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$SrSeO_3$ from a combined X-ray and neutron powder diffraction study

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Key indicators: powder neutron study; T = 295 K; mean σ(Se–O) = 0.004 Å; R factor = 0.064; wR factor = 0.082.

Strontium trioxoselenate(IV), $SrSeO_3$, crystallizes in the $KClO_3$ structure type and is isotypic with $BaSeO_3$, β-$PbSeO_3$ and the mineral scotlandite ($PbSO_3$). The Sr^{2+} cation is nine-coordinated by O atoms. The SrO_9 polyhedra are linked together by common edges to form a three-dimensional network, with channels running along the b axis where the Se^{4+} cations reside. They are coordinated by three O atoms to form one-sided SeO_3E pyramids (E = electron lone pair), with Se—O bond lengths of 1.672 (6) and 1.688 (3) Å (× 2). The SeO_3E pyramids are not connected to each other; instead, they share O atoms with the SrO_9 polyhedra. Except for one O atom, all other atoms (one Sr, one Se and the second O atom) are located on mirror planes.

Related literature

For precipitation of $SrSeO_3$ from aqueous solutions, see: Contineánu (1994); Fatu *et al.* (2003). The structure of $SrSeO_3$ is unrelated to that of the polymorphic $SrTeO_3$ (Yamada & Iwasaki, 1972; Elerman, 1993; Dityatiev *et al.*, 2006; Zavodnik *et al.*, 2007*a*,*b*), but crystallizes in the $KClO_3$ structure type (Danielsen *et al.* 1981). It is isotypic with $BaSeO_3$ (Giester & Lengauer, 1998), β-$PbSeO_3$ (Koskenlinna & Valkonen, 1977) and $PbSO_3$ (Pertlik & Zemann, 1985). The results of the present powder diffraction study are nearly the same as those of the independent single-crystal study of $SrSeO_3$ (Wildner & Giester, 2007). For structures of the MTeO$_3$ (M = Ca, Ba) homologues, see: Kocak *et al.* (1979); Folger (1975).

Experimental

Crystal data

$SrSeO_3$
M_r = 214.58
Monoclinic, $P2_1/m$
a = 6.5702 (4) Å
b = 5.4749 (3) Å
c = 4.4550 (3) Å
β = 107.419 (4)°
V = 152.90 (2) Å^3
Z = 2
Neutron radiation
λ = 1.59432 Å
μ = 0.02 mm^{-1}
T = 295 K
Specimen shape: cylinder
30 × 10 × 10 mm
Specimen prepared at ambient pressure
Specimen prepared at 473 K
Particle morphology: irregular, white

Data collection

D2b diffractometer at ILL, Grenoble
Specimen mounting: vanadium can
Specimen mounted in transmission mode
Scan method: step
Absorption correction: none
$2\theta_{min}$ = 5, 2°, $2\theta_{max}$ = 160°
Increment in 2θ = 0.05°

Refinement

R_p = 0.064
R_{wp} = 0.082
R_{exp} = 0.128
R_{F^2} = 0.093
S = 0.65
Excluded region(s): none
Profile function: CW Profile function number 2 with 18 terms. Profile coefficients for Simpson's rule integration of pseudo-Voigt function (Howard, 1982; Thompson *et al.*, 1987). 1(GU) = 89.779, 2(GV) = −57.381, 3(GW) = 105.091, 4(LX) = 20.389, 5(LY) = 0.000, 6(trns) = 0.000, 7(asym) = 12.8654, 8(shft) = 0.0000, 9(GP) = 0.000, 10(stec)= 0.00, 11(ptec)= 0.00, 12(sfec)= 0.00, 13(L11) = 0.000, 14(L22) = 0.000, 15(L33) = 0.000, 16(L12) = 0.000, 17(L13) = 0.000, 18(L23) = 0.000. Peak tails are ignored where the intensity is below 0.0005 times the peak. Aniso broadening axis 0.0 0.0 1.0
No. of reflections: 349
34 parameters
3 restraints
Preferred orientation correction: March–Dollase (Dollase, 1986), axis 1, ratio = 0.88823, h = 0.000, k = 1.000, l = 0.000. Preferred orientation correction range: Min = 0.83687, Max = 1.42785

Table 1
Selected geometric parameters (Å, °).

