

**La<sub>4.67</sub>(SiO<sub>4</sub>)<sub>3</sub>O** [1], apatite family; Sm<sub>4.67</sub>(SiO<sub>4</sub>)<sub>3</sub>O [1]

Structural features: Infinite columns of base-linked LaO<sub>6</sub>O<sub>3</sub> tricapped trigonal prisms (partial vacancies ignored) share atoms with SiO<sub>4</sub> tetrahedra to form a 3D-framework; additional O (trigonal coordination) in infinite columns of face-linked La<sub>6</sub> octahedra parallel to [001]. See Fig. IV.66.

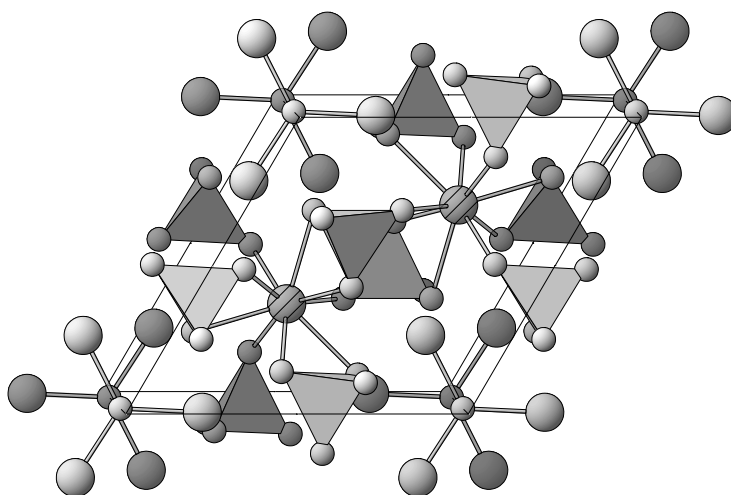


Fig. IV.66. **La<sub>4.67</sub>(SiO<sub>4</sub>)<sub>3</sub>O**

Arrangement of LaO<sub>6</sub>O<sub>3</sub> tricapped trigonal prisms (La atoms large hatched; partly occupied site), SiO<sub>4</sub> tetrahedra (O atoms small) and OLa<sub>3</sub> triangles (La atoms large).

Kuzmin E.A., Belov N.V. (1965) [1]

La<sub>4.67</sub>O<sub>13</sub>Si<sub>3</sub>

$a = 0.955$ ,  $c = 0.714$  nm,  $c/a = 0.748$ ,  $V = 0.5639$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12i	1	0.1	0.346	0.073		single atom Si
Si2	6h	$m..$	0.032	0.4	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
O3	6h	$m..$	0.124	0.592	$\frac{1}{4}$		single atom Si
La4	6h	$m..$	0.246	0.233	$\frac{1}{4}$		pentagonal bipyramid O <sub>7</sub>
O5	6h	$m..$	0.485	0.152	$\frac{1}{4}$		single atom Si
La6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0	0.833	tricapped trigonal prism O <sub>9</sub>
O7	2a	-6..	0	0	$\frac{1}{4}$		coplanar triangle La <sub>3</sub>

Transformation from published data: origin shift 0 0  $\frac{1}{2}$

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.113$

Remarks: Probably identical to the phase called monoclinic B-type La<sub>2</sub>O<sub>3</sub> in [2] and [3] (see a comparison of the powder patterns in [4]). In the reaction scheme on page 88 of [1] the chemical formula is misprinted as La<sub>4.33</sub>(SiO<sub>4</sub>)<sub>3</sub>O instead of La<sub>4.67</sub>(SiO<sub>4</sub>)<sub>3</sub>O (given elsewhere).

References: [1] Kuzmin E.A., Belov N.V. (1965), Dokl. Akad. Nauk SSSR 165, 88-90. [2] Daire M., Willer B. (1968), C. R. Seances Acad. Sci., Ser. C 266, 548-550. [3] Willer B., Daire M. (1969), Bull. Soc. Fr. Mineral. Cristallogr. 92, 33-37. [4] Kolitsch U., Seifert H.J., Aldinger F. (1995), J. Solid State Chem. 120, 38-42.