

OXYGEN OCTAHEDRAL ENVIRONMENTS IN THREE-LAYER AURIVILLIUS PHASES VIA COMBINED X-RAY AND NEUTRON POWDER DIFFRACTION

Eric J. Nichols, Scott T. Misture

Alfred University

Aurivillius phase oxides are members of the layered perovskite family of materials and consist of perovskite-like blocks interleaved with $[\text{Bi}_2\text{O}_2]^{2+}$ layers. Rietveld analysis of the three-layer Aurivillius phases $\text{Bi}_2\text{LnTi}_3\text{O}_{12}$ ($\text{Ln} = \text{La}_2, \text{Pr}_2, \text{Nd}_2, \text{LaPr}, \text{LaNd}$ and PrNd) and Bi_2Sr_2 - $x\text{A}_x\text{Nb}_2\text{TiO}_{12}$ ($\text{A} = \text{Ca}, \text{Ba}, x = 0, 0.5, 1$) will be discussed with special emphasis on local bonding environments within the TiO_6 and NbO_6 octahedra. Cation substitutions to the perovskite A-site ranging from 1.29-1.49 Å have been investigated. Planar to non-planar distortions of the equatorial oxygens contained within perovskite-like blocks have been shown to vary with an inverse proportionality to the average A-site cation radius. Non-planar distortions of up to 6° in this system have been linked to average A-site radii below 1.4 Å.