Sr1—O1^{i}	2.631 (6)	Sr1—O2^{ii}	2.633 (4)
Sr1—O1^{ii}	3.022 (3)	Se1—O1^{iv}	1.672 (6)
Sr1—O2	2.670 (4)	Se1—O2	1.688 (3)
Sr1—O2^{iii}	2.694 (5)		
O1^{iv}—Se1—O2	101.88 (19)	O2—Se1—O2^{v}	99.61 (26)

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

Table 2
Unit-cell parameters for isotypic MXO_3 compounds (M = Ba or Pb; X = S or Se) and Se(S)—O bond lengths (Å, °).

Compound	a	b	c	β	Se(S)—O
$BaSeO_3$^{a}	4.677	5.645	6.851	107.16	1.690, 1.693 (× 2)
β-$PbSeO_3$^{b}	4.5737	5.5137	6.634	106.547	1.674, 1.729 (× 2)
Scotlandite^{c}	4.505	5.333	6.405	106.24	1.507, 1.529 (× 2)

References: (*a*) Giester & Lengauer (1998); (*b*) Koskenlinna & Valkonen (1977); (*c*) Pertlik & Zemann (1985).

Data collection: local program at ILL; cell refinement: *GSAS* (Larson & Von Dreele, 1987); data reduction: local program at ILL; method used to solve structure: coordinates taken from an isotypic compound (Giester & Lengauer, 1998); program(s) used to refine structure: *GSAS*; molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *GSAS*.

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doi:10.1107/S1600536807025135

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2114).

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supplementary materials

Acta Cryst. (2007). E**63**, i149-i150 [**doi:10.1107/S1600536807025135**]

$SrSeO_3$ from a combined X-ray and neutron powder diffraction study

O. A. Dityatiev, **P. Lightfoot**, **P. S. Berdonosov** and **V. A. Dolgikh**

Comment

Multinary Te(IV) and Se(IV) oxides have been extensively studied in recent decades due to their potential non-linear optical and ferroelectric properties. The first tellurate(IV) where ferroelectric properties have been discovered is $SrTeO_3$ (Yamada & Iwasaki, 1972). It is polymorphic and has a relatively complex crystal structure (Elerman, 1993; Dityatiev *et al.* 2006; Zavodnik *et al.*, 2007), and no analogous structures have been reported so far. The alkaline earth homologues $MTeO_3$ (M = Ca, Ba) adopt different structures (Kocak *et al.*, 1979; Folger, 1975), and the crystal structure of the selenium homologue $SrSeO_3$ has not been structurally characterized so far.

During the review process we were notified that more or less simultaneously with our study the crystal structure of $SrSeO_3$ was determined independently from single-crystal X-ray data. The results of the single-crystal study and a comparative discussion of isotypic and related compounds under consideration of a stereochemical equivalence of $ESeO_3$ groups and tetrahedral TO_4 groups will be published soon (Wildner & Giester, 2007). In comparison with the somewhat more precise single-crystal data, the results of the present powder diffraction study are essentially the same.

In the $SrSeO_3$ structure the Sr^{2+} cation is coordinated by seven nearest O atoms up to 2.694 (5) Å and two more distant O atoms at 3.022 (2) Å (Table 1), which results in a distorted monocapped square antiprism as coordination polyhedron. The SrO_9 polyhedra are linked together by common edges to form a three-dimensional network with channels running along b, where the Se^{4+} atoms are located (Fig. 1a). They are coordinated by three O atoms forming SeO_3E pyramids (E = electron lone pair; Fig. 1 b) with basal oxygen planes parallel to each other (Fig. 2). Each pyramid is linked to six SrO_9 polyhedra, sharing O—O edges with three SrO_9 polyhedra and oxygen vertices with another three Sr polyhedra (Fig. 1 b). The Se—O bonds are directed to opposite sides of the Sr–O network channels and act as additional links (Fig. 1a). The remaining "empty" volume of the channels accommodates the stereochemically active lone pairs of the Se^{4+} cations.

