

The γ -phase of SrTeO₃ at 583 K¹Valery E. Zavodnik,^a Sergey A. Ivanov^{a,b} and Adam I. Stash^{a*}^aKarpov Institute of Physical Chemistry, 10 Vorontsovo Pole, 105064 Moscow, Russian Federation, and ^bMaterials Chemistry, Uppsala University, Box 538, SE-75121, Uppsala, Sweden

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Key indicators: single-crystal X-ray study; $T = 583$ K; mean $\sigma(\text{e}-\text{O}) = 0.027$ Å; R factor = 0.042; wR factor = 0.103; data-to-parameter ratio = 12.5.

As a part of current systematic investigations of strontium tellurite, SrTeO₃, with particular emphasis on crystal chemistry and phase transitions, the structure of the γ phase has been determined at 583 K using a single-crystal analysis. Both structural and nonlinear optical measurements indicate a β - γ first-order phase transition temperature that is close to 563 K. The structure of the γ phase is monoclinic (C_2) and does not differ essentially from the α phase (C_2). Comparison of the α and γ structures shows that the main atomic shifts and tiltings are connected with Te4, Te5 and Te6 pyramids.

Related literature

Single crystals of SrTeO₃ (STO) were prepared by Sadovskaya (1984). Structural phase transitions of STO have been studied by X-ray powder diffraction by Ismailzade *et al.* (1979) and Simon *et al.* (1979), by neutron powder diffraction by Dityatiev *et al.* (2006), and by second harmonic generation by Libertz & Sadovskaya (1980). The temperature dependence of physical properties of STO was analysed by Yamada & Iwasaki (1972, 1973), Yamada (1975) and Kudzin *et al.* (1988). For related literature, see: Antonenko *et al.* (1982); Avramenko *et al.* (1984); Kudzin *et al.* (1982); Zavodnik *et al.* (2007a,b).

Experimental

Crystal data

SrTeO ₃	$V = 2190.4$ (8) Å ³
$M_r = 263.22$	$Z = 24$
Monoclinic, C_2	Ag $K\alpha$ radiation
$a = 28.262$ (6) Å	$\mu = 12.04$ mm ⁻¹
$b = 5.935$ (1) Å	$T = 583$ (2) K
$c = 15.434$ (3) Å	$0.24 \times 0.22 \times 0.09$ mm
$\beta = 122.21$ (3)°	

Data collection

Enraf–Nonius CAD-4 diffractometer	2285 independent reflections
Absorption correction: analytical (Alcock, 1970)	1156 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.141$, $T_{\max} = 0.389$	$R_{\text{int}} = 0.079$
2335 measured reflections	3 standard reflections
	frequency: 60 min
	intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	183 parameters
$wR(F^2) = 0.103$	1 restraint
$S = 0.94$	$\Delta\rho_{\max} = 2.51$ e Å ⁻³
2285 reflections	$\Delta\rho_{\min} = -2.18$ e Å ⁻³

Data collection: *CAD-4-PC* (Enraf–Nonius, 1993); cell refinement: *CAD-4-PC*; data reduction: *CAD-4-PC*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2042).

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¹ On the thermal evolution of the crystal structure of SrTeO₃. Part III.

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The γ -phase of SrTeO₃ at 583 K

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Comment

Although ferroelectric STO has been under intensive investigation for a long time (Yamada & Iwasaki, 1972, 1973; Simon *et al.*, 1979; Libertz & Sadovskaya, 1980, Antonenko *et al.*, 1982; Kudzin *et al.*, 1988) there is still no a complete understanding of its rich polymorphism. Recently, in the two first papers of the present series the structures of α and β phases of STO were published (Zavodnik *et al.*, 2007a, 2007b). The purpose of this communication is to report on the structure of γ -phase. There is a number of experimental studies of physical properties near the reversible first order β - γ phase transition (Libertz & Sadovskaya, 1980; Kudzin *et al.*, 1982, 1988, Sadovskaya, 1984). All the measured constants exhibit abrupt changes, a small thermal hysteresis and a remarkably discontinuous volume change were found (Ismailzade *et al.*, 1979, Simon *et al.*, 1979, Dityatiev *et al.*, 2006). At 563 K the second harmonic generation (SHG) signal appeared, reflecting a transition to the noncentrosymmetric structure. The value of the spontaneous polarization along [010] polar axis was estimated as 0.037 c/m² at 585 K (Yamada & Iwasaki, 1972, 1973). It was determined (Sadovskaya, 1984, Kudzin *et al.*, 1988) that β - γ phase transition is connected with the formation and motion interfaces which are formed by crystallographic planes with indices (0 0 1) and (2 0 3). The peculiarities of the interface motion are the same as during the martensite transformation. No success was obtained in attempts to determine the γ -phase structure using X-ray and neutron powder diffraction (Simon *et al.*, 1979; Ismailzade *et al.*, 1979, Dityatiev *et al.*, 2006). Last investigator (Dityatiev *et al.*, 2006) believed that γ -STO at to be monoclinic *C2/c*. The polyhedral representation of γ -STO structure is presented on Figure 1. The current research indicates that γ -phase structure is supposed to be the same in many respects to α -phase structure. The Te—O bond lengths for Te3 and Te6 cations are located at distances greater than 2.7 Å and do not contribute to the first coordination sphere of Te⁴⁺. Figure 2 illustrates a comparison of α and γ -STO structures. The main atomic shifts and tiltings are connected with Te4, Te5 and Te6 pyramids while the maximum these values were observed for Te5 (O5 α -O5 γ 0.93 Å, O5 α -Te5—O5 γ 28.4°). It is not unreasonable to ask why the α and γ -phases separated by β -phase are structurally same. Full determination of the absolute configuration of γ -phase awaits the additional measurements and provides the means for tackling this important question. The relationship between the structures of the different phases will be describe later.

