Crystal Structure Refinements of the three-layer Aurivillius Phase $Bi_2LnTi_3O_{12}$ (Ln = La_2, LaPr, LaNd, Pr_2, PrNd, Nd_2) Utilizing Combined X-ray and Neutron Powder Diffraction

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Layered Aurivillius phases have in the past been shown to be photochemically active for hydrogen production, water purification, and similar applications. These phases consist of perovskite-like blocks sandwiched between $[Bi_2O_2]^{2+}$ layers. Cationic substitutions on the perovskite A-sites allow for the systematic manipulation of the band gap of these materials and have been shown previously to shift the optical absorption edge by as much as 0.3 eV over the range of substitutions from $Bi_2La_2Ti_3O_{12}$ to $Bi_2Nd_2Ti_3O_{12}$. Structural characterization of these materials via combined Rietveld refinements of x-ray and neutron powder diffraction patterns will be discussed with emphases on Ti-O bond length manipulation, static disorder between the cationic A-site positions and the $[Bi_2O_2]^{2+}$ layers, and bond valence sum calculations.