

High-Pressure Structural and Equation of State Study of Xenotime

Nancy L. Ross,¹ Jing Zhao,¹ Lynn A. Boatner,²

^[1] Department of Geosciences, Virginia Tech, Blacksburg, VA 24060, USA

^[2] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Xenotime has a wide range of formation temperatures in geological environments and is one of the most valuable minerals used for U-Pb geochronology. A major component of xenotime is YPO₄ which crystallizes in space group *I4₁/amd* (no. 141). The crystal structure of YPO₄ is composed of edge-sharing YO₈ dodecahedra and PO₄ tetrahedra that form chains running parallel to [001]. We studied the effect of pressure on the structure of YPO₄ to 9.1 GPa using single-crystal X-ray diffraction. The structure is stable throughout the pressure range studied. Axial compressibilities are anisotropic with [100] approximately 2.4 times more compressible than [001]. Volume reduction of the structure is accommodated by bond length shortening in both the PO₄ tetrahedra and YO₈ dodecahedra. Interestingly, the shorter Y-O bond lengths show a greater decrease with pressure than the longer Y-O bond lengths. A 3rd-order Birch-Murnaghan equation of state fit to the P-V data yielded $K=143.4(7)$ GPa with $dK/dP=7.0(2)$.

The results from this study are compared with high-pressure studies of other phosphates isostructural with xenotime as well as phosphates isostructural with monazite. Monazite, with ideal formula, CePO₄, is monoclinic and crystallizes in space group *P2₁/n* (no. 14) with PO₄ tetrahedra cross-linked by rare-earth cations in 9-fold coordination with oxygen. Whereas xenotime-type phosphates are known to accommodate smaller rare-earth cations (Tb to Lu), monazite-type phosphates accommodate larger rare-earth cations (Ce to Gd). The effect of cation size on the equations of state of these phosphates will be discussed.