Lists of atomic coordinates, displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: BM1119). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Strontium Metasilicate, $SrSiO_3$

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Abstract

Strontium silicon trioxide has been synthesized for the first time and its structure solved. It is isostructural with the germanium analogue $SrGeO_3$ reported by Hilmer [*Sov. Phys. Crystallogr.* (1963), **7**, 573–576], but the true symmetry is monoclinic, rather than hexagonal as reported earlier. The structure has alternate layers of ternary rings of SiO_4 groups and close-packed Sr atoms stacked along [001]. Viewed as a polytype, this compound has a six-layer structure and the calcium analogue α-$CaSiO_3$ [Yamanaka & Mori (1981). *Acta Cryst.* B**37**, 1010–1017] has a four-layer structure.

Comment

The title compound has been synthesized for the first time. Dornberger-Schiff (1962) discussed the symmetry of the analogous germanium compound $SrGeO_3$. Hilmer (1963) studied the structure of $SrGeO_3$ using a Weissenberg camera. He obtained the hexagonal lattice parameters $a = 7.29$, $c = 31.64$ Å and showed that the structure contained ternary rings of GeO_4 groups. In addition, he concluded that the structure was composed of alternating layers of $[Ge_3O_9]^{6-}$ rings and layers of Sr atoms. Nadezhina, Pobedimskaya, Ilyukhin & Belov (1981*a*,*b*) also studied $SrGeO_3$ and obtained the triclinic lattice parameters $a = 8.699$, $b = 9.935$, $c = 11.148$ Å, $\alpha = 106.04$, $\beta = 89.97$, $\gamma = 102.11°$. This structure also contained rings of GeO_4 groups. The configurations of the rings, however, were somewhat different from those in the study by Hilmer, and Nadezhina *et al.* stated that the different types of ternary rings in the two modifications of strontium metagermanate were undoubtedly the result of a difference in the structures of the cation layers. In addition, they called the form they had studied the low-temperature form (α'-$SrGeO_3$) and the form studied by Hilmer the high-temperature form (α-$SrGeO_3$).

Ito (1950) and Buerger & Prewitt (1961) discussed the analogous calcium compound $CaSiO_3$ (the high-pressure form). Trojer (1969) obtained the triclinic lattice parameters $a = 6.695$, $b = 9.257$, $c = 6.666$ Å, $\alpha = 86.5$, $\beta = 76.13$, $\gamma = 70.38°$ and solved its structure. He concluded that the basic features of this structure were irregular layers of Ca atoms, which were interconnected by pairs of Ca atoms, and Si_3O_9 rings, which were located in the remaining space between the layers. Yamanaka & Mori (1981) studied the structure of α-$CaSiO_3$ (pseudowollastonite) from the viewpoint of polytypism. In their definition, a layer comprises one layer of the ternary rings plus one layer of CaO_8 polyhedra. They concluded that α-$CaSiO_3$ has a four-layer structure and the form of $SrGeO_3$ studied by Hilmer has a six-layer structure.

The symmetry of the title compound, $SrSiO_3$, was found to be different not only to that of the form of $SrGeO_3$ studied by Hilmer but also to that of the form of $SrGeO_3$ studied by Nadezhina *et al.* $SrSiO_3$, however, is almost isostructural with the form of $SrGeO_3$ studied by Hilmer for two reasons. Firstly, $SrSiO_3$ has a pseudo-hexagonal cell which corresponds to the cell given by Hilmer. Secondly, all of the reflections observed by Hilmer can be indexed on the basis of the present monoclinic cell. On the contrary, the structure of $SrGeO_3$ reported by Nadezhina *et al.* is different. It can be concluded that there are two forms of $SrGeO_3$, but only one form of $SrSiO_3$ is known so far.

The arrangement of the ternary rings of SiO_4 groups and SrO_8 polyhedra is shown in Fig. 1. The polyhedron around Sr(1) is very irregular, but that around Sr(2) can be regarded as a distorted hexagonal bipyramid, with O(1) on either side of the hexagon. The SrO_8 polyhedra form a close-packed layer like the olivine structure. The layers of the ternary rings of SiO_4 groups and the layers of SrO_8 polyhedra are shown in Fig. 2. They are stacked

