Polymorphism and phase transitions of $K_3Lu(PO_4)_2$

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Alkali lanthanide double phosphates have been studied for uses as long-wavelength scintillators for γ-ray detection using Si photodiodes. This family of compounds exhibits layered crystal structures, in the sequence lanthanide, phosphate – alkali, alkali, alkali - phosphate. Current research has focused on $K_3Lu(PO_4)_2$. At room temperature, this compound is hexagonal, *P* –3 space group symmetry. The Lu ion is six-coordinated to the oxygen atoms of the phosphate groups. Our group has recently characterized two lower-temperature phases of $K_3Lu(PO_4)_2$ using single-crystal XRD and powder neutron diffraction. The first transition occurs at 230 K, with a transformation to monoclinic *P* 2_1/m space group symmetry, and the Lu still retains six coordination. Another transition occurs at 130 K, with a small change in the cell volume, keeping the same *P* 2_1/m space group symmetry; however, one of the phosphate groups rotates to increase the coordination of the Lu ion to seven. This new structure is isostructural with the room-temperature form of $K_3Yb(PO_4)_2$. A heat capacity versus temperature study of $K_3Lu(PO_4)_2$ confirms the transformations and indicates a large thermal hysteresis as the crystals are thermally cycled between 15 to 295 K. Research sponsored by the U.S. Department of Energy under contract DE-AC05-00OR22725 with the Oak Ridge National Laboratory, managed by UT-Battelle, LLC.