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Single-crystal X-ray diffraction of fluorapatite to 61 GPa

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Abstract

Apatite is a mineral of widespread importance in Earth and planetary science. Here we examine the behavior of a natural fluorapatite (FAp) crystal from Durango (Mexico) under compression to 61 GPa. Single-crystal X-ray diffraction experiments were carried out in a diamond-anvil cell using a synchrotron source. The apatite structure persists up to 32.4 GPa. Birch-Murnaghan equation of state parameters were fit to the pressure-volume data for fluorapatite for two cases: fixing V_0 at its measured ambient value resulted in a bulk modulus, K_{0T}, of 97.0(8) GPa and a pressure derivative of the bulk modulus, K'_{0T}, of 3.3(1), while fixing V_0 and K_{0T} at its ambient value 90.5 GPa (derived from ultrasonically measured elastic constants) resulted in a K'_{0T} value of 4.1(1). At 35.6 GPa, fluorapatite transforms to a triclinic phase ($P\bar{1}$, $Z = 4$), designated here as fluorapatite II (FAp-II). This phase persists up to at least 61 GPa. The major structural differences between FAp and FAp-II involve the buckling of the Ca polyhedra along the *c*-axis and changes in the number and coordination of the Ca sites. Our study extends the pressure range over which fluorapatite has been examined by more than a factor of three, providing new insights into its structural response to high-pressure conditions.

Keywords: Apatite, high-pressure, diamond anvil cell, single-crystal X-ray diffraction