

## **Phase transitions induced by solid solution in stuffed derivatives of quartz: A powder synchrotron XRD study of the $\text{LiAlSiO}_4\text{-SiO}_2$ join**

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### **ABSTRACT**

The crystal structures of stuffed derivatives of quartz within the  $\text{Li}_{1-x}\text{Al}_{1-x}\text{Si}_{1+x}\text{O}_4$  system have been refined by Rietveld analysis of powder synchrotron X-ray diffraction (XRD) data. Our results reveal an Al-Si order-disorder transition at  $x = \sim 0.3$  and a  $\beta$ - $\alpha$  displacive transformation at  $x = \sim 0.65$ . Structural variations across the series result from an interplay of three mechanisms: tetrahedral tilting associated with Al-Si order-disorder; Li positional disorder along structural channels parallel to  $c$ ; and tetrahedral rotation related to the  $\beta$ - $\alpha$  transition. At both microscopic (local bonding) and macroscopic (spontaneous strain) scales, the substitution of  $\text{Li}^+$  and  $\text{Al}^{3+}$  for  $\text{Si}^{4+}$  closely mimics temperature in its effect on the quartz framework.