High-pressure behavior of natural single-crystal epidote and clinozoisite up to 40 GPa

Fei Qin^{a,b}, Xiang Wu^a, Joshua P Townsend^b, Steven D. Jacobsen^b

^aKey Laboratory of Orogenic Belts and Crustal Evolution, MOE, Peking University and School of Earth and Space Sciences, Peking University, Beijing 100871, China ^bDepartment of Earth and Planetary Sciences, Northwestern University, Evanston, IL 60208, USA

Epidote group minerals are common hydrothermal alteration minerals in basaltic rocks and potentially important carriers of H₂O in subducted oceanic crust. Monoclinic epidote, including clinozoisite, occurs in high- and ultrahigh-pressure metamorphic rocks from a wide variety of geological settings. Al \leftrightarrow Fe³⁺ substitution along the clinozoisite-epidote join which affects the crystal structure and crystal chemistry. The concentration and valence state of iron in host minerals influences elastic properties, which can significantly affect the understanding of the geophysical and geochemical properties at high pressures and temperatures. Here, we determine the compressibility and vibrational properties of natural epidote and clinozoisite by synchrotron-based, single-crystal X-ray diffraction and Raman spectroscopy up to 40.6 GPa at room temperature. The lattice parameters of both phases exhibit continuous compression up to 30 GPa without phase transformation. Pressure-volume relationships of both phases were fitted to a third-order Birch-Murnaghan equation of state with $V_0 = 461.1(1) \text{ Å}^3$, $K_0 = 115(2)$ GPa, and $K_0 = 3.7(2)$ for epidote, and $V_0 =$ 457.8(1) Å³, $K_0 = 142(3)$ GPa, and $K'_0 = 5.2(4)$ for clinozoisite. Both epidote and clinozoisite exhibit anisotropic compression with the b-axis being the most incompressible. Raman spectra further suggest that the difference in compressibility between epidote and clinozoisite. The average pressure coefficient of Raman frequency shifts for M-O modes in epidote, 2.61(6) cm⁻¹/GPa, is larger than found for clinozoisite, 2.40(6) cm⁻¹/GPa, mainly due to the different compressibility of FeO₆ and AlO_6 octahedra in M3 sites. The calculated γ values for Si-O vibration are in the range of 0.5-0.8, which are typical for hydrous silicate minerals.