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In situ high-pressure single-crystal X-ray study of aegirine, $NaFe^{3+}Si_2O_6$, and the role of M1 size in clinopyroxene compressibility

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Abstract

The crystal structure of a synthetic aegirine crystal, $NaFe^{3+}Si_2O_6$, was studied at room temperature, under hydrostatic conditions, over the pressure range 0–11.55 GPa using single-crystal X-ray diffraction. Unit-cell data were determined at 16 pressures, and intensity data were collected at eight of these pressures. A third-order Birch-Murnaghan equation of state fit to the *P*-*V* data from 0–11.55 GPa yielded $K_0 = 117(1)$ GPa, $K_0' = 3.2(2)$, and $V_0 = 429.40(9)$ Å^3. Aegirine, like the other Na-clinopyroxenes that have been examined at high pressure, exhibits strongly anisotropic compression, with unit strain axial ratios $\varepsilon_1:\varepsilon_2:\varepsilon_3$ of 1.00:2.38:2.63. Silicate chains in aegirine become more O-rotated with pressure, reducing ∠O3-O3-O3 from 174.1(1)° at ambient pressure to 165.5(5)° at 10.82 GPa. No evidence of a phase transition was observed over the studied pressure range. The relationship between M1 cation radius and bulk modulus is examined for 14 clinopyroxenes, and two distinct trends are identified in a plot of these values. The distinction between these trends can be explained by the presence or absence of antipathetic bonds around M2, a feature first described by McCarthy et al. (2008). Aegirine, with Fe^{3+}, has nearly the same bulk modulus, within error, as hedenbergite, with Fe^{2+}, despite the difference in M2 bonding topology, M2 (Fe) valence and ambient unit-cell volume. Several explanations for this apparent paradox are considered.

Keywords: Aegirine, crystal structure, high pressure, single-crystal X-ray diffraction, clinopyroxene, compressibility, elasticity, bulk modulus