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## **Lattice simulation studies of the ferroelastic phase transitions in (Na,K)AlSi<sub>3</sub>O<sub>8</sub> and (Sr,Ca)Al<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> feldspar solid solutions**

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### **ABSTRACT**

Lattice-energy minimization calculations have been performed on the feldspar systems (Ca,Sr)Al<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> and disordered (Na,K)AlSi<sub>3</sub>O<sub>8</sub> as functions of composition to simulate the ferroelastic phase transitions  $I2/c-I\bar{1}$  and  $C2/m-C\bar{1}$ , respectively. In both cases the phase transition occurs as a function of composition and is driven by the vanishing of the quantity  $C_{44}C_{66} - C_{46}^2$ , without any of the individual elastic constants being strongly dependent on composition and without softening of an optic mode. In both cases, the strains  $\epsilon_4$  and  $\epsilon_6$  are proportional to each other for small values of strain, but nonlinear coupling becomes dominant when  $|\epsilon_4|$  becomes larger than about 0.02. The results are consistent with experimental data and explain the nature of coupling of the displacive transition to Al-Si ordering in Al:Si 2:2 feldspars.