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A powder diffraction study of $Sr_3Al_{10}SiO_{20}$

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Key indicators
Powder X-ray study
T = 293 K
Mean σ(Al–O) = 0.006 Å
R factor = 0.060
wR factor = 0.079

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In tristrontium decaaluminium silicon icosaoxide, $Sr_3Al_{10}SiO_{20}$, (Al,Si)O_4 tetrahedra and AlO_6 octahedra form a framework. Sr atoms occupy two large cavities of the framework. Sr2 and Al4 are on sites of $2/m$ symmetry, Al3 is on a twofold axis and Sr1 is on a mirror plane. The remaining Al and Si atoms are disordered over tetrahedral sites on general positions.

Comment

Al1 and Al2 are tetrahedrally coordinated with Si disordered over the two sites. These tetrahedra form six-membered rings in the *bc* plane which share corners with each other to form a chain parallel to the *c* axis. Individual chains are joined zigzag parallel to the *b* axis forming double layers by connecting the tetrahedra that point down in one chain with those that point up in the neighbouring chain. The Al3 and Al4 atoms are octahedrally coordinated. These octahedra share edges with each other and form a pillar parallel to the *c* axis. The pillars are separated from each other by the chains of six-membered rings and Sr2 atoms. The Sr atoms are inserted in cavities between the pillars and the chains and are arranged in columns parallel to the *c* axis. The Sr1 atoms are surrounded by one pillar and three chains and are coordinated by ten O atoms at an average Sr1—O distance of 2.881 (6) Å. The Sr2 atoms are surrounded by two pillars and two chains and are coordinated by eight O atoms at an average Sr2—O distance of 2.774 (7) Å. These distances are slightly longer than those of 2.67 (Sr1—O) and 2.70 Å (Sr2—O) found in $Sr_2Al_6O_{11}$, and 2.58 (Sr1—O) and 2.74 Å (Sr2—O) found in $Sr_4Al_{14}O_{21}$ (Smets *et al.*, 1989). The Al3—O distances (average 1.93 Å) are longer than the Al4—O distances (average 1.88 Å). The same effect can be seen in the case of $Sr_{1.33}Pb_{0.67}Al_6O_{11}$ (Plötz & Müller-Buschbaum, 1982) whose structure is the same as that of $Sr_2Al_6O_{11}$. In this compound, the Al—O distances in one of the octahedra are longer (average 1.93 Å) than those in the other (average 1.90 Å). In $Sr_2Al_6O_{11}$ and $Sr_4Al_{14}O_{21}$, the AlO_6 octahedra form walls parallel to the *bc* plane. In $Sr_2Al_6O_{11}$, (Al,Si)O_4 tetrahedra compose six-membered rings which are connected by sharing each corner and form walls parallel to the *bc* plane. On the other hand, in $Sr_4Al_{14}O_{21}$, there are no six-membered rings. In both compounds, Sr atoms are inserted in cavities between the tetrahedra and the walls formed by the octahedra.

Experimental

A powder specimen of $Sr_3Al_{10}SiO_{20}$ was obtained by solid-state reaction. The sample of $Sr_3Al_{10}SiO_{20}$ was prepared by mixing stoichiometric quantities of $SrCO_3$, SiO_2 and Al_2O_3 (Rare Metallic Co.,

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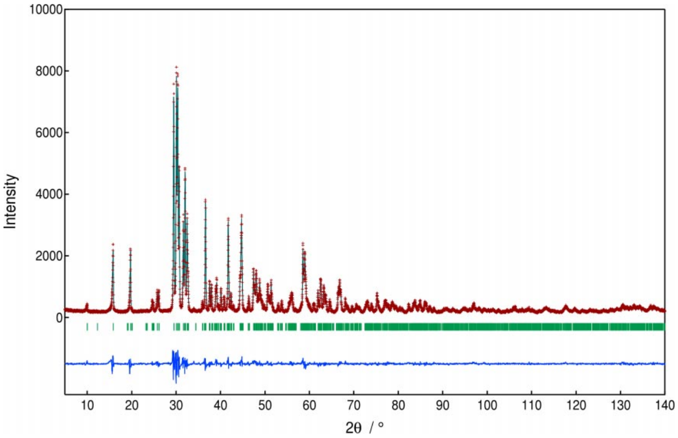

Figure 1
Comparison between the observed and calculated pattern and the difference curve.

