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ABSTRACT BOOK

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Polymorphic behavior of leucite under high-pressure and high-temperature conditions: insights from synchrotron single-crystal diffraction

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Leucite, KAlSi_2O_6 , is a key mineral phase in K-rich mafic to ultramafic volcanic rocks, commonly classified among feldspathoids or zeolites. Due to its widespread occurrence in alkaline magmatic systems, a detailed understanding of its thermodynamic stability, and structural evolution across a range of pressure-temperature (P - T) conditions, is crucial for interpreting petrological processes at depth. The mineral's physical and chemical properties are intrinsically linked to its crystal structure and the way it responds to changing P - T conditions.

Leucite displays a well-known sequence of temperature-induced phase transitions: it crystallizes in a high-temperature cubic structure (space group $Ia\bar{3}d$), but, upon cooling between ~ 620 and 670 °C, it sequentially transforms into two lower symmetry tetragonal polymorphs ($I4_1/acd$ and subsequently $I4_1/a$), with the latter being the stable ambient form (Hatch et al., 1990). These transformations are accompanied by complex twinning phenomena, which are further influenced by compositional variations and thermal history (Lange et al., 1986; Hatch et al., 1990; Palmer et al., 1997).

Under high pressure and room temperature, previous work has shown that the $I4_1/a$ tetragonal form undergoes a first-order phase transition near 2.4 GPa to a denser, metrically triclinic polymorph, tentatively indexed in the P -1 space group (Gatta et al., 2008). In our study, we re-examined this high-pressure behavior and, for the first time, extended the investigation to simultaneous high-pressure and high-temperature conditions, using *in situ* single-crystal synchrotron X-ray diffraction at the beamlines P02.2 (PETRA III) and ID15B (ESRF).

Our experiments reveal a previously unreported polymorphic transition of leucite from the ambient tetragonal $I4_1/a$ structure to a trigonal polymorph (space group $R\bar{3}$) at pressures exceeding 2.2–2.5 GPa. Remarkably, this transition occurs both at room temperature and under heating, suggesting that compression kinetics may play a key role in stabilizing this new structural form. These findings underscore the complex polymorphism of leucite and highlight the need for accurate structural characterization to fully understand its stability fields under deep Earth conditions. Our results open new perspectives for modeling K-rich magmatic systems and their evolution under variable geodynamic settings.

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