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Equations of state and structures of andalusite to 9.8 GPa and sillimanite to 8.5 GPa

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ABSTRACT

The equations of state and structures of andalusite and sillimanite have been determined using high-pressure single-crystal X-ray diffraction. A third-order Birch-Murnaghan equation-of-state fit to 14 *P-V* data points measured between 1 bar and 9.8 GPa for andalusite yields values of K_{T0} = 144.2(7) GPa and K' = 6.8(2). A similar analysis for sillimanite involving a fit to 13 *P-V* data points between 1 bar and 8.5 GPa results in K_{T0} = 164(1) GPa and K' = 5.0(3). The axial compression of both structures is nonlinear and highly anisotropic (~60%) with the *c*-axis being the least compressible axis in both structures. The axial moduli determined with a parameterized form of the third-order Birch-Murnaghan equation of state are: K_{a_0} = 163(1) GPa, K_{b_0} = 113.1(7) GPa, and K_{c_0} = 297(1) GPa with K'_{a_0} = 2.1(3), K'_{b_0} = 5.08(19), and K'_{c_0} = 11.1(4) for sillimanite, and K_{a_0} = 99.6(7) GPa, K_{b_0} = 152.2(9) GPa, and K_{c_0} = 236(3) GPa with K'_{a_0} = 5.83(19), K'_{b_0} = 7.6(3), and K'_{c_0} = 5.5(9) for andalusite. The major compression mechanism in both structures involves shortening of bond lengths within the AlO_6 octahedra with volume reductions of 7.4% and 5.1% in sillimanite and andalusite, respectively, over the pressure ranges studied. In andalusite there is also significant compression of the AlO_5 polyhedra and, to a lesser degree, the SiO_4 tetrahedra that display reductions of 5.0% and 3.1% in volume, respectively. In sillimanite there is no significant compression of either the AlO_4 or SiO_4 tetrahedra which behave as rigid, incompressible units.

Keywords: Andalusite, sillimanite, high-pressure studies, equation of state, XRD data, single crystal, crystal structure