The structure of $SrSeO_3$ is unrelated to that of the heavier homologue $SrTeO_3$, but crystallizes in the $KClO_3$ structure type (Danielsen *et al.*, 1981) and is isotypic with $BaSeO_3$ (Giester & Lengauer, 1998), β-$PbSeO_3$ (Koskenlinna & Valkonen, 1977) and the mineral scotlandite ($PbSO_3$) (Pertlik & Zemann, 1985). All the MXO_3 (M = Pb, Ba; X = Se, S) compounds (Table 2) are built up of MO_9 polyhedra forming the network, with channels occupied by the lone-pair cations X^{4+}. The M—O bond lengths are shown in Fig. 3, which reflects the distortions of the corresponding polyhedra. For the selenates(IV), the M-O coordination may be considered as 7 (2.53– 2.87 Å) + 2 (3.02–3.04 Å). If the degree of deformation (Δ) is estimated as the difference between the longest and the shortest M—O bonds, for M = Ba and Sr Δ amounts to 0.392 and 0.326 Å, respectively, but for $PbSeO_3$ Δ is much larger (0.511 Å). The discrepancy may be explained by the presence of Pb^{2+} with its additional electron lone pair. On the other hand, for scotlandite Δ is 0.304 Å which is even smaller than that estimated for related alkaline earth selenites.

Experimental

Hot aqueous solutions of Na_2SeO_3 and $Sr(NO_3)_2$ (both chemically pure) were mixed in the stoichiometric ratio 1:1 which resulted in slow precipitation of a fine white powder. The product with the best crystallinity was obtained by mixing the hot solutions (acidified to pH $\simeq$ 1) and by subsequent slow neutralization with an aqueous solution of ammonia. The product was then repeatedly washed with hot water and decanted, and finally dried at 423–473 K.

The IR spectrum, recorded as a hexachlorobenzene suspension placed between two NaCl disks on a "Specord" spectrophotometer, showed no absorption bands in the 4000–2000 cm^{-1} region, thus ruling out incorporation of OH^- or water. Thermal analysis performed on a Perkin-Elmer TG7 derivatograph in air up to 1323 K showed absence of any phase transitions, oxidation or decomposition reactions.

Our results disagree with those given by Continéanu (1994) and Fatu *et al.* (2003) who obtained $SrSeO_3{\cdot}4.5H_2O$ under similar conditions. It is most likely that strontium selenate(IV) crystallizes from aqueous solutions as $SrSeO_3{\cdot}4.5H_2O$ at room temperature, but as anhydrous $SrSeO_3$ at about 373 K. Indeed, the sample precipitated at room temperature had a different X-ray pattern, however, with rather poor quality which prevented further X-ray studies.

Refinement

The X-ray data for structure determination were collected on a Stoe Stadi/P transmission system, using monochromatic Cu Kα1 radiation, over the range of 5–120°/2θ with a step size of 0.02°. Satisfactory *R* values (*R* = 18%) were found when the atomic parameters of the heavy atoms of the isotypic $BaSeO_3$ (Giester & Lengauer, 1998) were used as a starting model. However, we were not able to localize all oxygen atoms. Therefore we have supplemented our investigation with a neutron powder diffraction study which helped to refine the O atoms. The powder neutron diffraction data were collected on the high-flux powder diffractometer D2b at ILL, Grenoble. The $SrSeO_3$ sample was loaded into a vanadium can, and data were collected at 295 K for about 2 h. In the final refinement cycles, all atoms were refined with isotropic temperature factors. The March–Dollase model (Dollase, 1986) showed the [010] direction for preferred orientation with a ratio of 0.88. The final Rietveld refinement plot (neutron data) for $SrSeO_3$ is displayed in Fig. 4.

Figures

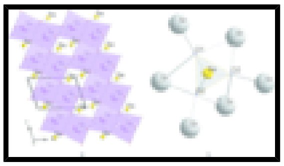


Fig. 1. The crystal structure of $SrSeO_3$: a) The network of SrO_9 polyhedra with the Se atoms located in the channels; b) The SeO_3E pyramid linked to the SrO_9 polyhedra.