Experimental

The single crystals of STO were grown by Czochralski technique as described earlier (Libertz & Sadovskaya, 1980; Avramenko *et al.*, 1984). The products were characterized in a scanning electron microscope (Jeol 820) with an energy-dispersive spectrometer (LINK AN10000), confirming the presence and stoichiometry of Sr and Te. SHG measurements showed that there is no a symmetry centre in γ -phase which is stable between 563 K and 633 K with small thermal hysteresis (near 5 K). This conclusion is in a full agreement with the results of Libertz & Sadovskaya (1980). A special Enraf–Nonius mini-heater based on a goniometer head was used. The tested single-crystal was maintained by a special high-temperature silicate-based glue. The temperature interval of existence of the γ -phase was controlled by well calibrated thermocouple and with help of an appearance (or vanishing) of superstructural reflections (for example, (021) diffraction peak).

Refinement

The structure of STO was solved by the direct method in space group C2 where the atomic coordinates of all Sr and Te cations were found. The O atoms were localized by difference Fourier maps. The selection of space group C2 for description of crystal structure of γ -phase STO was based on the experimental data of second harmonic generation (SHG) obtained on tested single crystals. The temperature dependence of SHG signal confirms that the structure of γ -phase STO is non-centrosymmetric with the polar axis along (010) direction. The choice of the portion of reciprocal space ($k > 0$), used in our experiments results from the constructional features of high-temperature equipment. Secondly, the data collection of two equivalent sets of reflections was used for a performance evaluation of empirical absorption correction because the *HABIT-US* of tested single-crystal was very far from a proper polyhedral shape. Absorption coefficient for used crystal is very high ($\mu=12.3 \text{ mm}^{-1}$ for Ag-radiation and $\mu=22.8 \text{ mm}^{-1}$ for Mo-radiation). We were unable to rely on the possibility to fix the effect of anomalous scattering using Ag-radiation because the maximum value Δf for Te cations is equal to -1.212 (only 2.3%). Several additional experiments at 583 K on Mo-radiation were performed (as a supplementary to our experiment on Ag-radiation) using the identical single crystals with a significantly less size because of very strong absorption. In this case the maximum value of Δf for Sr cations is equal to -1.657 (4.5%). The absolute configuration of this phase was determined making use of anomalous scattering. For these additional data collections, the special modifications of Enraf–Nonius mini-heater were made in order to determine the intensities of Friedel pairs (hkl) and ($-h-k-l$). For the experiment with best accuracy the following results were obtained: 1857 non-zero reflections including the Friedel pairs, the agreement factors- 0.041 and 0.045, Flack parameters- 0.11 (3) and 0.72 (4) for absolute and inverted structures, correspondingly. Precise X-ray diffraction study of single crystals at high temperatures is a challenging task because there is usually only a small number of measured X-ray reflections in the data and they cover a rather limited range of $\sin\theta/\lambda$. The thermal vibration parameters for oxygen anions were very high and strongly anisotropic. It was difficult to use an anisotropic approximation in these high-temperature refinements because the ratio of statistically reliable reflections to a number of refined parameters was very far from an optimal value. A positive definite refinements with anisotropic atomic displacement parameters were impossible for O atoms at 583 K. It was a main reason why the oxygen atoms were refined isotropically. A special attention must be given to the accuracy of interatomic distances of Te—O which are not rather similar as in the case of room temperature experiment for α -phase (Zavodnik *et al.*, 2007a). But all these Te—O bond lengths can be found acceptable if we take into account the standard deviation. For polar space group C2 the origin was fixed along the polar b axis in least square refinements. The highest residual electron density peak is located 0.92 \AA from atom Te6 and the deepest hole is located 0.74 \AA from atom O22. Several atoms (Te4, Te5, Sr6, O12, O42 and O52) have increased isotropic atomic displacement parameters. These atoms are located inside significant voids which are larger than the voids for the rest of the atoms. The same peculiarity was also observed for the α - and β -STO structures. At the heating of γ -phase there is structural phase transition $C2 \rightarrow C2/m$ and at 583 K some indicators on the mirror plane m are remarkable.

