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The pressure behavior of clinozoisite and zoisite: An X-ray diffraction study

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Abstract

Compressibility data of clinozoisite and zoisite were measured by single-crystal X-ray diffraction in a diamond-anvil cell up to a pressure of about 50 kbar. In both polymorphs, the unit cell parameters varied linearly with pressure but in an anisotropic pattern: β_a = 2.1(1) × 10^{-4}, β_b = 2.8(1) × 10^{-4}, β_c = 3.3(1) × 10^{-4} $kbar^{-1}$ for clinozoisite, and β_a = 2.3(2) × 10^{-4}, β_b = 2.9(1) × 10^{-4}, β_c = 3.7(2) × 10^{-4} $kbar^{-1}$ for zoisite. The principal coefficients of the strain ellipsoid of clinozoisite are β_1 = 2.0 × 10^{-4}, β_2 = 2.7 × 10^{-4}, β_3 = 3.3 × 10^{-4} $kbar^{-1}$; β_1 and β_3 were symmetrically oriented in the (010) plane with an angle of about 12° between β_1 and the *a* axis, whereas β_2 coincides with the *b* axis. Bulk moduli calculated as the reciprocal of cell-volume compressibility were 1300(20) kbar for the monoclinic and 1140(20) for the orthorhombic polymorph. K_0, determined by fitting the unit-cell parameters with a third-order Birch-Murnaghan equation of state, was 1270(45) kbar, with K' = 0.5(2) for clinozoisite and 1020(65) kbar with K' = 4.8(4) for zoisite.

Structural refinements of clinozoisite performed at 0.5, 19.4, and 42 kbar, and also under ambient conditions, showed that the compression mechanism included both shrinking of the polyhedra (i.e., octahedra and Ca polyhedra) and tilting of the Si_2O_7 group, with reduction of the Si-O-Si angle. The different effect of these mechanisms explains the anisotropic compressional pattern in clinozoisite and the similar behavior observed in the two polymorphs.

Comparison of high-pressure and high-temperature data for clinozoisite showed that a given increase in pressure produced structural effects very similar to those seen after a proportional decrease in temperature. The calculated volume-expansivity–to–compressibility ratio of 38 bar/K indicates that the cell volume of clinozoisite remains unchanged with geothermal gradients of about 10 °C/km. The crystallographic data support the results of experimental petrology in indicating that epidote is a good candidate for transporting H_2O in down-going subduction slabs.