Barrier et al., 2006; Weil \& Stöger, 2007) and $\mathrm{SrTe}_{5} \mathrm{O}_{11}$ (Burckhardt \& Trömel, 1983). Solid reaction products containing Se-phases were not detected. Platy $\mathrm{Sr}_{5} \mathrm{Te}_{4} \mathrm{O}_{12}(\mathrm{OH})_{2}$ crystals were present in only minor amounts, and were manually separated for structure determination from the other solid products.

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. Some of the O atoms showed physically unreasonable behaviour when refined with anisotropic displacement parameters. Hence, for the final model all O atoms were refined with individual isotropic displacement parameters. The H atom of the OH group (or positionally disordered parts) could not be located and thus was not included in the model. Twinning by inversion was also taken into account, with a contribution of the minor twin component of about $6 \%$. The maximum and minimum remaining electron densities are found 2.34 and $0.96 \AA$, respectively, from $\operatorname{Sr} 3$.

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The X-ray centre of the Vienna University of Technology is acknowledged for providing access to the single-crystal diffractometer.

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## supporting information

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## Crystal structure of $\mathrm{Sr}_{5} \mathrm{Te}_{4} \mathrm{O}_{12}(\mathrm{OH})_{2}$, the first basic strontium oxotellurate(IV)

## Matthias Weil and Mahdi Shirkhanlou

## Computing details

Data collection: APEX2 (Bruker, 2012); cell refinement: SAINT (Bruker, 2012); data reduction: SAINT (Bruker, 2012); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL2014 (Sheldrick, 2015); molecular graphics: ATOMS (Dowty, 2006); software used to prepare material for publication:
publCIF (Westrip, 2010).
Pentastrontium tetrakis[oxotellurate(IV)] dihydroxide

## Crystal data

$\mathrm{Sr}_{5} \mathrm{Te}_{4} \mathrm{O}_{12}(\mathrm{OH})_{2}$
$M_{r}=1174.52$
Monoclinic, C2
Hall symbol: C 2 y
$a=16.0785$ (10) $\AA$
$b=5.7927$ (5) A
$c=8.9262(7) \AA$
$\beta=107.542$ (4) ${ }^{\circ}$
$V=792.71(11) \AA^{3}$
$Z=2$

## Data collection

Bruker APEXII CCD
diffractometer
Radiation source: fine-focus sealed tube
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan
(SADABS; Bruker, 2012)
$T_{\text {min }}=0.099, T_{\text {max }}=0.795$
12913 measured reflections

## Refinement

Refinement on $F^{2}$
Least-squares matrix: full
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.042$
$w R\left(F^{2}\right)=0.085$
$S=1.02$
1914 reflections
71 parameters
1 restraint
$F(000)=1024$
$D_{\mathrm{x}}=4.921 \mathrm{Mg} \mathrm{m}^{-3}$
Mo $K \alpha$ radiation, $\lambda=0.71073 \AA$
Cell parameters from 2028 reflections
$\theta=4.2-33.0^{\circ}$
$\mu=23.99 \mathrm{~mm}^{-1}$
$T=295 \mathrm{~K}$
Plate, colourless
$0.18 \times 0.06 \times 0.01 \mathrm{~mm}$

1914 independent reflections
1319 reflections with $I>2 \sigma(I)$
$R_{\text {int }}=0.088$
$\theta_{\text {max }}=28.0^{\circ}, \theta_{\text {min }}=2.4^{\circ}$
$h=-20 \rightarrow 21$
$k=-7 \rightarrow 7$
$l=-11 \rightarrow 11$

H -atom parameters not defined
$w=1 /\left[\sigma^{2}\left(F_{0}^{2}\right)+(0.0236 P)^{2}+0.7139 P\right]$
where $P=\left(F_{\mathrm{o}}^{2}+2 F_{\mathrm{c}}^{2}\right) / 3$
$(\Delta / \sigma)_{\max }<0.001$
$\Delta \rho_{\max }=2.31 \mathrm{e} \AA^{-3}$
$\Delta \rho_{\text {min }}=-1.78$ e $\AA^{-3}$
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.058 (18)

