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High-pressure behavior of kyanite: Compressibility and structural deformations

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ABSTRACT

The lattice parameters of kyanite were measured at various pressures up to about 60 kbar by single-crystal X-ray diffraction in a diamond anvil cell. Unit-cell dimensions decreased linearly with an almost uniform rate:

$\beta_a = 2.00(8) \times 10^{-4}$, $\beta_b = 1.90(4) \times 10^{-4}$, $\beta_c = 2.00(4) \times 10^{-4}$ kbar^{-1}. The principal compressibility coefficients were $\beta_1 = 2.23 \times 10^{-4}$, $\beta_2 = 2.04 \times 10^{-4}$, $\beta_3 = 1.65 \times 10^{-4}$ kbar^{-1}, with β_1 forming an angle of 35° with the *c* axis. K_0, calculated by fitting pressure-volume data to a third-order Birch-Murnaghan equation of state, was 1560(100) kbar, with K' 5.6(5.5); when K' was set at 4, K_0 became 1600(30) kbar.

Structural refinements were carried out on data collected at 0.001 kbar with the crystal in air and at 0.1, 25.4, 37, and 47 kbar with the crystal in the diamond anvil cell. Whereas the Si tetrahedra and Al4 octahedron were incompressible in this *P* range, the polyhedral bulk modulus for Al1 and Al2 was 1280(150) kbar and 2380(200) kbar for Al3. These octahedra became more regular with increasing pressure.

The almost isotropic compression pattern was due to the many shared edges between the polyhedra, uniformly distributed in the cell. The evolution of Al-Al separation showed that the largest reduction regarded the Al2-Al3 and Al2-Al4 distances, whereas the average Al1-Al2 distance was almost unchanged, resulting from linkage with Si tetrahedra having rigid edges. The result was that the largest reduction did not occur along the *c* axis but along the Al4-Al1–Al2-Al3 directions.

The geometrical structural invariance, expressed by the β_V/α_V ratio and obtained from the average compressibility and average thermal expansion of the cell volume (Winter and Ghose 1979), was 23 °C/kbar. The following equation of state, which applies in crustal *P-T* conditions, may be defined as: $V/V_0 = 1 + 3.00(7) \times 10^{-5}\ T - 5.8(1) \times 10^{-4}\ P$, where *T* is in °C and *P* in kbar.

The present volume-pressure data support multi-anvil experiments by Schmidt et al. (1997) defining the *P-T* conditions necessary for decomposition of kyanite into stishovite + corundum.