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High-pressure and low-temperature behaviour of trigonal kalsilite

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Kalsilite (ideal formula KAlSiO4) is a framework silicate belonging to the "feldspathoid group". Kalsilite occurs mainly in K-rich and silica under-saturated volcanic rocks and is usually associated with olivine, melilite, clinopyroxene, phlogopite, nepheline, and leucite. Kalsilite also occurs in metamorphic rocks. The tetrahedral framework of kalsilite is isotypic with tridymite. The thermo-elastic behavior and the structural evolution of a natural metamorphic kalsilite from the Punalur district in Kerala (southern India), with P31c symmetry and a K/Na molar ratio of ∼350, were investigated by in-situ single-crystal X-ray diffraction up to 7 GPa and down to 100K. At low-temperature, the variations of the unit-cell parameters are continuous, and show no evidence of any phase-transitions in this temperature range. An expansion is observed along [0001] with decreasing temperature. The axial and volume thermal expansion coefficients between 298 and 100K, calculated by weighted linear regression through the data points, are alpha(a)=alpha(b)=1.30(6)•10-5, alpha(c)= -1.5(1)•10-5, alpha(V)=1.1(2)•10-5 K-1. The main structural change on decreasing temperature is a cooperative anti-rotation of tetrahedra forming the 6-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 oxygens. A small decrease in the tetrahedra tilts perpendicular to [0001] is responsible for the negative thermal expansion along [0001]. At high-pressure, a first-order phase-transition is observed at about 3.5 GPa. The high-pressure polymorph maintains a metrically trigonal lattice. The elastic behavior of both the polymorphs was described with a 3rd-order Birch-Murnaghan Equation-of-State. Fitting the P-V data, the refined parameters are: V0=201.17(1)Å3, KT0= 59.7(5) GPa, K'=3.5(3) for the low-P polymorph, and V0=200.1(13)Å3, KT0= 44(8) GPa, K'=6.4(20) for the high-P polymorph. The pressure-induced structural evolution in kalsilite up to 7 GPa appears to be completely reversible.