Figures

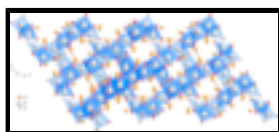


Fig. 1. The crystal structure of γ -SrTeO₃ at 583 K. The sequence of Sr polyhedra are presented, Te cations occupy two different kinds of voids in a three-dimensional lattice.

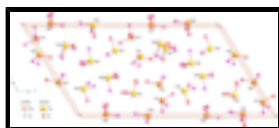


Fig. 2. A comparison of crystal structure of α and γ phases of STO. The TeO₃ units are shown. The Sr positions have been omitted for clarity.

strontium tellurite

Crystal data

SrTeO ₃	$F_{000} = 2736$
$M_r = 263.22$	$D_x = 4.789 \text{ Mg m}^{-3}$
Monoclinic, <i>C2</i>	Ag <i>K</i> α radiation
Hall symbol: <i>C 2y</i>	$\lambda = 0.56086 \text{ \AA}$
$a = 28.262 (6) \text{ \AA}$	Cell parameters from 24 reflections
$b = 5.935 (1) \text{ \AA}$	$\theta = 12.3\text{--}14.5^\circ$
$c = 15.434 (3) \text{ \AA}$	$\mu = 12.04 \text{ mm}^{-1}$
$\beta = 122.21 (3)^\circ$	$T = 583 (2) \text{ K}$
$V = 2190.4 (8) \text{ \AA}^3$	Prism, colourless
$Z = 24$	$0.24 \times 0.22 \times 0.09 \text{ mm}$

Data collection

Enraf–Nonius CAD-4 with high-temperature device diffractometer	$R_{\text{int}} = 0.079$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 20.0^\circ$
Monochromator: β-filter	$\theta_{\text{min}} = 2.1^\circ$
$T = 583(2) \text{ K}$	$h = -30 \rightarrow 34$
$\omega/2\theta$ scans	$k = -7 \rightarrow 0$
Absorption correction: analytical (Alcock, 1970)	$l = -15 \rightarrow 18$
$T_{\text{min}} = 0.141$, $T_{\text{max}} = 0.389$	3 standard reflections
2335 measured reflections	every 60 min
2285 independent reflections	intensity decay: none
1156 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2]$
$wR(F^2) = 0.103$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 0.94$	$\Delta\rho_{\text{max}} = 2.51 \text{ e \AA}^{-3}$
2285 reflections	$\Delta\rho_{\text{min}} = -2.18 \text{ e \AA}^{-3}$
183 parameters	Extinction correction: SHELXL97, $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
1 restraint	Extinction coefficient: 0.00036 (5)

