## Si-Al order and the *I*1-*I*2/*c* structural phase transition in synthetic CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>-SrAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> feldspar: A <sup>29</sup>Si MAS-NMR spectroscopic study

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## ABSTRACT

We present <sup>20</sup>Si MAS-NMR spectroscopic data for a series of synthetic feldspar samples along the join CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>-SrAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>, from which the composition dependence and coupling of order parameters describing Si-Al order and the triclinic-monoclinic displacive transition were determined. Spectra of SrAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> contain narrow peaks for the two crystallographic Si sites, plus additional peaks for Si having three and two Al nearest neighbors, indicating the presence of approximately 0.14 Al-O-Al linkages per formula unit and a value of  $\sigma = 0.93$  for the short-range order parameter. For the triclinic feldspar samples, short-range Si-Al order increases continuously with Sr content from  $\sigma = 0.89(3)$  for CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> to 0.97(1) for Sr<sub>0.85</sub>Ca<sub>0.15</sub>Al<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> to SrAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>. The variation of peak positions with composition is consistent with a structural phase transition near Sr<sub>0.85</sub>Ca<sub>0.15</sub> Al<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> from *I* 1 to *I2/c*. The order parameter for this displacive transition is reflected by the chemical shift of the T1mz crystallographic site, and its composition dependence gives an order-parameter critical exponent of  $\beta = 0.49(2)$ , indicating classical second-order behavior.