

Synthesis and crystal structure of the feldspathoid CsAlSiO₄: An open-framework silicate and potential nuclear waste disposal phase

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ABSTRACT

Crystalline CsAlSiO₄ was synthesized from a stoichiometric mixture of Al₂O₃ + SiO₂ + Cs₂O (plus excess water) in Ag-capsules at hydrostatic pressure of 0.1 GPa and temperature of 695 °C. The duration of synthesis was 46 h. The crystal structure of CsAlSiO₄ was investigated by single-crystal X-ray diffraction. The structure is orthorhombic with *Pc2₁n* space group and lattice parameters: *a* = 9.414(1), *b* = 5.435(1), and *c* = 8.875(1) Å. Because of the orthohexagonal relation between *b* and *a* (*a* ≈ *b*√3), within the standard uncertainty on the lattice parameters, a hexagonal superlattice exists, which is responsible for twinning. The crystals are twinned by reflection, with twin planes (110) and (310): twinning in both cases is by reticular merohedry with twin index 2 and hexagonal twin lattice (**L_T**). The transformation from the lattice of the individual (**L_{ind}**) to **L_T** is given by: **a_T** = **a_{ind}** – **b_{ind}**, **b_T** = 2**b_{ind}**, and **c_T** = **c_{ind}**. The refinement was initiated using the previously published atomic coordinates for RbAlSiO₄. The final least-square cycles were conducted with anisotropic displacement parameters. *R*₁ = 3.04% for 66 parameters and 2531 unique reflections. For a more reliable crystallographic comparison the crystal structure of RbAlSiO₄ is reinvestigated here adopting the same data collection and least-squares refinement strategy as for CsAlSiO₄.

The crystal structure of the CsAlSiO₄ feldspathoid is built on an ABW framework type, showing a fully ordered Si/Al-distribution in the tetrahedral framework. The only extra-framework site is occupied by Cs, lying off-center in the 8mR-channels. CsAlSiO₄ is more likely to retain Cs when immersed in a fluid phase, relative to several other Cs-bearing zeolites. The topological configuration of the Cs-polyhedron (and its bonding environment), the small dimension of the pores and the high flexibility of the ABW framework type would imply a better thermal and elastic stability of CsAlSiO₄ than those of the zeolitic Cs-aluminosilicates. In this light, CsAlSiO₄ can be considered as a functional material potentially usable for fixation and deposition of radioactive isotopes of Cs and can also be considered as a potential solid host for a ¹³⁷Cs γ-radiation source to be used in sterilization applications.

Keywords: CsAlSiO₄, RbAlSiO₄, ABW framework type, feldspathoid, crystal structure, nuclear waste disposal phase