## 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.
Refinement. Refined as a 2-component inversion twin

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

|  | $x$ | $y$ | $z$ | $U_{\text {iso }} * / U_{\mathrm{eq}}$ |
| :--- | :--- | :--- | :--- | :--- |
| Sr1 | $0.16911(10)$ | $0.0360(4)$ | $0.4988(2)$ | $0.0097(5)$ |
| Sr2 | 0.0000 | $0.5471(4)$ | 0.5000 | $0.0094(8)$ |
| Sr3 | $0.27399(11)$ | $0.0613(2)$ | $0.1447(2)$ | $0.0071(5)$ |
| Te1 | $0.10820(7)$ | $0.52512(19)$ | $0.16455(15)$ | $0.0081(3)$ |
| Te2 | $-0.05011(7)$ | $0.0246(2)$ | $0.17800(14)$ | $0.0091(3)$ |
| O1 | $-0.0998(7)$ | $-0.1557(19)$ | $0.3050(14)$ | $0.015(3)^{*}$ |
| O2 | $0.2040(8)$ | $0.3491(18)$ | $0.2785(14)$ | $0.017(3)^{*}$ |
| O3 | $0.0218(7)$ | $0.2152(19)$ | $0.3350(14)$ | $0.013(3)^{*}$ |
| O4 | $-0.1423(7)$ | $0.2229(19)$ | $0.0869(14)$ | $0.018(3)^{*}$ |
| O5 | $0.0964(7)$ | $0.7088(19)$ | $0.3320(14)$ | $0.017(3)^{*}$ |
| O6 | $0.1651(7)$ | $0.7327(19)$ | $0.0690(14)$ | $0.014(3)^{*}$ |
| O7 | $0.1881(7)$ | $0.4343(18)$ | $0.5881(13)$ | $0.017(3)^{*}$ |

Atomic displacement parameters $\left(\AA^{2}\right)$

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Sr 1 | $0.0090(8)$ | $0.0107(11)$ | $0.0086(10)$ | $-0.0015(8)$ | $0.0013(7)$ | $-0.0017(9)$ |
| Sr 2 | $0.0108(13)$ | $0.006(2)$ | $0.0134(14)$ | 0.000 | $0.0063(10)$ | 0.000 |
| Sr 3 | $0.0055(8)$ | $0.0035(13)$ | $0.0127(10)$ | $-0.0001(7)$ | $0.0036(6)$ | $-0.0012(9)$ |
| Te 1 | $0.0066(6)$ | $0.0084(8)$ | $0.0087(6)$ | $0.0003(6)$ | $0.0014(4)$ | $0.0000(6)$ |
| Te 2 | $0.0092(6)$ | $0.0062(7)$ | $0.0126(7)$ | $-0.0013(7)$ | $0.0041(4)$ | $-0.0024(8)$ |

Geometric parameters $\left({ }^{A},{ }^{\circ}\right)$

| Sr1-O7 | 2.430 (12) | Sr3-O2 | 2.507 (11) |
| :---: | :---: | :---: | :---: |
| Sr1-O5 ${ }^{\text {i }}$ | 2.476 (12) | $\mathrm{Sr} 3-\mathrm{O} 4^{\text {vi }}$ | 2.517 (11) |
| $\mathrm{Sr} 1-\mathrm{O} 1^{\text {ii }}$ | 2.593 (12) | Sr3-O6 ${ }^{\text {i }}$ | 2.536 (11) |
| Sr1-O3 | 2.596 (11) | $\mathrm{Sr} 3-06{ }^{\text {vii }}$ | 2.590 (12) |
| $\mathrm{Sr} 1-\mathrm{O} 2^{\text {iii }}$ | 2.616 (12) | $\mathrm{Sr} 3-\mathrm{O} 4^{\text {viii }}$ | 2.644 (11) |
| Sr1-O7 $7^{\text {iii }}$ | 2.700 (11) | Sr3-O1 $1^{\text {ix }}$ | 2.666 (11) |
| Sr1-O2 | 2.852 (12) | Te1-O6 | 1.865 (11) |
| $\mathrm{Sr} 2-\mathrm{O} 3$ | 2.510 (11) | $\mathrm{Te} 1-\mathrm{O} 2$ | 1.871 (11) |
| $\mathrm{Sr} 2-\mathrm{O} 3{ }^{\text {ii }}$ | 2.510 (11) | Te1-O5 | 1.890 (12) |
| $\mathrm{Sr} 2-\mathrm{O} 1^{\text {iv }}$ | 2.624 (12) | Te2-O4 | 1.858 (11) |
| $\mathrm{Sr} 2-\mathrm{O} 1^{\text {v }}$ | 2.624 (11) | Te2-O3 | 1.882 (11) |
| Sr2-O5 | 2.633 (12) | Te2-O1 | 1.886 (11) |
| $\mathrm{Sr} 2-\mathrm{O} 5{ }^{\text {ii }}$ | 2.633 (12) | $\mathrm{O} 7-\mathrm{Ol}^{\text {iv }}$ | 3.063 (11) |
| Sr2-O7ii | 2.960 (11) | O7-O2 | 2.893 (12) |


