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Crystal chemistry and thermodynamics of HREE (Er, Yb) mixing in xenotime solid solution

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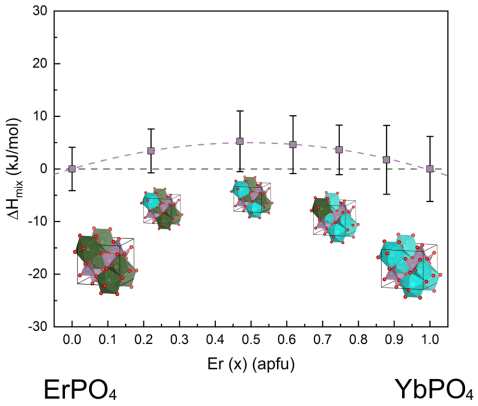

Rare earth elements (REE), the thirteen naturally occurring lanthanides, plus yttrium and scandium, are ubiquitously utilized in modern life as they are critical components of many advanced devices and technologies. However, the demand for REE is not equal, with the heavy rare earth elements (HREE) having a higher demand. Xenotime ($HREEPO_4$) is an important HREE ore mineral and globally is an economical source of HREE. Most of the crystallographic and thermodynamic properties of xenotime endmembers have been determined through calorimetric, solubility, and high-pressure studies. However, endmembers are rarely encountered in natural systems, but solid solutions of HREE are more commonly observed. In this work, we characterize the crystal chemistry, thermodynamics of HREE mixing, and high temperature material behaviors and thermochemistry of a synthetic erbium (Er)- ytterbium (Yb) binary xenotime solid solution series ($Er_{(x)}Yb_{(1-x)}PO_4$) using a suite of experimental techniques, including X-ray fluorescence spectrometry, synchrotron X-ray powder diffraction implemented with Rietveld analysis, Fourier transform infrared spectroscopy coupled with attenuated total reflectance, Raman spectroscopy, thermogravimetric analysis coupled with differential scanning calorimetry, and high temperature oxide melt drop solution calorimetry. Studying of these HREE solid solutions generates important implications on the natural occurrence of xenotime minerals and their industrial applications as thermal coating materials.