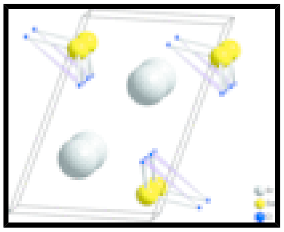


Fig. 2. Arrangement of the oxygen basal planes of the SeO_3 groups in $SrSeO_3$.

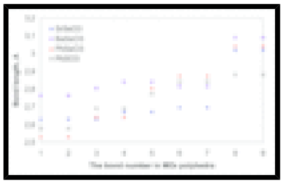


Fig. 3. The M—O distances in isotypic MXO_3 (M = Sr, Ba, Pb; X =Se, S) compounds.

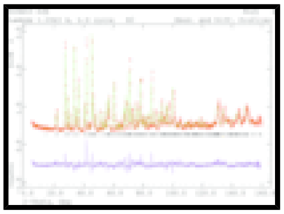


Fig. 4. Final Rietveld refinement plot for $SrSeO_3$ from neutron data.

Strontium trioxoselenate(IV)

Crystal data

$SrSeO_3$	D_x = 4.661 Mg m^{-3}
M_r = 214.58	Neutron radiation λ = 1.59432 Å
Monoclinic, $P2_1/m$	μ = 0.02 mm^{-1}
Hall symbol: -P 2yb	T = 295 K
a = 6.5702 (4) Å	Specimen shape: cylinder
b = 5.4749 (3) Å	30 × 10 × 10 mm
c = 4.4550 (3) Å	Specimen prepared at ambient kPa
β = 107.419 (4)°	Specimen prepared at 473 K
V = 152.90 (2) Å^3	Particle morphology: irregular, white
Z = 2	

Data collection

D2b at ILL diffractometer	T = 295 K
Specimen mounting: vanadium can	$2\theta_{min}$ = ?, $2\theta_{max}$ = ?°
Specimen mounted in transmission mode	Increment in 2θ = ?°
Scan method: step	

Refinement

Least-squares matrix: full	Profile function: CW Profile function number 2 with 18 terms Profile coefficients for Simpson's rule integration of pseudovoigt function (Howard, 1982; Thompson *et al.*, 1987). #1(GU) = 89.779 #2(GV) = -57.381 #3(GW) = 105.091 #4(LX) = 20.389 #5(LY) = 0.000 #6(trns) = 0.000 #7(asym) = 12.8654 #8(shft) = 0.0000 #9(GP) = 0.000 #10(stec)= 0.00 #11(ptec)= 0.00 #12(sfec)= 0.00 #13(L11) = 0.000 #14(L22) = 0.000 #15(L33) = 0.000 #16(L12) = 0.000 #17(L13) = 0.000 #18(L23) = 0.000 Peak tails are ignored where the intensity is below 0.0005 times the peak Aniso. broadening axis 0.0 0.0 1.0

R_{p} = 0.064

R_{wp} = 0.082

R_{exp} = 0.128

R_{B} = ?

S = 0.65

Wavelength of incident radiation: ? Å

Excluded region(s): none

34 parameters

3 restraints

? ?

$(\Delta/\sigma)_{\text{max}}$ = 0.03

Extinction correction: none

Preferred orientation correction: March–Dollase (Dollase, 1986) AXIS 1 Ratio = 0.88823 h = 0.000 k = 1.000 l = 0.000 Prefered orientation correction range: Min = 0.83687, Max = 1.42785

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sr1	0.7016 (5)	0.25	0.3473 (9)	0.0070 (8)*
Se1	0.1566 (5)	0.25	0.0639 (8)	0.0104 (7)*
O1	0.1081 (8)	0.25	0.6735 (11)	0.0220 (12)*
O2	0.3287 (4)	0.4855 (4)	0.1743 (8)	0.0078 (6)*

Geometric parameters (Å, °)