supplementary materials

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Te1	-0.01952 (6)	0.4326 (9)	0.14806 (10)	0.0371 (4)
Te2	0.49454 (5)	0.4367 (8)	0.65532 (10)	0.0286 (4)
Te3	0.11356 (5)	-0.0611 (7)	0.27897 (10)	0.0267 (4)
Te4	0.35558 (6)	-0.0645 (9)	0.22906 (13)	0.0434 (5)
Te5	0.14933 (6)	0.9420 (9)	-0.00044 (10)	0.0406 (4)
Te6	0.26226 (5)	0.4413 (7)	0.41764 (9)	0.0236 (3)
Sr1	0.12299 (7)	0.4497 (9)	0.42053 (14)	0.0296 (5)
Sr2	0.24724 (8)	0.4533 (9)	0.11004 (15)	0.0295 (5)
Sr3	0.24269 (9)	-0.0454 (11)	0.27598 (14)	0.0370 (6)
Sr4	0.37712 (8)	0.4159 (8)	0.39581 (16)	0.0282 (8)
Sr5	0.12480 (7)	0.4440 (12)	0.15394 (14)	0.0356 (6)
Sr6	0.0000	-0.079 (2)	0.0000	0.0601 (16)
Sr7	0.5000	0.9165 (19)	0.5000	0.0445 (15)
O11	0.0545 (8)	0.508 (4)	0.2171 (13)	0.048 (5)*
O12	-0.0152 (16)	0.145 (7)	0.108 (3)	0.133 (14)*
O13	-0.0485 (10)	0.573 (5)	0.0288 (17)	0.067 (7)*
O21	0.4447 (10)	0.656 (4)	0.5752 (18)	0.048 (7)*
O22	0.5460 (8)	0.527 (4)	0.6244 (14)	0.046 (5)*
O23	0.4556 (13)	0.202 (5)	0.564 (2)	0.065 (9)*
O31	0.1610 (9)	0.183 (4)	0.3309 (15)	0.037 (5)*
O32	0.0979 (7)	-0.011 (4)	0.1455 (11)	0.040 (5)*
O33	0.1708 (14)	-0.268 (6)	0.315 (2)	0.084 (10)*
O41	0.3210 (12)	-0.307 (5)	0.249 (2)	0.051 (8)*
O42	0.4061 (12)	0.010 (6)	0.363 (2)	0.103 (10)*
O43	0.3094 (11)	0.151 (5)	0.231 (2)	0.050 (8)*
O51	0.1802 (9)	0.719 (4)	0.1100 (16)	0.039 (5)*
O52	0.2047 (13)	1.015 (6)	-0.024 (2)	0.105 (11)*
O53	0.1681 (11)	1.195 (5)	0.0773 (19)	0.061 (8)*
O61	0.2331 (5)	0.418 (5)	0.2787 (9)	0.028 (3)*
O62	0.3166 (10)	0.657 (4)	0.4485 (18)	0.034 (6)*
O63	0.3064 (9)	0.190 (3)	0.4327 (16)	0.023 (5)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te1	0.0249 (6)	0.0491 (13)	0.0340 (7)	-0.001 (3)	0.0136 (6)	0.002 (3)
Te2	0.0245 (7)	0.0286 (10)	0.0334 (6)	-0.003 (2)	0.0160 (5)	0.001 (2)
Te3	0.0261 (7)	0.0251 (9)	0.0321 (6)	0.008 (2)	0.0176 (5)	0.012 (2)
Te4	0.0353 (8)	0.0342 (11)	0.0720 (11)	-0.003 (3)	0.0361 (8)	-0.002 (3)
Te5	0.0302 (7)	0.0469 (11)	0.0319 (7)	0.003 (3)	0.0079 (6)	0.005 (2)
Te6	0.0187 (5)	0.0240 (8)	0.0278 (6)	-0.004 (2)	0.0122 (5)	-0.004 (2)
Sr1	0.0267 (9)	0.0209 (13)	0.0326 (9)	-0.008 (2)	0.0099 (7)	-0.002 (2)
Sr2	0.0266 (9)	0.0217 (14)	0.0423 (10)	0.005 (2)	0.0197 (8)	0.002 (2)
Sr3	0.0384 (10)	0.0375 (17)	0.0323 (9)	0.001 (3)	0.0169 (8)	-0.002 (3)
Sr4	0.0218 (8)	0.024 (2)	0.0374 (9)	-0.0008 (14)	0.0151 (8)	0.0041 (15)
Sr5	0.0261 (9)	0.0453 (16)	0.0329 (9)	0.011 (3)	0.0141 (8)	0.010 (3)
Sr6	0.0311 (15)	0.077 (5)	0.0444 (17)	0.000	0.0016 (13)	0.000
Sr7	0.0217 (13)	0.062 (4)	0.0467 (16)	0.000	0.0161 (12)	0.000

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

Te1—O13	1.77 (2)	Sr4—O43	2.72 (3)
Te1—O11	1.827 (19)	Sr4—O21	2.78 (2)
Te1—O12	1.84 (4)	Sr5—O53 ^v	2.58 (3)
Te2—O21	1.83 (2)	Sr5—O51	2.59 (2)
Te2—O22	1.84 (2)	Sr5—O13 ^{vii}	2.59 (2)
Te2—O23	1.86 (3)	Sr5—O61	2.611 (12)
Te3—O31	1.84 (2)	Sr5—O11	2.66 (2)
Te3—O33	1.86 (4)	Sr5—O33 ⁱⁱⁱ	2.71 (3)
Te3—O32	1.886 (16)	Sr5—O32	2.79 (2)
Te4—O42	1.84 (3)	Sr5—O31	2.82 (2)
Te4—O43	1.84 (3)	Sr5—O32 ⁱⁱⁱ	3.31 (2)
Te4—O41	1.85 (3)	Sr6—O12	2.34 (4)
Te5—O53	1.81 (3)	Sr6—O12 ^{vii}	2.34 (4)
Te5—O52	1.84 (3)	Sr6—O32	2.496 (16)
Te5—O51	1.96 (2)	Sr6—O32 ^{vii}	2.496 (16)
Te6—O61	1.848 (12)	Sr6—O13 ^{viii}	2.65 (3)
Te6—O62	1.85 (2)	Sr6—O13 ^v	2.65 (3)
Te6—O63	1.88 (2)	Sr7—O42 ^{ix}	2.42 (3)
Sr1—O63 ⁱ	2.52 (2)	Sr7—O42 ⁱⁱⁱ	2.42 (3)
Sr1—O62 ⁱⁱ	2.52 (2)	Sr7—O23 ^{ix}	2.60 (3)
Sr1—O21 ⁱⁱ	2.61 (3)	Sr7—O23 ⁱⁱⁱ	2.60 (3)
Sr1—O31	2.68 (2)	Sr7—O22 ^{vi}	2.84 (2)
Sr1—O11	2.692 (18)	Sr7—O22	2.84 (2)
Sr1—O23 ⁱ	2.79 (3)	Sr7—O21	2.85 (3)
Sr1—O33 ⁱⁱⁱ	3.10 (4)	Sr7—O21 ^{vi}	2.85 (3)
Sr2—O52 ^{iv}	2.37 (3)	O13—Sr5 ^{vii}	2.59 (2)