| Sr2-07 | 2.960 (11) |
| :---: | :---: |
| Sr3-O7 ${ }^{\text {iii }}$ | 2.393 (11) |
| O7-Sr1-O5 ${ }^{\text {i }}$ | 156.1 (4) |
| $\mathrm{O} 7-\mathrm{Sr} 1-\mathrm{O} 1^{\text {ii }}$ | 102.8 (4) |
| $\mathrm{O} 5-\mathrm{Sr} 1-\mathrm{O} 1^{\text {ii }}$ | 81.8 (4) |
| O7-Sr1-O3 | 79.0 (4) |
| O5 ${ }^{\text {i }} \mathrm{Sr} 1-\mathrm{O} 3$ | 77.4 (4) |
| O1ii-Sr1-O3 | 92.7 (4) |
| O7-Sr1-O2 ${ }^{\text {iii }}$ | 98.7 (4) |
| $\mathrm{O} 5^{\text {i }}-\mathrm{Sr} 1-\mathrm{O} 2{ }^{\text {iii }}$ | 105.0 (4) |
| $\mathrm{O} 1^{\text {ii- }} \mathrm{Sr} 1-\mathrm{O} 2{ }^{\text {iii }}$ | 72.8 (4) |
| $\mathrm{O} 3-\mathrm{Sr} 1-\mathrm{O} 2^{\text {iii }}$ | 164.5 (4) |
| O7-Sr1-O7 ${ }^{\text {iii }}$ | 105.5 (3) |
| $\mathrm{O} 5^{\text {i }}-\mathrm{Sr} 1-\mathrm{O} 7{ }^{\text {iii }}$ | 87.0 (4) |
| $\mathrm{O} 1^{\text {ii- }} \mathrm{Sr} 1-\mathrm{O} 7^{\text {iii }}$ | 132.6 (4) |
| $\mathrm{O} 3-\mathrm{Sr} 1-\mathrm{O} 7{ }^{\text {iii }}$ | 129.5 (4) |
| $\mathrm{O} 2{ }^{\text {iii }}-\mathrm{Sr} 1-\mathrm{O} 7{ }^{\text {iii }}$ | 65.9 (4) |
| $\mathrm{O} 7-\mathrm{Sr} 1-\mathrm{O} 2$ | 65.9 (4) |
| $\mathrm{O} 5-\mathrm{Sr} 1-\mathrm{O} 2$ | 103.2 (4) |
| $\mathrm{O} 1 \mathrm{ii}-\mathrm{Sr} 1-\mathrm{O} 2$ | 162.2 (4) |
| $\mathrm{O} 3-\mathrm{Sr} 1-\mathrm{O} 2$ | 72.1 (3) |
| $\mathrm{O} 2{ }^{\text {iii }}-\mathrm{Sr} 1-\mathrm{O} 2$ | 121.1 (2) |
| $\mathrm{O} 7{ }^{\text {iii }}-\mathrm{Sr} 1-\mathrm{O} 2$ | 65.2 (3) |
| $\mathrm{O} 3-\mathrm{Sr} 2-\mathrm{O} 3{ }^{\text {ii }}$ | 80.0 (5) |
| $\mathrm{O} 3-\mathrm{Sr} 2-\mathrm{O} 1^{\text {iv }}$ | 136.6 (4) |
