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Lattice compression and structural behavior of $NaVSi_2O_6$ clinopyroxene to 11 GPa

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ABSTRACT

High-pressure behavior of a synthetic single crystal of the $C2/c$ clinopyroxene $NaVSi_2O_6$ was investigated using X-ray diffraction and Raman spectroscopy in combination with diamond-anvil cell techniques. Lattice-parameters, single-crystal intensity data, and Raman spectra were collected up to pressures of about 11 GPa, revealing no discontinuity in the evolution of the lattice with increasing pressure. The fit of a third-order Birch-Murnaghan equation of state to the pressure-volume data yields a bulk modulus of $K_0 = 114.7$ (1.8) GPa with its pressure derivative $K' = 5.4$ (4). Strain analysis reveals compressional anisotropy with unit strain axial ratios of 1:2.9:3.1. The direction of largest compression was found to be perpendicular to the $(\bar{3}02)$ plane, which matches closely the direction of largest interlayer spacing between oxygen monolayers forming the structure of clinopyroxenes. The relatively large pressure dependency of the bulk modulus, compared to that of isostructural transition-metal compounds, was related to an increase in stiffness of the M2 polyhedron occurring above 4.6 GPa.

Keywords: Clinopyroxene, compressibility, high pressure, single crystal, X-ray diffraction