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Sr2—O51	2.47 (2)	O13—Sr6 ⁱⁱⁱ	2.65 (3)
Sr2—O41 ⁱⁱⁱ	2.49 (3)	O21—Sr1 ⁱ	2.61 (3)
Sr2—O43	2.51 (3)	O22—Sr4 ^{vi}	2.44 (2)
Sr2—O53 ^v	2.53 (3)	O23—Sr7 ^v	2.60 (3)
Sr2—O61	2.844 (13)	O23—Sr1 ⁱⁱ	2.79 (3)
Sr2—O52 ^v	3.14 (3)	O32—Sr5 ^v	3.31 (2)
Sr3—O63	2.53 (2)	O33—Sr5 ^v	2.71 (3)
Sr3—O43	2.61 (3)	O33—Sr1 ^v	3.10 (4)
Sr3—O51 ^v	2.61 (2)	O41—Sr2 ^v	2.49 (3)
Sr3—O33	2.75 (4)	O41—Sr4 ^v	2.55 (3)
Sr3—O61	2.77 (3)	O42—Sr7 ^v	2.42 (3)
Sr3—O41	2.91 (3)	O51—Sr3 ⁱⁱⁱ	2.61 (2)
Sr3—O62 ^v	2.94 (2)	O52—Sr2 ^x	2.37 (3)
Sr3—O53 ^v	3.00 (3)	O52—Sr2 ⁱⁱⁱ	3.14 (3)
Sr3—O31	3.16 (2)	O53—Sr2 ⁱⁱⁱ	2.53 (3)
Sr3—O61 ^v	3.20 (3)	O53—Sr5 ⁱⁱⁱ	2.58 (3)
Sr4—O22 ^{vi}	2.44 (2)	O53—Sr3 ⁱⁱⁱ	3.00 (3)
Sr4—O41 ⁱⁱⁱ	2.55 (3)	O61—Sr3 ⁱⁱⁱ	3.20 (3)
Sr4—O62	2.67 (3)	O62—Sr1 ⁱ	2.52 (2)
Sr4—O23	2.67 (3)	O62—Sr3 ⁱⁱⁱ	2.94 (2)
Sr4—O42	2.68 (4)	O63—Sr1 ⁱⁱ	2.52 (2)
Sr4—O63	2.71 (2)		
O13—Te1—O11	104.0 (10)	O22 ^{vi} —Sr4—O62	130.8 (7)
O13—Te1—O12	99.3 (15)	O41 ⁱⁱⁱ —Sr4—O62	74.3 (9)
O11—Te1—O12	99.4 (14)	O22 ^{vi} —Sr4—O23	85.3 (8)
O21—Te2—O22	92.8 (11)	O41 ⁱⁱⁱ —Sr4—O23	165.8 (9)
O21—Te2—O23	95.1 (9)	O62—Sr4—O23	107.0 (8)
O22—Te2—O23	104.6 (12)	O22 ^{vi} —Sr4—O42	80.6 (9)
O31—Te3—O33	94.2 (12)	O41 ⁱⁱⁱ —Sr4—O42	121.4 (9)
O31—Te3—O32	92.5 (9)	O62—Sr4—O42	148.2 (9)
O33—Te3—O32	95.2 (12)	O23—Sr4—O42	65.0 (9)
O42—Te4—O43	86.8 (14)	O22 ^{vi} —Sr4—O63	165.1 (7)
O42—Te4—O41	99.3 (13)	O41 ⁱⁱⁱ —Sr4—O63	109.1 (8)
O43—Te4—O41	95.5 (10)	O62—Sr4—O63	62.3 (5)
O53—Te5—O52	87.6 (14)	O23—Sr4—O63	83.3 (8)
O53—Te5—O51	98.4 (11)	O42—Sr4—O63	85.9 (8)
O52—Te5—O51	107.6 (12)	O22 ^{vi} —Sr4—O43	105.5 (8)
O61—Te6—O62	98.4 (10)	O41 ⁱⁱⁱ —Sr4—O43	75.5 (6)
O61—Te6—O63	86.5 (10)	O62—Sr4—O43	110.3 (8)
O62—Te6—O63	96.4 (8)	O23—Sr4—O43	116.1 (9)
O63 ⁱ —Sr1—O62 ⁱⁱ	78.2 (6)	O42—Sr4—O43	55.8 (8)
O63 ⁱ —Sr1—O21 ⁱⁱ	126.5 (8)	O63—Sr4—O43	71.3 (8)