Sr1—O1$^{\text{i}}$	2.631 (6)	Sr1—O2$^{\text{v}}$	2.694 (5)
Sr1—O1$^{\text{ii}}$	3.022 (3)	Sr1—O2$^{\text{vi}}$	2.633 (4)
Sr1—O1$^{\text{iii}}$	3.022 (3)	Sr1—O2$^{\text{vii}}$	2.670 (4)
Sr1—O2	2.670 (4)	Se1—O1$^{\text{viii}}$	1.672 (6)
Sr1—O2$^{\text{iv}}$	2.694 (5)	Se1—O2	1.688 (3)
Sr1—O2$^{\text{ii}}$	2.633 (4)	Se1—O2$^{\text{vii}}$	1.688 (3)
O1$^{\text{ii}}$—Sr1—O1$^{\text{iii}}$	129.8 (2)	O2$^{\text{ii}}$—Sr1—O2$^{\text{vi}}$	66.72 (16)
O1$^{\text{ii}}$—Sr1—O2	141.34 (14)	O2$^{\text{ii}}$—Sr1—O2$^{\text{ix}}$	71.51 (13)
O1$^{\text{ii}}$—Sr1—O2$^{\text{iv}}$	53.94 (11)	O2$^{\text{v}}$—Sr1—O2$^{\text{vi}}$	113.49 (8)
O1$^{\text{ii}}$—Sr1—O2$^{\text{ii}}$	70.05 (11)	O2$^{\text{v}}$—Sr1—O2$^{\text{ix}}$	100.73 (13)
O1$^{\text{ii}}$—Sr1—O2$^{\text{v}}$	112.64 (14)	O2$^{\text{vi}}$—Sr1—O2$^{\text{ix}}$	102.35 (12)
O1$^{\text{ii}}$—Sr1—O2$^{\text{vi}}$	130.92 (16)	Sr1—Se1—O1$^{\text{viii}}$	103.7 (2)
O1$^{\text{ii}}$—Sr1—O2$^{\text{ix}}$	84.61 (11)	Sr1—Se1—O2	49.98 (13)
O1$^{\text{iii}}$—Sr1—O2	84.61 (11)	Sr1—Se1—O2$^{\text{ix}}$	49.98 (13)
O1$^{\text{iii}}$—Sr1—O2$^{\text{iv}}$	112.64 (14)	O1$^{\text{viii}}$—Se1—O2	101.88 (19)
O1$^{\text{iii}}$—Sr1—O2$^{\text{ii}}$	130.92 (16)	O1$^{\text{viii}}$—Se1—O2$^{\text{ix}}$	101.88 (19)
O1$^{\text{iii}}$—Sr1—O2$^{\text{v}}$	53.94 (11)	O2—Se1—O2$^{\text{ix}}$	99.61 (26)
O1$^{\text{iii}}$—Sr1—O2$^{\text{vi}}$	70.05 (11)	Sr1$^{\text{x}}$—O1—Sr1$^{\text{ii}}$	110.12 (11)
O1$^{\text{iii}}$—Sr1—O2$^{\text{ix}}$	141.34 (14)	Sr1$^{\text{x}}$—O1—Sr1$^{\text{iii}}$	110.12 (11)
O2—Sr1—O2$^{\text{iv}}$	100.73 (13)	Sr1$^{\text{x}}$—O1—Se1$^{\text{xi}}$	114.9 (3)
O2—Sr1—O2$^{\text{ii}}$	102.35 (12)	Sr1$^{\text{ii}}$—O1—Sr1$^{\text{iii}}$	129.8 (2)
O2—Sr1—O2$^{\text{v}}$	70.55 (11)	Sr1$^{\text{ii}}$—O1—Se1$^{\text{xi}}$	94.58 (14)
O2—Sr1—O2$^{\text{vi}}$	71.51 (13)	Sr1$^{\text{iii}}$—O1—Se1$^{\text{xi}}$	94.58 (14)

