

Compressibility and crystal structure of kyanite, Al_2SiO_5 , at high pressure

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ABSTRACT

The unit-cell dimensions and crystal structure of kyanite at various pressures up to 4.56 GPa were refined from single-crystal X-ray diffraction data. The bulk modulus is 193(1) GPa, assuming $K' = 4.0$. Calculated unit-strain tensors show that kyanite exhibits more isotropic compressibility than andalusite or sillimanite. The most and least compressible directions in the kyanite structure correspond approximately to the most and the least thermally expandable directions. The analysis of the distortion of the closest packing in kyanite indicates that the most compressible direction of the structure (along [012]) corresponds to the direction along which the closest-packed O monolayers are stacked. The bulk moduli for the Al1, Al2, Al3, and Al4 octahedra are 274(43), 207(14), 224(26), and 281(24) GPa, respectively, and those for the Si1 and Si2 tetrahedra are 322(80) and 400(95) GPa, respectively. Four AlO_6 octahedra that all become less distorted at higher pressures do not display clearly dominant compression directions. The average unshared O-O distance for each octahedron is considerably more compressible than the shared O-O distance. The high-pressure behaviors of the Al1 and Al4 octahedra are very similar but different from those of the Al2 and Al3 octahedra. Bulk moduli for the three Al_2SiO_5 polymorphs (kyanite, sillimanite, and andalusite), as well as those for the AlO_6 octahedra in their structures, appear to decrease linearly as their volumes increase. The significantly larger bulk modulus and more isotropic compressibility for kyanite than for andalusite or sillimanite are a consequence of the nearly cubic close-packed arrangement of O atoms and the complex edge-sharing among four distinct AlO_6 octahedra in the kyanite structure.