| O3ii- ${ }^{\text {ii }} 2-\mathrm{O} 1^{\text {iv }}$ | 106.2 (3) |
| $\mathrm{O} 3-\mathrm{Sr} 2-\mathrm{O} 1^{\text {v }}$ | 106.2 (3) |
| $\mathrm{O} 3{ }^{\text {iii }} \mathrm{Sr} 2-\mathrm{Ol}^{\text {v }}$ | 136.6 (4) |
| $\mathrm{O} 1^{\text {iv }}-\mathrm{Sr} 2-\mathrm{O} 1^{\text {v }}$ | 98.0 (5) |
| O3-Sr2-O5 | 74.2 (3) |
| O3ii-Sr2-O5 | 144.8 (4) |
| $\mathrm{O} 1^{\text {iv }}-\mathrm{Sr} 2-\mathrm{O} 5$ | 78.3 (4) |
| $\mathrm{O1}^{\mathrm{v}}$ - $\mathrm{Sr} 2-\mathrm{O} 5$ | 74.7 (3) |
| $\mathrm{O} 3-\mathrm{Sr} 2-\mathrm{O} 5^{\text {ii }}$ | 144.8 (4) |
| $\mathrm{O} 3{ }^{\text {iii }}$ - $\mathrm{Sr} 2-\mathrm{O} 5^{\text {ii }}$ | 74.2 (3) |
| $\mathrm{O} 1^{\text {iv }}-\mathrm{Sr} 2-\mathrm{O} 5^{\text {ii }}$ | 74.7 (3) |
| $\mathrm{O1}^{\mathrm{v}}-\mathrm{Sr} 2-\mathrm{O} 5^{\text {ii }}$ | 78.3 (4) |
| O5-Sr2-O5 ${ }^{\text {ii }}$ | 138.3 (5) |
| $\mathrm{O} 3-\mathrm{Sr} 2-\mathrm{O} 7{ }^{\text {ii }}$ | 89.3 (3) |
| $\mathrm{O} 3{ }^{\text {iii }}-\mathrm{Sr} 2-\mathrm{O} 7^{\text {ii }}$ | 71.0 (3) |
| $\mathrm{O} 1^{\text {iv }}-\mathrm{Sr} 2-\mathrm{O} 7^{\text {ii }}$ | 133.8 (3) |
| $\mathrm{O1}^{\mathrm{v}}-\mathrm{Sr} 2-\mathrm{O} 7^{\text {ii }}$ | 66.2 (3) |
| $\mathrm{O} 5-\mathrm{Sr} 2-\mathrm{O} 7^{\text {ii }}$ | 131.1 (3) |
| $\mathrm{O} 5^{\text {iii }} \mathrm{Sr} 2-\mathrm{O} 7^{7 i}$ | 60.0 (3) |
| $\mathrm{O} 3-\mathrm{Sr} 2-\mathrm{O} 7$ | 71.0 (3) |
| $\mathrm{O} 3{ }^{\text {iii }}-\mathrm{Sr} 2-\mathrm{O} 7$ | 89.3 (3) |
| $\mathrm{O} 1^{\mathrm{iv}}-\mathrm{Sr} 2-\mathrm{O} 7$ | 66.2 (3) |