O2—Sr1—O2^{ix}	57.75 (12)	Sr1—O2—Sr1^{xii}	109.45 (11)
O2^{iv}—Sr1—O2^{ii}	113.49 (8)	Sr1—O2—Sr1^{iii}	108.49 (13)
O2^{iv}—Sr1—O2^{v}	65.02 (13)	Sr1—O2—Se1	101.06 (15)
O2^{iv}—Sr1—O2^{vi}	171.8 (2)	Sr1^{xii}—O2—Sr1^{iii}	113.49 (8)
O2^{iv}—Sr1—O2^{ix}	70.55 (11)	Sr1^{xii}—O2—Se1	106.80 (19)
O2^{ii}—Sr1—O2^{v}	171.8 (2)	Sr1^{iii}—O2—Se1	116.72 (17)

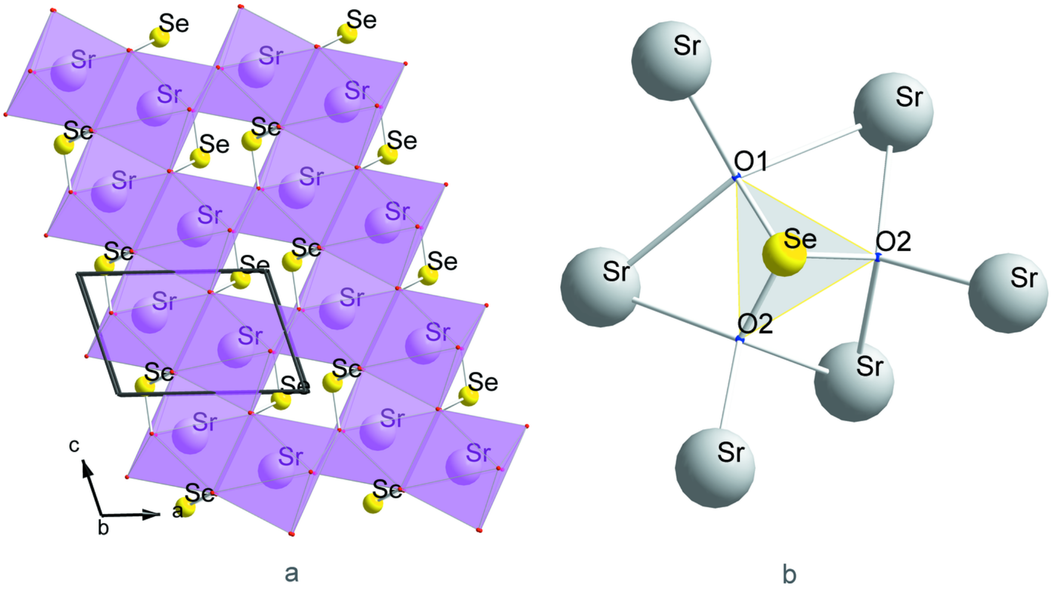
Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, *y*−1/2, −*z*+1; (iii) −*x*+1, *y*+1/2, −*z*+1; (iv) −*x*+1, *y*−1/2, −*z*; (v) −*x*+1, −*y*+1, −*z*; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) *x*, −*y*+1/2, *z*; (viii) *x*, *y*, *z*−1; (ix) *x*, −*y*+3/2, *z*; (x) *x*−1, *y*, *z*; (xi) *x*, *y*, *z*+1; (xii)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

The unit-cell parameters for isotypic MXO_3 compounds (M = Ba or Pb; X = S or Se) and the lengths of the Se(S)—O bonds (Å, °)

Compound	a	b	c	β	Se(S)—O
$BaSeO_3$[a]	4.677	5.645	6.851	107.16	1.690, 1.693 (× 2)
β-$PbSeO_3$[b]	4.5737	5.5137	6.634	106.547	1.674, 1.729 (× 2)
Scotlandite[c]	4.505	5.333	6.405	106.24	1.507, 1.529 (× 2)

Notes: (*a*) Giester & Lengauer (1998); (*b*) Koskenlinna & Valkonen (1977); (*c*) Pertlik & Zemann (1985).

