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Isothermal compression of staurolite: A single-crystal study

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ABSTRACT

The response of staurolite to pressure was studied by single crystal X-ray diffraction (XRD) in a diamond-anvil cell, using crystals with composition: $(Fe_{3.365}Zn_{0.025}Li_{0.114}Co_{0.009}\,Mn_{0.034})$[T2, M4] $(Al_2Mg_{0.307})$[M3] $(Al_{15.491}Fe^{3+}_{0.104}Mg_{0.394}Cr_{0.004}Ti_{0.07})$[M1, M2] $(Si_{7.534}\,Al_{0.466})$[T1] $O_{48}H_3$.

Lattice parameters, measured at various pressure up to 7.264(6) GPa, were fitted using a third-order Birch-Murnaghan equation of state (EoS). The resulting EoS parameters are: V_0 = 740.85(7) Å^3, K_0 = 180(2) GPa and K' = 4.7(6), a_0 = 7.8723 (2) Å, K_0 = 189(2) GPa, and K'_a = 4.1 (6), b_0 = 16.62453(1) Å, K_0 = 179(2) GPa, K'_b = 6.1(6) and c_0 = 5.6604 (4) Å, K_0 = 179(5) GPa, K'_c = 2(1); whereas the angle β remained almost constant with increasing pressure. These data suggest an almost isotropic compressibility.

Structural evolution was studied by comparison of structural refinements carried out with data collected at 0.0001, 2.48, 4.15, 5.43, 6.84, and 8.74 GPa. All refinements were made in the *Ccmm* space group. Polyhedral evolution with *P* is a function of occupancy: whereas the T1 tetrahedron and the M1 and M2 octahedra, occupied by Si and Al, are practically incompressible, the T2 tetrahedron, and the M4 and M3 octahedra, only partially occupied principally by Fe (the first two) and by Al (the last), show larger changes as a function of pressure. As a consequence, the two kyanite and Fe-Al hydroxide layers, which can be used to describe the staurolite structure, have different compressibilities.