O62 ⁱⁱ —Sr1—O21 ⁱⁱ	73.2 (8)	O22 ^{vi} —Sr4—O21	78.7 (7)
O63 ⁱ —Sr1—O31	117.1 (7)	O41 ⁱⁱⁱ —Sr4—O21	109.0 (8)
O62 ⁱⁱ —Sr1—O31	73.7 (7)	O62—Sr4—O21	68.4 (8)
O21 ⁱⁱ —Sr1—O31	96.9 (8)	O23—Sr4—O21	60.0 (6)
O63 ⁱ —Sr1—O11	135.2 (7)	O42—Sr4—O21	122.2 (8)
O62 ⁱⁱ —Sr1—O11	141.5 (8)	O63—Sr4—O21	103.7 (8)
O21 ⁱⁱ —Sr1—O11	92.0 (7)	O43—Sr4—O21	174.4 (8)
O31—Sr1—O11	73.2 (6)	O53 ^v —Sr5—O51	74.9 (7)
O63 ⁱ —Sr1—O23 ⁱ	84.5 (8)	O53 ^v —Sr5—O13 ^{vii}	89.6 (8)
O62 ⁱⁱ —Sr1—O23 ⁱ	122.2 (9)	O51—Sr5—O13 ^{vii}	78.3 (7)
O21 ⁱⁱ —Sr1—O23 ⁱ	74.4 (8)	O53 ^v —Sr5—O61	69.3 (7)
O31—Sr1—O23 ⁱ	156.7 (7)	O51—Sr5—O61	66.2 (7)
O11—Sr1—O23 ⁱ	85.4 (7)	O13 ^{vii} —Sr5—O61	142.1 (7)
O63 ⁱ —Sr1—O33 ⁱⁱⁱ	78.9 (8)	O53 ^v —Sr5—O11	151.6 (8)
O62 ⁱⁱ —Sr1—O33 ⁱⁱⁱ	119.7 (9)	O51—Sr5—O11	132.7 (7)
O21 ⁱⁱ —Sr1—O33 ⁱⁱⁱ	154.4 (8)	O13 ^{vii} —Sr5—O11	90.3 (7)
O31—Sr1—O33 ⁱⁱⁱ	68.9 (6)	O61—Sr5—O11	123.2 (5)
O11—Sr1—O33 ⁱⁱⁱ	64.0 (7)	O53 ^v —Sr5—O33 ⁱⁱⁱ	132.1 (10)
O23 ⁱ —Sr1—O33 ⁱⁱⁱ	110.1 (10)	O51—Sr5—O33 ⁱⁱⁱ	77.3 (9)
O52 ^{iv} —Sr2—O51	124.7 (10)	O13 ^{vii} —Sr5—O33 ⁱⁱⁱ	121.8 (10)
O52 ^{iv} —Sr2—O41 ⁱⁱⁱ	85.8 (11)	O61—Sr5—O33 ⁱⁱⁱ	63.9 (9)
O51—Sr2—O41 ⁱⁱⁱ	85.7 (9)	O11—Sr5—O33 ⁱⁱⁱ	70.2 (9)
O52 ^{iv} —Sr2—O43	98.3 (11)	O53 ^v —Sr5—O32	66.9 (7)
O51—Sr2—O43	133.6 (9)	O51—Sr5—O32	141.8 (6)
O41 ⁱⁱⁱ —Sr2—O43	80.4 (8)	O13 ^{vii} —Sr5—O32	100.7 (7)
O52 ^{iv} —Sr2—O53 ^v	133.5 (10)	O61—Sr5—O32	99.2 (7)
O51—Sr2—O53 ^v	77.9 (7)	O11—Sr5—O32	85.3 (6)
O41 ⁱⁱⁱ —Sr2—O53 ^v	139.7 (9)	O33 ⁱⁱⁱ —Sr5—O32	129.7 (8)
O43—Sr2—O53 ^v	84.8 (9)	O53 ^v —Sr5—O31	96.5 (8)
O52 ^{iv} —Sr2—O61	157.2 (8)	O51—Sr5—O31	130.0 (6)
O51—Sr2—O61	64.2 (7)	O13 ^{vii} —Sr5—O31	151.6 (7)
O41 ⁱⁱⁱ —Sr2—O61	73.5 (8)	O61—Sr5—O31	64.8 (6)
O43—Sr2—O61	69.4 (8)	O11—Sr5—O31	71.4 (6)
O53 ^v —Sr2—O61	66.3 (7)	O33 ⁱⁱⁱ —Sr5—O31	73.0 (8)
O52 ^{iv} —Sr2—O52 ^v	83.7 (8)	O32—Sr5—O31	57.5 (5)
O51—Sr2—O52 ^v	120.4 (8)	O53 ^v —Sr5—O32 ⁱⁱⁱ	134.3 (7)
O41 ⁱⁱⁱ —Sr2—O52 ^v	153.1 (9)	O51—Sr5—O32 ⁱⁱⁱ	62.1 (6)
O43—Sr2—O52 ^v	76.7 (9)	O13 ^{vii} —Sr5—O32 ⁱⁱⁱ	68.2 (7)
O53 ^v —Sr2—O52 ^v	51.7 (9)	O61—Sr5—O32 ⁱⁱⁱ	104.0 (7)
O61—Sr2—O52 ^v	110.6 (8)	O11—Sr5—O32 ⁱⁱⁱ	71.0 (6)
O63—Sr3—O43	76.0 (8)	O33 ⁱⁱⁱ —Sr5—O32 ⁱⁱⁱ	53.7 (8)