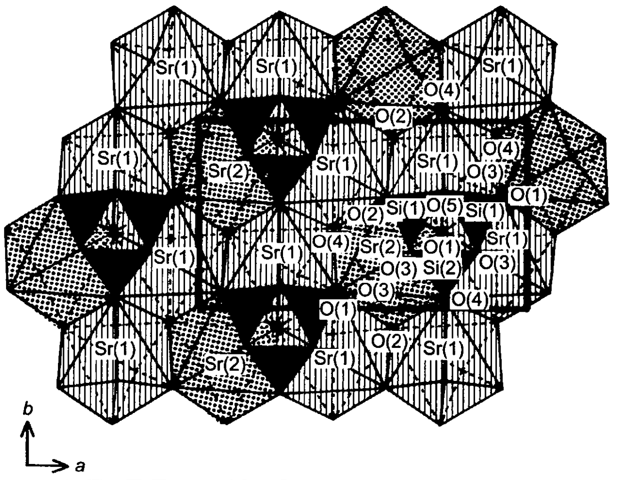

Fig. 1. The $SrSiO_3$ structure viewed along [001]. The arrangement of the Si_3O_9 rings (black triangles) at $z \simeq 3/4$ and the SrO_8 polyhedra [Sr(1) and Sr(2)] at $z \simeq \frac{1}{2}$ is shown.

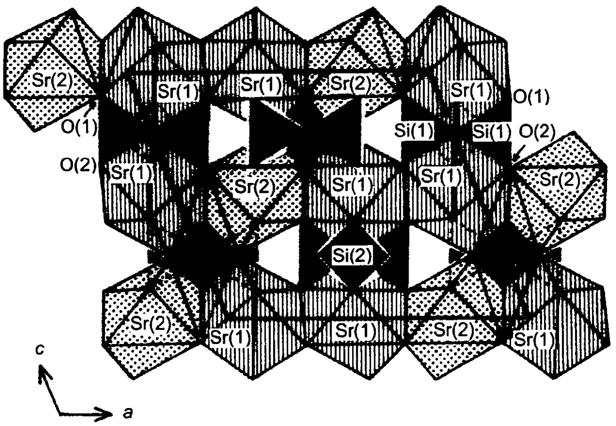

Fig. 2. The $SrSiO_3$ structure viewed down the *b* axis. The stacking of the layers of Si_3O_9 rings (black triangles and black squares) and SrO_8 polyhedra [Sr(1) and Sr(2)] is shown.

alternately along [001]. $SrSiO_3$ can be said to have a six-layer structure because the seventh layer is located just above the first along the stacking direction.

The Si—O—Si angles in the rings are 135.0 (6) and 135.6 (8)° (Table 2). These angles may be compared with those in other ternary rings of SiO_4 and GeO_4 groups, which lie within the ranges 122–124, 118.3–121.2 and 121.2 (4)–123.8 (5)° in the high-pressure form of $CaSiO_3$ (Trojer, 1969), α'-$SrGeO_3$ (Nadezhina *et al.*, 1981*a*,*b*) and $SrGe_4O_9$ (Nishi, 1996), respectively. The present values are distinctly larger and are close to those in α-$CaSiO_3$ (134.5–135.6°; Yamanaka & Mori, 1981) suggesting that $SrSiO_3$ contains the same kind of ternary rings as α-$CaSiO_3$. It is notable that α-$CaSiO_3$ has a four-layer structure and $SrSiO_3$ has a six-layer stucture, which raises the question of how many layers $Ca_xSr_{1-x}SiO_3$ ($0 < x < 1$) would contain. It is intended to clarify this problem in the near future.

Experimental

Single crystals of strontium metagermanate were synthesized from a stoichiometric mixture of $SrCl_2$ and SiO_2 at 1720 K. Electron microprobe analyses of the crystals showed that they had the chemical formula $SrSiO_3$.

Crystal data

$SrSiO_3$
$M_r = 163.71$
Monoclinic
$C2/c$
$a = 12.333\,(2)$ Å
$b = 7.146\,(1)$ Å
$c = 10.885\,(1)$ Å
$\beta = 111.57\,(1)°$
$V = 892.1\,(2)$ Å^3
$Z = 12$
$D_x = 3.67$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 33.15$–$34.10°$
$\mu = 16.32$ mm^{-1}
$T = 293$ K
Sphere
0.14 mm (radius)
Colourless

Data collection

Rigaku AFC-5 diffractometer
$\omega/2\theta$ scans
Absorption correction: spherical
$T_{min} = 0.141$, $T_{max} = 0.168$
2253 measured reflections
2029 independent reflections
1006 reflections with $I > 3\sigma(I)$

