

## **Compressibility trends of the clinopyroxenes, and in-situ high-pressure single-crystal X-ray diffraction study of jadeite**

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### **ABSTRACT**

The crystal structure of a natural jadeite, NaAlSi<sub>2</sub>O<sub>6</sub>, was studied at room temperature over the pressure range 0–9.17 GPa using single-crystal X-ray diffraction. Unit-cell data were determined at 16 pressures, and intensity data were collected at nine of these pressures. A third-order Birch-Murnaghan equation of state fit to the *P-V* data yielded  $V_0 = 402.03(2) \text{ \AA}^3$ ,  $K_0 = 136.5(14) \text{ GPa}$ , and  $K'_0 = 3.4(4)$ . Jadeite exhibits strongly anisotropic compression with unit strain axial ratios of 1.00:1.63:2.10. Silicate chains become more O-rotated with pressure, reducing  $\angle O3-O3-O3$  from  $174.7(1)^\circ$  at ambient pressure to  $169.2(6)^\circ$  at 9.17 GPa and bringing the anions of jadeite closer to a cubic closest-packed arrangement. No evidence of a phase transition was observed over the studied pressure range.

In an effort to understand pyroxene compressibilities, selected clinopyroxene bulk moduli were plotted against ambient unit-cell volumes. Two trends were identified and are explained in terms of differences in M2-O3 bonding topologies and the geometric relationship of the bonds with tetrahedral rotation in the silicate chains. Bonds positioned to favor the tetrahedral rotation upon compression are termed “sympathetic,” whereas bonds positioned to resist the rotation are termed “antipathetic.” Examination of the different pyroxene structures indicates that structures containing antipathetic M2-O3 bonds are less compressible than those with only sympathetic M2-O3 bonds. This behavior has not been previously recognized.

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