

**Structural behavior, crystal chemistry, and phase transitions in substituted leucite:
High-resolution neutron powder diffraction studies**

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ABSTRACT

High-resolution neutron powder diffraction was used to study phase transitions in the leucite phases of KAlSi_2O_6 , $\text{RbAlSi}_2\text{O}_6$, $\text{CsAlSi}_2\text{O}_6$, and KFeSi_2O_6 . The temperature-dependent structural behavior involves two mechanisms: relaxation of the tetrahedral framework about channel cations, and slowly changing T-O bond lengths. The high-temperature cubic phase is characterized by a fully-extended tetrahedral framework; thermal expansion occurs by an increase in mean T-O bond lengths. On decreasing temperature, a displacive phase transition to tetragonal symmetry is manifested by an optic instability; twisting of tetragonal prisms of corner-linked $(\text{Al,Si})\text{O}_4$ tetrahedra about $[001]$ leads to collapse of the $\langle 111 \rangle$ structural channels and concomitant volume reduction.