



Leucite at high-pressure: elastic behavior and phase stability

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Elastic and structural behavior of a natural tetragonal leucite from the volcanic Lazium district (Italy) were investigated at high pressure by *in-situ* single-crystal X-ray diffraction with a diamond anvil cell under hydrostatic conditions. A first-order phase transition, never reported in the literature, was observed at $P=2.4\pm 0.2$ GPa from tetragonal ($I4_1/a$) to triclinic symmetry (diffraction intensities analysis suggests $P\bar{1}$), accompanied by a drastic increase of density, about 4.7%. The transition pressure was bracketed by several measurements in compression and decompression. No further phase-transition has been observed up to 7 GPa. Fitting a second-order Birch-Murnaghan Equation-of-State (BM-EoS) to the pressure-volume data of the tetragonal polymorph, we obtain: $K_0=41.9(6)$ GPa and $K''=4$ (fixed). In the case of the triclinic polymorph, a second-order BM-EoS gives: $K_0=33.2(5)$ GPa. The eulerian finite strain (fe) vs normalised stress (Fe) curves were calculated for the low- and high- P polymorphs, providing $Fe(0)=42(1)$ and $Fe(0)=33.2(4)$ GPa, respectively. The axial bulk modulus values of the tetragonal polymorph, calculated with a linearised BM-EoS, are: $K_0(a)=34.5(5)$ GPa and $K_0(c)=78(1)$ GPa. For the triclinic polymorph, we obtain: $K_0(a)=35.9(5)$ GPa, $K_0(b)=34.9(7)$ GPa and $K_0(c)=35.5(7)$ GPa. The elastic behavior of the low- P polymorph appears to be drastically more anisotropic than that of the high- P polymorph. The HP-crystal structure evolution of the tetragonal polymorph of leucite was studied on the basis of six structural refinements at different pressures between 0.0001-1.8 GPa. The main deformation mechanisms at high-pressure are due to tetrahedral tilting, giving rise to an increase of the ellipticity of the 4- and 6-membered rings of the tetrahedral framework. The tetrahedral T-O bond

distances are almost invariant within the stability field of the tetragonal polymorph. The complex P -induced twinning, due to the tetragonal-to-triclinic phase-transition, and the low quality of the diffraction data at pressure above the phase-transition, did not allow the refinement of the crystal structure of the triclinic polymorph.