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$Sr_3Al_{10}SiO_{20}$ from single-crystal data

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Single crystals of tristrontium decaaluminum silicon icosaoxide were synthesized by local flux growth with H_3BO_3 as mineralizer. Lattice parameters and refinement data indicate no significant incorporation of B in the structure. Pairs of AlO_6 octahedra are located between layers of edge-linked Al/Si–O_4 tetrahedra. The Sr1 (2/*m* symmetry) and Sr2 (mirror plane) sites are orientated in layers perpendicular to the layers of Al/Si–O polyhedra.

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(Al–O) = 0.002 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.032
Data-to-parameter ratio = 11.9

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

Comment

Recently, $Sr_3Al_{10}SiO_{20}$ doped with Tb, Eu or Eu/Ho was discovered to be a blue-emitting long-lasting phosphor for optical applications, such as TFT screens and LEDs (Kuang *et al.* 2005, 2006;Kubota & Shimada, 2002; Kubota *et al.*, 2002). $Sr_3Al_{10}SiO_{20}$ is isostructural with $Pb_3Al_{10}GeO_{20}$ (monoclinic, *C*2/*m;* Vinek *et al.*, 1970). The first structure refinement of $Sr_3Al_{10}SiO_{20}$ was performed by Kubota *et al.* (2001) using powder diffraction data by Rietveld refinement based on $Pb_3Al_{10}GeO_{20}$ by replacing Pb sites with Sr. In order to obtain a more precise structure determination, we synthesized single crystals of $Sr_3Al_{10}SiO_{20}$ (SR3). The published results from powder data agree very well with our single-crystal measure-

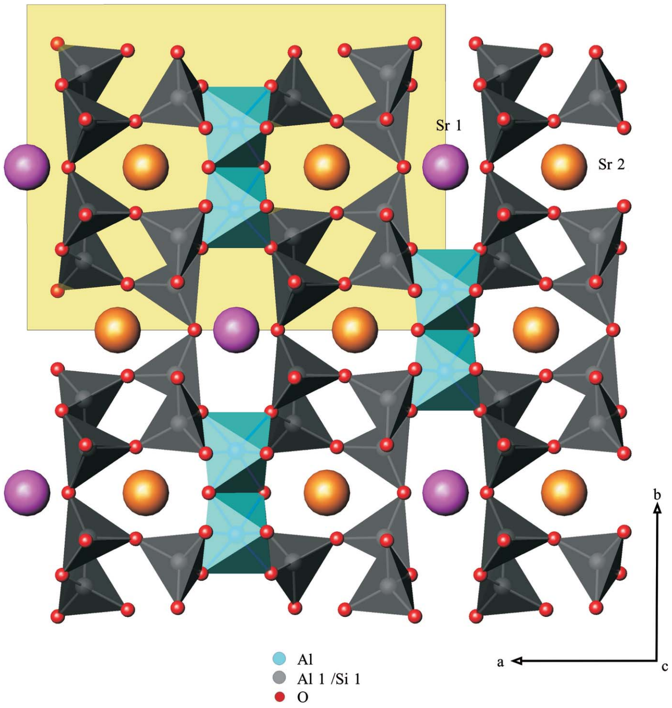

Figure 1
Pairs of Al octahedra (blue) and layers of mixed Al/Si tetrahedra (grey) building a three-dimensional framework, viewed down [001]. The yellow rectangle marks one unit cell.

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ments. The lattice parameters of the single crystal (see *Crystal data*) agree with the literature [a = 15.1416 (18), b = 11.1843 (12), c = 4.9026 (13) Å, β = 108.117 (5)° and V = 789.06 (16) Å^3; Kubota *et al.* 2001]. Capron *et al.* (2002) puplished a powder diffraction study with a refinement in space group $I2/m$ [a = 14.394 (2), b = 11.189 (2), c = 4.904 (1) Å, β = 90.793 (1)°, V = 789.74 Å^3]. The refinement of the structure model against single-crystal data was performed using *Xtal* 3.2 (Hall *et al.*, 1992) to a final R = 0.036. The good correlation between the powder and single-crystal data excludes any incorporation of B, even in small amounts. B tends to replace the tetravalent or octahedral Al position, and at least a reduction of the unit cell in the a-axis direction (due to deformations of the octahedral chains in this direction) should be observed.

A detailed description of the structure was reported by Kubota *et al.* (2001). The matrix is composed of corner-linked Al/Si tetrahedra arranged in layers along the c axis, connected to isolated pairs of edge-linked Al octahedra (see Fig. 1). These octahedra show distortion in all bond lengths and angles. Selected bond distances are given in Table 1. The averaged Al/Si—O bond distances are almost the same for both tetrahedral Al/Si positions [Al1/Si1—O 1.745 (6), Al2/Si2—O 1.737 (6) Å] and an identical substitution ratio is assumed. The occupancy factor for Si1,2 refined to 0.125 (subsequently set at this value) and is the same as is given in the literature. In the original $Pb_3Al_{10}GeO_{20}$ compound, all Al sites were substituted by a small amount (s.o.f. 0.091) of Ge.

