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X-ray study of the trigonal → hexagonal phase transition in metamorphic kalsilite

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ABSTRACT

High-temperature annealing experiments on metamorphic kalsilite ($KAlSiO_4$) indicate that there is an irreversible phase transition from the $P31c$ to $P6_3$ structure at ~200 °C. Powder X-ray investigations indicate that the transformation is incomplete. The proportion of $P6_3$ phase increases as a function of temperature, attaining 70% for the powdered sample at ~500 °C. At higher temperatures, the fraction of sample transforming to $P6_3$ phase seems to be independent of temperature, and probably depends on the structural state of the starting material as influenced by mechanical grinding. Transformation proceeds by tetrahedral rotation such that successive (001) sheets undergo opposite-sense rotations. The transition behavior differs for single crystals, which had not been mechanically ground; at 500 °C single crystals transformed completely into the $P6_3$ phase. Single-crystal structure refinements of the $P6_3$ phase indicate that the structure is similar to that of volcanic kalsilite. Both apical and basal O atoms show large anisotropic displacement parameters, but the displacement of the apical oxygen does not exhibit the trigonal distribution that has been observed in volcanic kalsilite. The more pronounced positional disorder in volcanic kalsilite is due to the presence of sodium.