

Direct Methods, ab-initio Structure Solution from Powder Data, Synchrotron vs Neutron Powder Diffraction data

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Abstract No. unde2099

Beamline(s): **X7A**

Abstract: Three quaternary compounds $\text{Ba}_2\text{Nb}_2\text{TeO}_{10}$, $\text{Bi}_4\text{Sr}_3\text{Te}_5\text{O}_{19}$, and $\text{Bi}_2\text{SrTeO}_7$ were synthesized in air using conventional solid-state synthetic techniques. All three compounds have been previously reported in the literature, but the structures of the latter two compounds were unknown. Ab-initio structure solution was performed in each case using direct methods using the Sirpow97 software suite. The structures obtained from direct methods were subsequently refined using Rietveld methods. Both synchrotron x-ray and neutron powder diffraction data were collected. The major focus of the study was to determine the effectiveness of synchrotron diffraction versus neutron diffraction analysis for ab-initio structure solution using direct methods. Peak intensities were extracted using a LeBail algorithm, as implemented in the GSAS software suite. The relative success of the direct methods approach using the two diffraction techniques will be discussed.