| O7-O2 ${ }^{\text {x }}$ | 2.991 (11) |
| :---: | :---: |
| O7-O5 | 2.808 (12) |
| $\mathrm{O} 2-\mathrm{Sr} 3-\mathrm{O}^{\text {i }}$ | 104.7 (4) |
| $\mathrm{O} 4{ }^{\text {vi}}-\mathrm{Sr} 3-\mathrm{O} 6^{\text {i }}$ | 74.3 (3) |
| $\mathrm{O} 7^{\text {iiii }}$ - $\mathrm{Sr} 3-\mathrm{Ob}^{\text {vii }}$ | 144.4 (4) |
| $\mathrm{O} 2-\mathrm{Sr} 3-\mathrm{O} 6{ }^{\text {vii }}$ | 114.8 (4) |
| $\mathrm{O} 4{ }^{\text {vi }}-\mathrm{Sr} 3-\mathrm{O} 6^{\text {vii }}$ | 78.7 (4) |
| O6--Sr3-O6 ${ }^{\text {vii }}$ | 118.4 (3) |
| O7 ${ }^{\text {iii- }}$-Sr3-O4 ${ }^{\text {viii }}$ | 142.3 (4) |
| $\mathrm{O} 2-\mathrm{Sr} 3-\mathrm{O} 4{ }^{\text {viii }}$ | 76.6 (4) |
| $\mathrm{O} 4{ }^{\text {vi }}-\mathrm{Sr} 3-\mathrm{O} 4^{\text {viii }}$ | 117.8 (3) |
| $\mathrm{O} 6^{\text {i }}$ - $\mathrm{Sr} 3-\mathrm{O} 4{ }^{\text {viii }}$ | 74.4 (3) |
| O6 ${ }^{\text {vii }}$ - $\mathrm{Sr} 3-\mathrm{O} 4{ }^{\text {viii }}$ | 71.3 (3) |
| O7iii- $\mathrm{Sr} 3-\mathrm{O} 1^{\text {ix }}$ | 74.3 (4) |
| $\mathrm{O} 2-\mathrm{Sr} 3-\mathrm{O} 1^{\text {ix }}$ | 73.4 (4) |
| $\mathrm{O} 4{ }^{\text {vi }}-\mathrm{Sr} 3-\mathrm{O} 1^{\text {ix }}$ | 102.8 (3) |
| O6--Sr3-O1 ${ }^{\text {ix }}$ | 163.2 (4) |
| O6 ${ }^{\text {vii }}$-Sr3-O1 $1^{\text {ix }}$ | 76.3 (3) |
| $\mathrm{O} 4{ }^{\text {viii }}-\mathrm{Sr} 3-\mathrm{O} 1^{\text {ix }}$ | 120.2 (3) |
| $\mathrm{O} 6-\mathrm{Te} 1-\mathrm{O} 2$ | 99.4 (4) |
| O6-Te1-O5 | 100.3 (5) |
| $\mathrm{O} 2-\mathrm{Te} 1-\mathrm{O} 5$ | 98.0 (5) |
| $\mathrm{O} 4-\mathrm{Te} 2-\mathrm{O} 3$ | 101.1 (5) |
| $\mathrm{O} 4-\mathrm{Te} 2-\mathrm{O} 1$ | 100.3 (5) |
| $\mathrm{O} 3-\mathrm{Te} 2-\mathrm{O} 1$ | 98.8 (5) |
| Te2-O1-Sr1 ${ }^{\text {ii }}$ | 121.0 (5) |
| Te2-O1-Sr2 ${ }^{\text {i }}$ | 118.5 (5) |
| $\mathrm{Sr} 1^{\text {iii }}-\mathrm{O} 1-\mathrm{Sr} 2^{\mathrm{i}}$ | 97.7 (4) |
| $\mathrm{Te} 2-\mathrm{O} 1-\mathrm{Sr} 3^{\text {xi }}$ | 114.2 (5) |
| $\mathrm{Sr} 1^{\text {ii }}-\mathrm{O} 1-\mathrm{Sr} 3{ }^{\text {xi }}$ | 102.3 (4) |
| $\mathrm{Sr} 2^{\mathrm{i}}-\mathrm{O} 1-\mathrm{Sr}^{\text {3i }}$ | 99.6 (4) |
| Te1-O2-Sr3 | 121.2 (6) |
| $\mathrm{Te} 1-\mathrm{O} 2-\mathrm{Sr} 1^{\text {x }}$ | 120.9 (5) |
| $\mathrm{Sr} 3-\mathrm{O} 2-\mathrm{Sr}^{\text {x }}$ | 106.2 (4) |
| Te1-O2-Sr1 | 114.9 (5) |
| $\mathrm{Sr} 3-\mathrm{O} 2-\mathrm{Sr} 1$ | 96.6 (3) |
| $\mathrm{Sr} 1^{\mathrm{x}}-\mathrm{O} 2-\mathrm{Sr} 1$ | 90.5 (4) |
| Te2-O3-Sr2 | 136.3 (5) |
| $\mathrm{Te} 2-\mathrm{O} 3-\mathrm{Sr} 1$ | 115.9 (5) |
| $\mathrm{Sr} 2-\mathrm{O} 3-\mathrm{Sr} 1$ | 103.9 (4) |
| Te2-O4-Sr3 ${ }^{\text {xii }}$ | 142.8 (6) |
| $\mathrm{Te} 2-\mathrm{O} 4-\mathrm{Sr} 3{ }^{\text {viii }}$ | 117.9 (5) |
| $\mathrm{Sr} 3{ }^{\text {xii }}$-O4- $\mathrm{Sr}^{\text {viii }}$ | 94.8 (4) |
| Te1-O5-Sr1 ${ }^{\text {v }}$ | 139.9 (6) |
| Te1-O5-Sr2 | 117.8 (5) |
| $\mathrm{Sr}^{2}-\mathrm{O} 5-\mathrm{Sr} 2$ | 100.5 (4) |
| Te1-O6- $\mathrm{Sr}^{\text { }}$ | 139.1 (6) |