supplementary materials

O63—Sr3—O51 ^v	176.9 (7)	O32—Sr5—O32 ⁱⁱⁱ	153.2 (6)
O43—Sr3—O51 ^v	100.8 (8)	O31—Sr5—O32 ⁱⁱⁱ	122.2 (6)
O63—Sr3—O33	106.8 (9)	O12—Sr6—O12 ^{vii}	111 (2)
O43—Sr3—O33	177.1 (10)	O12—Sr6—O32	78.8 (11)
O51 ^v —Sr3—O33	76.4 (8)	O12 ^{vii} —Sr6—O32	90.8 (11)
O63—Sr3—O61	57.4 (5)	O12—Sr6—O32 ^{vii}	90.8 (11)
O43—Sr3—O61	69.4 (7)	O12 ^{vii} —Sr6—O32 ^{vii}	78.8 (11)
O51 ^v —Sr3—O61	121.8 (6)	O32—Sr6—O32 ^{vii}	161.6 (12)
O33—Sr3—O61	112.7 (8)	O12—Sr6—O13 ^{viii}	150.5 (10)
O63—Sr3—O41	102.9 (7)	O12 ^{vii} —Sr6—O13 ^{viii}	90.9 (12)
O43—Sr3—O41	59.2 (6)	O32—Sr6—O13 ^{viii}	81.5 (7)
O51 ^v —Sr3—O41	75.1 (7)	O32 ^{vii} —Sr6—O13 ^{viii}	113.5 (7)
O33—Sr3—O41	118.9 (10)	O12—Sr6—O13 ^v	90.9 (12)
O61—Sr3—O41	128.3 (6)	O12 ^{vii} —Sr6—O13 ^v	150.5 (10)
O63—Sr3—O62 ^v	70.5 (4)	O32—Sr6—O13 ^v	113.5 (7)
O43—Sr3—O62 ^v	104.1 (8)	O32 ^{vii} —Sr6—O13 ^v	81.5 (7)
O51 ^v —Sr3—O62 ^v	110.4 (7)	O13 ^{viii} —Sr6—O13 ^v	77.1 (12)
O33—Sr3—O62 ^v	76.3 (9)	O42 ^{ix} —Sr7—O42 ⁱⁱⁱ	153.4 (18)
O61—Sr3—O62 ^v	127.8 (5)	O42 ^{ix} —Sr7—O23 ^{ix}	69.8 (10)
O41—Sr3—O62 ^v	65.2 (7)	O42 ⁱⁱⁱ —Sr7—O23 ^{ix}	92.6 (11)
O63—Sr3—O53 ^v	118.0 (7)	O42 ^{ix} —Sr7—O23 ⁱⁱⁱ	92.6 (11)
O43—Sr3—O53 ^v	74.3 (8)	O42 ⁱⁱⁱ —Sr7—O23 ⁱⁱⁱ	69.8 (10)
O51 ^v —Sr3—O53 ^v	60.8 (6)	O23 ^{ix} —Sr7—O23 ⁱⁱⁱ	98.5 (14)
O33—Sr3—O53 ^v	104.7 (9)	O42 ^{ix} —Sr7—O22 ^{vi}	132.3 (10)
O61—Sr3—O53 ^v	61.4 (6)	O42 ⁱⁱⁱ —Sr7—O22 ^{vi}	72.7 (10)
O41—Sr3—O53 ^v	106.3 (8)	O23 ^{ix} —Sr7—O22 ^{vi}	114.5 (7)
O62 ^v —Sr3—O53 ^v	170.0 (7)	O23 ⁱⁱⁱ —Sr7—O22 ^{vi}	130.4 (8)
O63—Sr3—O31	75.8 (6)	O42 ^{ix} —Sr7—O22	72.7 (10)
O43—Sr3—O31	127.9 (8)	O42 ⁱⁱⁱ —Sr7—O22	132.3 (10)
O51 ^v —Sr3—O31	106.5 (6)	O23 ^{ix} —Sr7—O22	130.4 (8)
O33—Sr3—O31	54.2 (7)	O23 ⁱⁱⁱ —Sr7—O22	114.5 (7)
O61—Sr3—O31	58.5 (5)	O22 ^{vi} —Sr7—O22	70.9 (8)
O41—Sr3—O31	171.2 (7)	O42 ^{ix} —Sr7—O21	110.7 (9)
O62 ^v —Sr3—O31	106.5 (6)	O42 ⁱⁱⁱ —Sr7—O21	84.0 (9)
O53 ^v —Sr3—O31	81.6 (7)	O23 ^{ix} —Sr7—O21	172.1 (11)
O63—Sr3—O61 ^v	124.0 (5)	O23 ⁱⁱⁱ —Sr7—O21	73.6 (7)
O43—Sr3—O61 ^v	121.9 (7)	O22 ^{vi} —Sr7—O21	71.4 (7)
O51 ^v —Sr3—O61 ^v	57.4 (6)	O22—Sr7—O21	55.7 (7)
O33—Sr3—O61 ^v	56.0 (8)	O42 ^{ix} —Sr7—O21 ^{vi}	84.0 (9)
O61—Sr3—O61 ^v	168.6 (5)	O42 ⁱⁱⁱ —Sr7—O21 ^{vi}	110.7 (9)
O41—Sr3—O61 ^v	63.1 (6)	O23 ^{ix} —Sr7—O21 ^{vi}	73.6 (7)