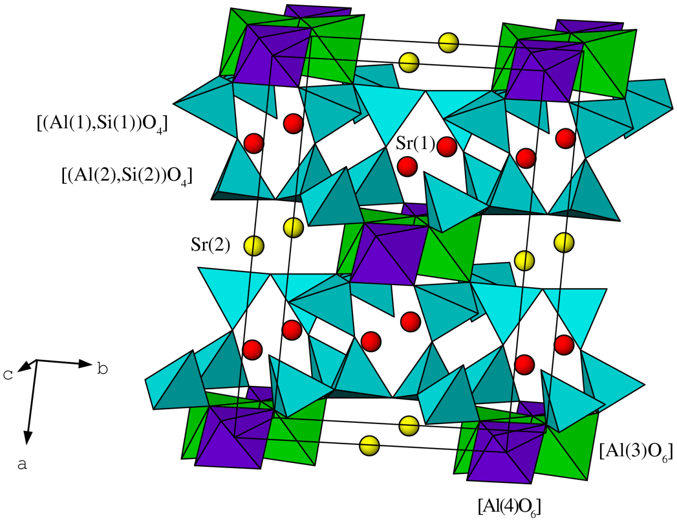

Figure 2
The structure of $Sr_3Al_{10}SiO_{20}$.

Ltd, purity >99.99%). A pressed pellet mixture was fired for 3 h at 1773 K, which is below the melting point, and quenched. The procedure was followed by regrinding, repelleting, and refiring twice.

Crystal data

$Sr_3Al_{10}SiO_{20}$
$M_r = 880.75$
Monoclinic, $C2/m$
$a = 15.1416\ (18)$ Å
$b = 11.1843\ (12)$ Å
$c = 4.9025\ (6)$ Å
$\beta = 108.117\ (5)^\circ$
$V = 789.06\ (16)$ Å^3
$Z = 2$

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
$\mu = 20.39\ \mathrm{mm}^{-1}$
$T = 293$ K
Specimen shape: flat sheet
20 × 25 × 0.5 mm
Specimen prepared at 1773 K
White powder

Data collection

Rigaku RINT2500V diffractometer
IMRAM, Tohoku University, Japan
Specimen mounted in reflection mode

$T = 293$ K
$2\theta_{\min} = 5$, $2\theta_{\max} = 140^\circ$
Increment in $2\theta = 0.02^\circ$

Refinement

Refinement on $I_{\rm net}$
$R_p = 0.0596$
$R_{\rm wp} = 0.0790$
$R_{\rm exp} = 0.0507$
Wavelength of incident radiation: 1.5418 Å

Profile function: pseudo–Voigt and Person 7 function
41 parameters
Weighting scheme based on measured s.u.'s
Preferred orientation correction: none

Table 1
Selected bond lengths (Å).

Sr1—O5	2.401 (8)	Al1—O3$^{\rm iv}$	1.749 (5)
Sr1—O2	2.686 (6)	Al2—O2	1.711 (6)
Sr1—O3$^{\rm i}$	2.740 (6)	Al2—O3	1.720 (6)
Sr1—O4$^{\rm ii}$	2.866 (6)	Al2—O6	1.732 (4)
Sr1—O2$^{\rm i}$	3.201 (6)	Al2—O1$^{\rm v}$	1.754 (6)
Sr1—O6	3.408 (8)	Al3—O4$^{\rm vi}$	1.908 (6)
Sr2—O6$^{\rm iii}$	2.540 (8)	Al3—O5	1.925 (5)
Sr2—O3$^{\rm iv}$	2.710 (6)	Al3—O1	1.957 (6)
Sr2—O6$^{\rm iv}$	3.137 (8)	Al4—O5	1.841 (8)
Al1—O4$^{\rm iv}$	1.710 (6)	Al4—O4$^{\rm iv}$	1.892 (5)
Al1—O2	1.728 (6)	Al4—O4$^{\rm vii}$	1.892 (5)
Al1—O1	1.734 (6)		

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

Diffraction data were obtained on a Rigaku RINT 2500V diffractometer system at 293 K. The Cu $K\alpha$ radiation was selected by means of a graphite monochromator. A system of diverging, anti-scattering and receiving slits of 0.5°, 0.5° and 0.15 mm, respectively, was used; two Soller slits were positioned both on the incident beam, before the divergent slit, and on the diffracted beam before the monochromator. In order to confirm the unit-cell parameters determined from the X-ray powder pattern, electron-diffraction patterns of $Sr_3Al_{10}SiO_{20}$ were recorded. The electron diffraction patterns were studied with a Jeol JEM-2000EX microscope (of Electron Microscope Laboratory of Tohoku University) operating at 200 kV. Fine powder specimens for electron microscopic observations were prepared by crushing the sintered products in an agate mortar. They were then mounted on collodion film meshes. Most of the electron-diffraction patterns could be indexed using the above lattice parameters.

Data collection: *RINT2500V Diffractometer Software* (Rigaku, 1995); cell refinement: *ITO* (Visser, 1969); data reduction: *RINT2500V Diffractometer Software*; program(s) used to solve structure: *EXPO* (Altomare *et al.*, 1994, 1995); program(s) used to refine structure: *Rietan* 2000 (Izumi & Ikeda, 2000); molecular graphics: *ATOMS* (Dowty, 1999); software used to prepare material for publication: *WORD*97.

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