| O1 ${ }^{\text {v }}$ - $\mathrm{Sr} 2-\mathrm{O} 7$ | 133.8 (3) | Te1-O6-Sr3 ${ }^{\text {xiii }}$ | 115.9 (5) |
| :---: | :---: | :---: | :---: |
| O5-Sr2-O7 | 60.0 (3) | Sr3 ${ }^{\text {v }}-\mathrm{O} 6-\mathrm{Sr} 3{ }^{\text {xiii }}$ | 95.7 (4) |
| $\mathrm{O} 5 \mathrm{ii}-\mathrm{Sr} 2-\mathrm{O} 7$ | 131.1 (3) | Sr3 ${ }^{\text {- }}$ O7-Sr1 | 126.0 (5) |
| $\mathrm{O} 7 \mathrm{ii}-\mathrm{Sr} 2-\mathrm{O} 7$ | 154.5 (4) | $\mathrm{Sr} 3{ }^{\mathrm{x}}-\mathrm{O} 7-\mathrm{Sr} 1^{\mathrm{x}}$ | 103.7 (4) |
| $\mathrm{O} 7 \mathrm{iii}-\mathrm{Sr} 3-\mathrm{O} 2$ | 75.2 (4) | $\mathrm{Sr} 1-\mathrm{O} 7-\mathrm{Sr}^{1}{ }^{\text {a }}$ | 98.5 (4) |
| $\mathrm{O} 7{ }^{\text {iii }}-\mathrm{Sr} 3-\mathrm{O} 4^{\text {vi }}$ | 88.5 (4) | $\mathrm{Sr} 3 \times-\mathrm{O} 7-\mathrm{Sr} 2$ | 97.4 (4) |
| $\mathrm{O} 2-\mathrm{Sr} 3-\mathrm{O} 4^{\text {vi }}$ | 163.7 (4) | $\mathrm{Sr} 1-\mathrm{O} 7-\mathrm{Sr} 2$ | 96.0 (4) |
| O7 ${ }^{\text {iii }}-\mathrm{Sr} 3-\mathrm{O}^{\text {i }}$ | 89.0 (4) | $\mathrm{Sr} 1^{\mathrm{x}}-\mathrm{O} 7-\mathrm{Sr} 2$ | 139.9 (4) |

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

Hydrogen-bond geometry ( $\AA$ )

| $D-\mathrm{H} \cdots A$ | D $\cdots$ A |
| :---: | :---: |
| O7‥05 | 2.808 (12) |
| O7‥02 | 2.893 (12) |
| O7‥02 ${ }^{\text {x }}$ | 2.991 (11) |
| O7 $\cdots$ O1 ${ }^{\text {iv }}$ | 3.063 (11) |

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