$R_{int} = 0.030$
$\theta_{max} = 35°$
$h = -19 \rightarrow 18$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 17$
3 standard reflections every 150 reflections intensity decay: 0.5%

Refinement

Refinement on F
$R = 0.056$
$wR = 0.067$
$S = 1.34$
1006 reflections
72 parameters
$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max} = 0.06$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Extinction correction: isotropic (Zachariasen, 1963)
Extinction coefficient: $3.1\,(4) \times 10^{-6}$
Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Sr(1)	0.0873 (1)	0.2396 (2)	0.4992 (2)	0.0051 (2)
Sr(2)	1/4	1/4	0	0.0050 (3)
Si(1)	0.1241 (3)	0.4574 (5)	0.2460 (4)	0.0031 (5)
Si(2)	0	0.8319 (7)	1/4	0.0035 (7)
O(1)	0.1272 (9)	0.4067 (15)	0.1045 (9)	0.0087 (15)
O(2)	0.2220 (8)	0.4059 (16)	0.3832 (11)	0.0102 (16)
O(3)	0.1072 (8)	0.6903 (13)	0.2495 (10)	0.0049 (13)
O(4)	0.0468 (8)	0.9342 (14)	0.3888 (9)	0.0069 (14)
O(5)	0	0.369 (2)	1/4	0.006 (2)

Table 2. *Selected geometric parameters (Å, °)*

Sr(1)—O(4$^{\rm i}$)	2.453 (11)	Sr(2)—O(4$^{\rm vii}$)	2.692 (9)
Sr(1)—O(2$^{\rm ii}$)	2.457 (9)	Sr(2)—O(4$^{\rm viii}$)	2.692 (9)
Sr(1)—O(5)	2.688 (5)	Sr(2)—O(2$^{\rm vii}$)	2.731 (12)
Sr(1)—O(3$^{\rm iii}$)	2.691 (11)	Sr(2)—O(2$^{\rm viii}$)	2.731 (12)
Sr(1)—O(4$^{\rm iv}$)	2.692 (11)	Si(1)—O(2)	1.580 (10)
Sr(1)—O(2)	2.703 (13)	Si(1)—O(1)	1.596 (12)
Sr(1)—O(1$^{\rm v}$)	2.739 (10)	Si(1)—O(5)	1.671 (7)
Sr(1)—O(1$^{\rm iii}$)	2.744 (11)	Si(1)—O(3)	1.679 (10)
Sr(2)—O(1)	2.471 (12)	Si(2)—O(4)	1.584 (10)
Sr(2)—O(1$^{\rm vi}$)	2.471 (12)	Si(2)—O(4$^{\rm v}$)	1.584 (10)
Sr(2)—O(3$^{\rm vii}$)	2.681 (9)	Si(2)—O(3)	1.666 (11)
Sr(2)—O(3$^{\rm viii}$)	2.681 (9)	Si(2)—O(3$^{\rm v}$)	1.666 (11)
O(2)—Si(1)—O(1)	125.3 (7)	O(4)—Si(2)—O(3)	105.8 (5)
O(2)—Si(1)—O(3)	105.5 (5)	O(4)—Si(2)—O(3$^{\rm v}$)	106.8 (6)
O(2)—Si(1)—O(5)	106.0 (5)	O(4$^{\rm v}$)—Si(2)—O(3)	106.8 (6)
O(1)—Si(1)—O(3)	107.1 (6)	O(4$^{\rm v}$)—Si(2)—O(3$^{\rm v}$)	105.8 (5)
O(1)—Si(1)—O(5)	106.7 (4)	O(3)—Si(2)—O(3$^{\rm v}$)	105.2 (6)
O(3)—Si(1)—O(5)	104.6 (7)	Si(2)—O(3)—Si(1)	135.0 (6)
O(4)—Si(2)—O(4$^{\rm v}$)	125.0 (6)	Si(1)—O(5)—Si(1$^{\rm v}$)	135.6 (8)

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

The intensities of the reflections were measured at the X-ray Laboratory of Nihon University, Japan.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992*a*). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1992*b*). Program(s) used to solve structure: *MITHRIL* (Gilmore, 1983) in *TEXSAN*. Program(s) used to refine structure: *LINUS* (Coppens & Hamilton, 1970). Program(s) used to calculate Fourier maps: *ORFFE* (Busing, Martin & Levy, 1964).

Lists of displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: TA1133). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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