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Compressibility and pressure-induced structural evolution of kokchetavite, hexagonal polymorph of $KAlSi_3O_8$, by single-crystal X-ray diffraction

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Abstract

Compressibility and pressure-induced structural evolution of kokchetavite, the hexagonal polymorph of $KAlSi_3O_8$, has been studied up to 11.8 GPa using synchrotron single-crystal X-ray diffraction. Two phase transitions were observed at pressures of ~0.3 and 10.4 GPa. Kokchetavite-I (as-synthesized, *P*6/*mcc*) transforms into kokchetavite-II with the $P\bar{6}c2$ space group. Kokchetavite-II → kokchetavite-III phase transition at ~10.4 GPa is accompanied by a change of symmetry to probably orthorhombic. After pressure release, kokchetavite reverts to the initial single-crystal state with *P*6/*mcc* space group. A second-order Birch-Murnaghan equation of state was calculated for phase kokchetavite-II with coefficients $V_0 = 1486(3)$ Å^3, $K_0 = 59(2)$ GPa.

Keywords: Kokchetavite; synchrotron X-ray diffraction, high-pressure crystallography, $KAlSi_3O_8$, K-cymrite, feldspar polymorphism