Fig. 1



a

b

Fig. 2

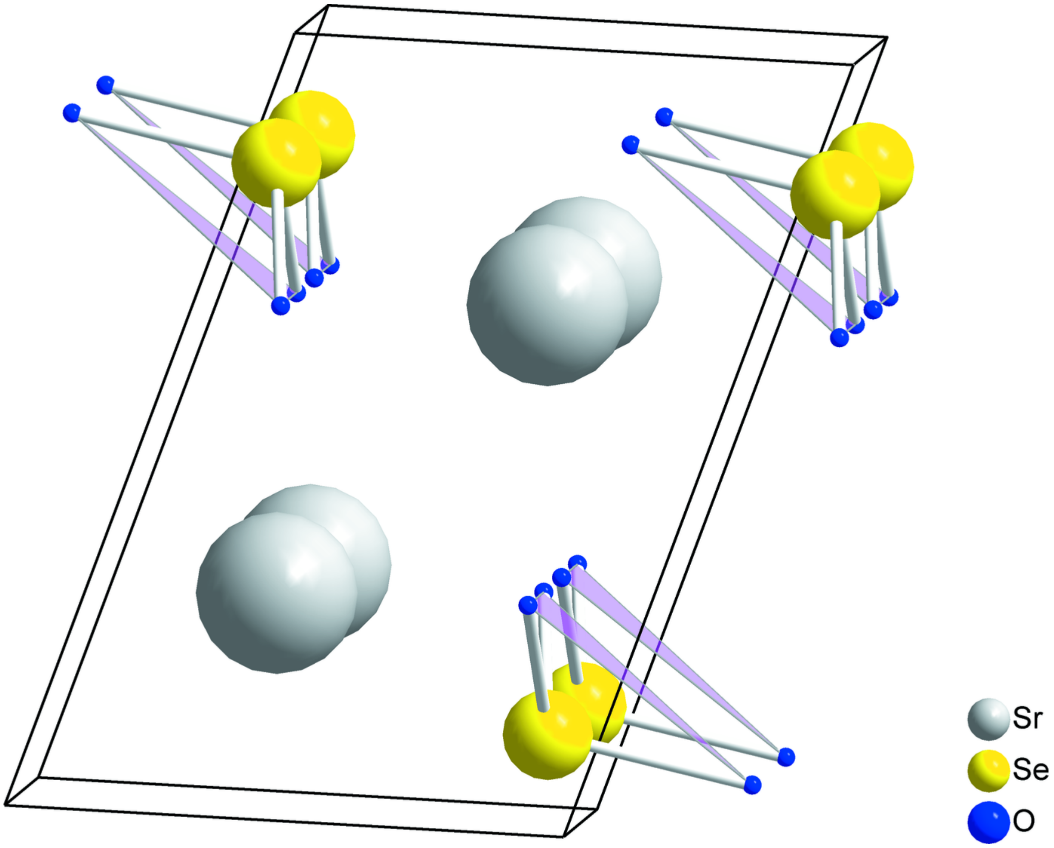


Fig. 3

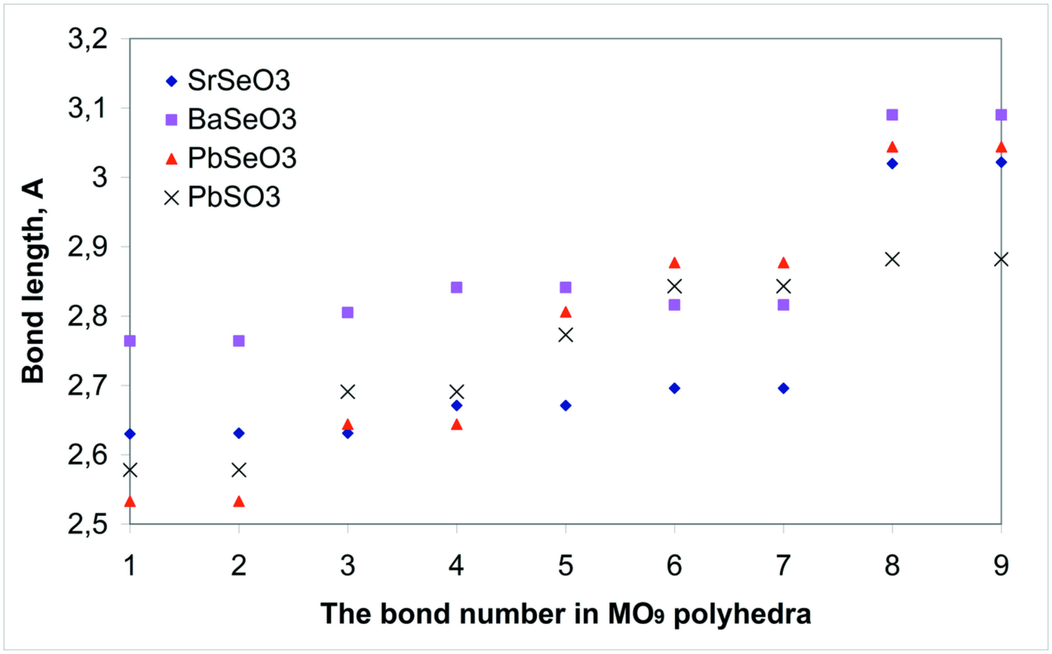
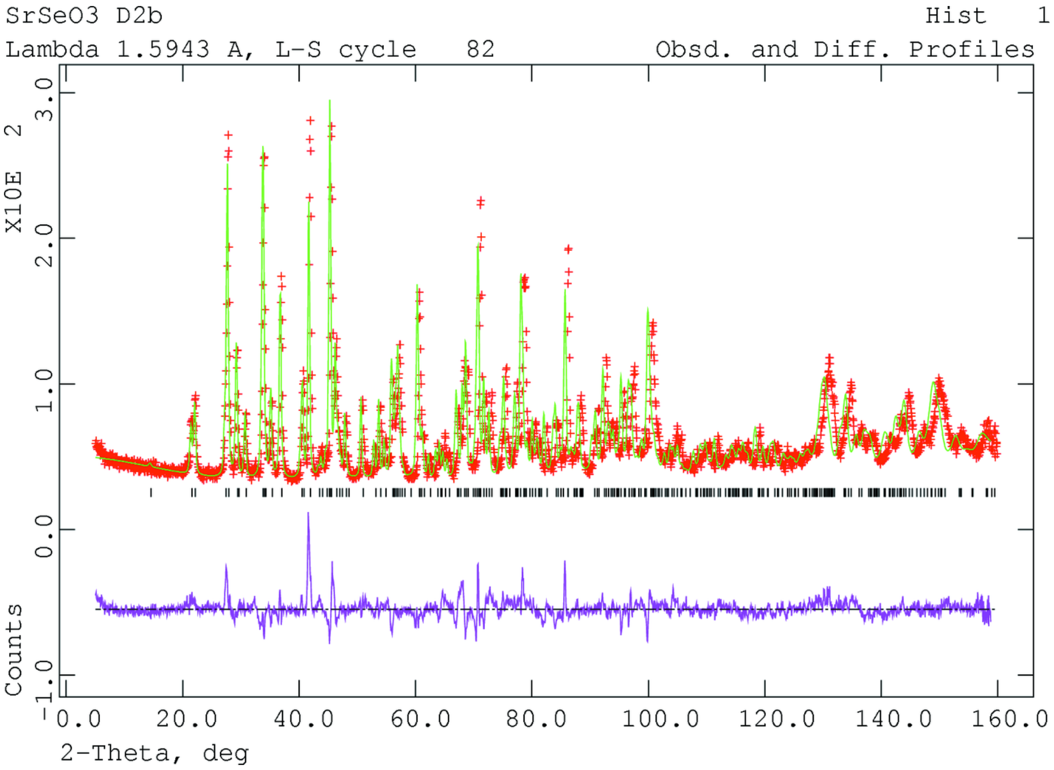

3,2
3,1
3
2,9
2,8
2,7
2,6
2,5
Bond length, A
1
2
3
4
5
6
7
8
9
The bond number in MO9 polyhedra
◆ SrSeO3
■ BaSeO3
▲ PbSeO3
× PbSO3

Fig. 4


SrSeO3 D2b
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Obsd. and Diff. Profiles
X10E 2
Counts
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0.0
-1.0
0.0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
2-Theta, deg