

High-pressure behavior and structural transition of beryl-type johnkoivulaite, $\text{Cs}(\text{Be}_2\text{B})\text{Mg}_2\text{Si}_6\text{O}_{18}$

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ABSTRACT

The beryl-group mineral johnkoivulaite, $\text{Cs}(\text{Be}_2\text{B})\text{Mg}_2\text{Si}_6\text{O}_{18}$, was compressed hydrostatically in a diamond-anvil cell up to 10.2 GPa. In situ Raman spectroscopy and X-ray crystallography revealed a $P6/mcc$ -to- $P\bar{3}c1$ (second-order) phase transition on isothermal compression at the critical transition pressure $P_c = 4.13 \pm 0.07$ GPa. The elastic parameters determined for the volume elasticity of the two polymorphs correspond to a Birch-Murnaghan equation of state with $K_0 = 148 \pm 2$ GPa and $K' = 0$ for $P < P_c$ and $K_0 = 75.5 \pm 0.9$ GPa with $K' = 4$ for $P > P_c$. The low- P polymorph shows anomalously linear compression behavior, as reported for several other beryl-derived framework structures. The high- P polymorph, which was found to follow a $a' = a \cdot \sqrt{3}$, $c' = c$ superstructure according to $P\bar{3}c1$, is almost twice as compressible as its low- P form. This is unique for any beryl-derived structure and can be attributed to the high degree of freedom for atomic displacements in the superstructure. The reduced symmetry can also be understood as the effect of the driving mechanism of the transformation. The extra-framework Cs channel components counteract any lateral deformation of the channels parallel to [0001] within the microporous framework and, similar to pezzottaite, are responsible for maintaining the trigonal/hexagonal lattice metrics.

Keywords: Beryl-type structure, johnkoivulaite, high pressure, structural transition, second-order phase transition, superstructure; Microporous Materials: Crystal-chemistry, Properties, and Utilizations