

Equation of state and crystal structure of a new germanate post-titanite phase

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ABSTRACT

The compressibility and crystal structure of a recently discovered post-titanite phase of CaGe_2O_5 was investigated by single-crystal X-ray diffraction to 8.6 GPa at room temperature in a diamond-anvil cell. Unit-cell parameters decrease non-linearly with increasing pressure and do not show any discontinuity in the pressure range investigated. The unit-cell volume decreases by about 4.6% to 8.6 GPa. The P - V data were fit using a third-order Birch-Murnaghan equation of state giving the following coefficients: $V_0 = 345.65(4) \text{ \AA}^3$, $K_{T0} = 159(1) \text{ GPa}$, and $K' = 5.0(3)$. A parameterized form of the same equation of state was used to obtain the axial moduli for a , b , and c . The room-pressure ratios of axial compressibility are 2.64:1.00:1.42, indicating strong compression anisotropy, with b the stiffest direction and a the most compressible one. The crystal-structure data confirm that no change in symmetry occurs at high-pressure. Most of the compression to 8.6 GPa is accommodated by the CaO_8 and GeO_5 polyhedra, with reductions in volume of 5.6 and 4.6%, respectively. The analysis of the individual bond-lengths with pressure is discussed to explain the observed strong axial anisotropy. A comparison with the closely related crystal structure of andalusite shows that the post-titanite phase is less compressible by about 10%. A further comparison with other titanite phases studied at high-pressures allows us to obtain a qualitative model capable of predicting their bulk moduli when unit-cell volume at ambient conditions is known.

Keywords: Post-titanite, single crystal, high pressure, X-ray diffraction