Remarkable in this structure is the short distance between Sr1 and O5 of only 2.392 (3) Å; the sum of ionic radii for Sr^{2+} and O^{2-} is 2.58 Å (Shannon, 1976). Capron *et al.* (2002) report an even shorter Sr—O distance of 2.388 (8) Å. For Sr1, CN 12 and for Sr2, CN (4 + 4 + 4) is observed. The other Sr—O distances (Table 2) are within or longer than the range expected from the atomic radii [Sr(x)—O(y) > 2.68 Å].

Experimental

Single crystals were synthesized from well ground analytical $SrCO_3$, $Al(OH)_3$ (both Merck) and SiO_2 (Fluka) by adding 10% by weight of H_3BO_3 (Aldrich). The carefully homogenized mixture of educts was pressed into pellets and fired at 1723 K (180 K h^{-1}) in a corundum crucible for 24 h. The samples were slowly cooled down to room temperature with a cooling rate of 180 K h^{-1}. To improve yield and crystal growth, samples were crushed, refired and repelleted after 12 h of heating. The hard sintered pellets were crushed carefully in a mortar into smaller fragments. Under polarized light, microscopic crystals showing homogeneous extinction were separated and prepared for single-crystal measurements.

Crystal data

$Sr_3Al_{10}SiO_{20}$
M_r = 880.75
Monoclinic, $C2/m$
a = 15.1438 (18) Å
b = 11.1858 (13) Å
c = 4.9018 (6) Å
β = 108.137 (2)°
V = 789.09 (16) Å^3

Z = 2
D_x = 3.707 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 10.86 mm^{-1}
T = 298 K
Splinter, colourless
0.14 × 0.11 × 0.09 mm

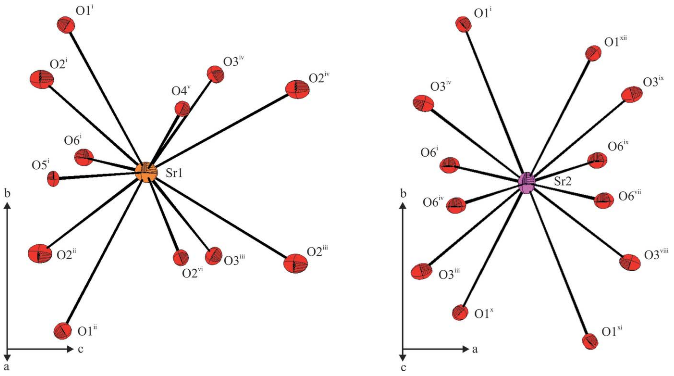

Figure 2
Coordination environments for Sr1 and Sr2. Symmetry codes: (i) $\frac{1}{2} + x, \frac{1}{2} + y, z$; (ii) $\frac{1}{2} + x, \frac{1}{2} - y, z$; (iii) $\frac{1}{2} + x, \frac{1}{2} - y, 1 + z$; (iv) $\frac{1}{2} + x, \frac{1}{2} + y, 1 + z$; (v) $1 - x, y, 1 - z$; (vi) $1 - x, 1 - y, 1 - z$; (vii) $\frac{3}{2} - x, \frac{1}{2} + y, 2 - z$; (viii) $\frac{3}{2} - x, \frac{1}{2} - y, 1 - z$; (ix) $\frac{3}{2} - x, \frac{1}{2} + y, 1 - z$; (x) $\frac{1}{2} + x, \frac{3}{2} - y, z$; (xi) $\frac{1}{2} - x, \frac{3}{2} - y$,-$z$; (xii) $\frac{1}{2} - x, \frac{1}{2} + y$,-$z$. Displacement ellipsoids are drawn at the 50% probability level.

Data collection

Siemens SMART APEX diffractometer
ω scans
Absorption correction: spherical (Tibballs, 1982)
T_{min} = 0.302, T_{max} = 0.318

4207 measured reflections
1261 independent reflections
1022 reflections with $I > 3\sigma(I)$
R_{int} = 0.033
θ_{max} = 30.5°

Refinement

Refinement on F
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.032
S = 1.70
1022 reflections

86 parameters
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.66 e Å^{-3}
$\Delta\rho_{min}$ = −1.15 e Å^{-3}

Table 1
Selected bond lengths (Å).

$Sr1^{i}$—$O5^{i}$	2.3932 (17)	$Sr1^{i}$—$O1^{i}$	3.4812 (14)
$Sr1^{i}$—$O2^{i}$	2.6832 (18)	$Sr2^{iv}$—$O6^{i}$	2.527 (2)
$Sr1^{i}$—$O3^{ii}$	2.7018 (15)	$Sr2^{iv}$—$O3^{v}$	2.6781 (16)
$Sr1^{i}$—$O4^{iii}$	2.8420 (16)	$Sr2^{iv}$—$O6^{vi}$	3.158 (3)
$Sr1^{i}$—$O2^{ii}$	3.1967 (18)	$Sr2^{i}$—$O1^{vii}$	3.5126 (14)
$Sr1^{i}$—$O6^{i}$	3.410 (3)		

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

The highest peak is located 0.00 Å from atom Sr2 and the deepest hole is located 1.02 Å from atom O5.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 1999); data reduction: *Xtal3*.2 (Hall *et al.*, 1992); program(s) used to solve structure: *Xtal3*.2; program(s) used to refine structure: *Xtal3*.2; molecular graphics: *Xtal3*.2; software used to prepare material for publication: *Xtal3*.2.

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