

Compressibility of synthetic potassium-rich clinopyroxene: In-situ high-pressure single-crystal X-ray study

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ABSTRACT

The crystal structure of a synthetic potassium-rich clinopyroxene, $(\text{Ca}_{0.88}\text{K}_{0.12})(\text{Mg}_{0.83}\text{Al}_{0.17})(\text{Si}_{1.98}\text{Al}_{0.02})\text{O}_6$, was studied using high-pressure single-crystal X-ray diffraction methods. A four-pin diamond anvil cell with 4:1 methanol:ethanol pressure medium was used to achieve pressures to 9.72 GPa. Unit-cell data were measured at 17 pressures, and intensity data were collected at 6 pressures. Fitting the P - V data to the third-order Birch-Murnaghan equation of state yields $V_0 = 435.49(3) \text{ \AA}^3$, $K_0 = 129(1) \text{ GPa}$, $K' = 2.7(3)$. Anisotropic compression was observed with unit strain axial ratios of 1:1.94:1.90. Unit-cell parameters decrease gradually as a function of pressure with axial compressibilities $\beta_b > \beta_c \sim \beta_a$. They match those found for kosmochlor but are stiffer than those observed for synthetic diopside and hedenbergite. Compressibilities of the bond distances within the M2, M1, and T polyhedra show significant anisotropy. The incorporation of K into the clinopyroxene structure has little effect on its compressibility, although the concomitant substitution of Al in M1 from the K-Jd component reduces its compressibility. The K atom is softer than the M2 polyhedron and thus shrinks enough at high pressure to fit into the pyroxene structure.

Keywords: High-pressure studies, clinopyroxene, crystal structure, XRD data, chemical mineral analysis