O62 ^v —Sr3—O61 ^v	54.1 (5)	O23 ⁱⁱⁱ —Sr7—O21 ^{vi}	172.1 (11)
O53 ^v —Sr3—O61 ^v	118.0 (6)	O22 ^{vi} —Sr7—O21 ^{vi}	55.7 (7)
O31—Sr3—O61 ^v	110.2 (5)	O22—Sr7—O21 ^{vi}	71.4 (7)
O22 ^{vi} —Sr4—O41 ⁱⁱⁱ	83.5 (8)	O21—Sr7—O21 ^{vi}	114.3 (11)

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

Fig. 1

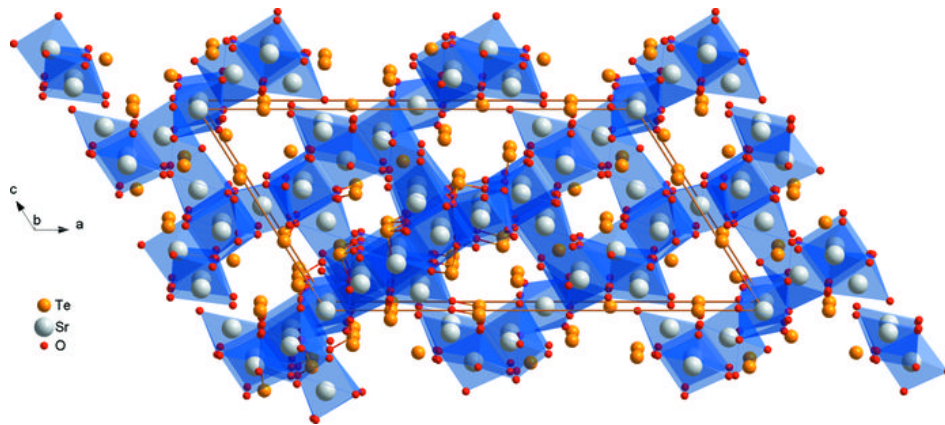


Fig. 2

