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Low-temperature behavior of natural kalsilite with *P*31*c* symmetry: An in situ single-crystal X-ray diffraction study

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Abstract

The low-temperature behavior of a natural kalsilite (ideal formula $KAlSiO_4$) with *P*31*c* symmetry has been investigated by in situ single-crystal diffraction. A series of intensity data collections and structural refinements have been performed at 298, 250, 200, 150, and 100 K on decreasing temperature, and 175, 225, and 275 K on increasing *T*. The variations of the unit-cell parameters of kalsilite as a function of *T* are continuous, and show no evidence of any phase transitions or thermo-elastic anomalies in this temperature range. An expansion is observed along [0001] with decreasing temperature. The axial and volume thermal expansion coefficients ($\alpha_j = l_j^{-1} \cdot \partial l_j / \partial T$, $\alpha_V = V^{-1} \cdot \partial V / \partial T$) between 298 and 100 K, calculated by weighted linear regression through the data points, are $\alpha_a = \alpha_b = 1.30(6) \cdot 10^{-5}$, $\alpha_c = -1.5(1) \cdot 10^{-5}$, $\alpha_V = 1.1(2) \cdot 10^{-5}$ K^{-1}. The main structural change on decreasing temperature is a cooperative anti-rotation of tetrahedra forming the six-membered rings lying parallel to (0001). This tetrahedral rotation is coupled with a change in the distances between the extra-framework cations and the framework O atoms. A small decrease in the tetrahedral tilts perpendicular to [0001] is responsible for the negative thermal expansion along [0001]; the implications of these mechanisms for thermal expansion in nephelines and kalsilites are discussed.

Keywords: Kalsilite, feldspathoids, low temperature, single-crystal X-ray diffraction, thermal expansion