Poster Presentation

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Petalite Under Pressure

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The lithium aluminosilicate mineral petalite ($LiAlSi_4O_{10}$) has been studied using high-pressure single-crystal X-ray diffraction up to 5 GPa. Petalite is a layered silicate mineral. The layers comprise puckered double-sheets of corner-sharing SiO_4 tetrahedra. Corner-sharing AlO_4 tetrahedra bridge neighboring layers and complete the 3D architecture. The charge is balanced by lithium cations that reside within channels that propagate through the structure. Petalite undergoes two pressure-induced phase transitions at ca. 1.5 and 2.5 GPa. The first of these transforms the low-pressure α-phase of petalite (P2/c) to an intermediate β' phase that then fully converts to the high-pressure β phase at ca. 2.5 GPa. The α→β transition is isomorphic with a commensurate modulation that triples the unit cell volume. Measurement of the unit cell parameters of petalite as a function of pressure, and fitting of the data with 3rd order Birch-Murnaghan equations of state, has provided revised elastic constants for petalite. The bulk moduli of the α- and β-phases are 49(1) and 35(3) GPa, respectively. These values indicate that petalite is one of the most compressible lithium aluminosilicate minerals. The α-phase structure has been refined at five different pressures, revealing a compression mechanism that is driven by the rigid body movement of the Si_2O_7 units from which the silicate double-layers are constructed. The structure of the β' phase was not determined. The structure of the β phase was determined at 2.71 GPa. Although the fundamental structural features of petalite are retained in the α → β phase transition, subtle alterations occur in the internal structure of the silicate double-layers.

Keywords: phase transition