High-pressure structural evolution and equation of state of analbite

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ABSTRACT

The volume and unit-cell parameters of analbite (i.e., NaAlSi₃O₈ with complete Al,Si disorder) have been determined by single-crystal X-ray diffraction to a maximum pressure of ~8.71 GPa. The volume variation with pressure is described by a fourth-order Birch-Murnaghan equation of state with K_{0T} = 50.3(5) GPa, K'_0 = 8.9(5), and K''_0 = -2.4(3) GPa⁻¹. The value of the room-pressure bulk modulus is ~4% lower than that of low albite, and the onset of volume softening in analbite is at ~6.7 GPa, some 1.7 GPa higher than the onset in albite. The anisotropy of compression of analbite is less than that in albite.

Single-crystal structure determinations of analbite to \sim 9.4 GPa show that there is no significant detectable compression of the T-O bonds within the structure, and the compression of the framework of tetrahedra is therefore accommodated by changes in the T-O-T angles, which result in significant compression of the "crankshaft chains" within the framework. No significant shear of the tetrahedral rings of analbite was detected, in contrast to the structural compression of albite. Overall, the structural changes that occur in analbite from 0.0001 to 9.4 GPa resemble those seen in ordered albite over the pressure range 0.0001–4 GPa. Therefore analbite shows a significantly greater structural rigidity than low albite up to pressures of 9.4 GPa.

Keywords: Analbite, equation of state, high pressure, X-ray structure, single crystal