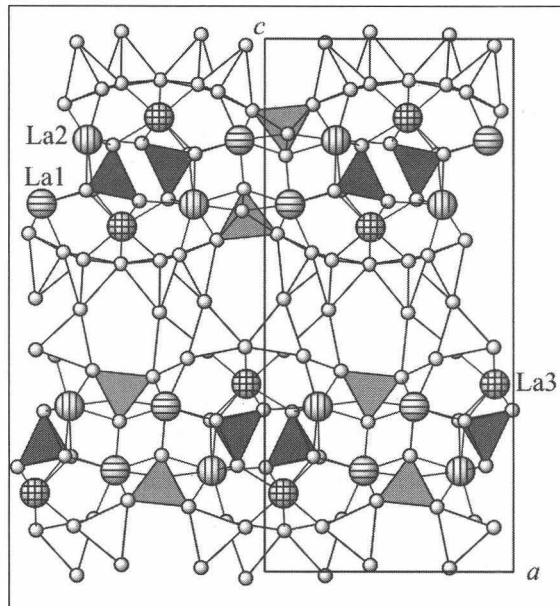


SYNTHETIC LaAlSiO_5 : A MIXED-ANION RARE EARTH ALUMOSILICATE

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The crystal structure of a new synthetic lanthanum alumosilicate with composition LaAlSiO_5 has been investigated using single crystal diffraction data collected at room conditions. LaAlSiO_5 crystallizes in the non-centrosymmetric orthorhombic space group $P2_12_12_1$ with twelve formula units per cell ($a = 11.0525(7) \text{ \AA}$, $b = 5.2261(3) \text{ \AA}$, $c = 23.7049(21) \text{ \AA}$, $V = 1369.2(3) \text{ \AA}^3$, $R(|F|) = 0.023$ for 2875 independent observed reflections) and belongs to the group of mixed anion alumosilicates. Basic building units are isolated $[\text{SiO}_4]$ groups as well as tetrahedral double layers of composition $[(\text{Al},\text{Si})_5\text{O}_{11}]$. The two single layers comprising a single double layer are related by 2_1 screw axes running along $[100]$. Each of these two layers can be thought of as being built from the condensation of unbranched as well as open-branched *zweier* single chains running parallel $[010]$. Therefore, the whole anion can be classified as a hybrid *zweier* double layer. Stacking of the layers parallel to $[001]$ results in the formation of a three-dimensional structure in which lanthanum cations and isolated SiO_4 -groups are incorporated for charge compensation. The three crystallographically independent La-atoms are coordinated by 7–8 oxygen ligands. Concerning the connectedness of tetrahedra in the structure of LaAlSiO_5 one singular (Q^0), one primary (Q^1) and four quaternary (Q^4) groups can be distinguished (cf. Figure 1).



Bond valence calculations were performed to obtain the Al/Si distributions for the symmetrically independent T-sites. Four out of six tetrahedra show a strong preference for either Al or Si, whereas the remaining two tetrahedral centers show a Al:Si ratio close to 1:1. Using the silicate classification procedure introduced by Liebau the structural formula of the present compound can be written as $\text{La}_3\{hB, 2_x^2\} [(\text{Al},\text{Si})_5\text{O}_{11}][\text{SiO}_4]$.

Figure 1
 Projection of the crystal structure of LaAlSiO_5 parallel $[010]$. White, medium and dark grey tetrahedra correspond to Q^0 , Q^1 and Q^4 units.