Phase transition behavior of the layered perovskite $CsBi_{0.6}La_{0.4}Nb_2O_7$: a hybrid improper ferroelectric

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Supplementary Material

Synthesis: The $CsBi_{1-x}La_xNb_2O_7$ solid solution was synthesised using traditional ceramic methods. Stoichiometric amounts of La_2O_3 (99.9 % Sigma-Aldrich), Nb_2O_5 (99.9 % Alfa Aesar) and a 20 % excess of Cs_2CO_3 (99 % Alfa Aesar) were dried at 100 °C for 24 hours. The loose powders were ground for a period of 30 minutes and pressed into pellets of approximately 10 mm diameter and 5 mm thickness. The pellets were annealed at 1000 °C for a period of 24 hours with a cooling rate of 10 $°min^{-1}$.

Powder Diffraction: X-ray powder diffraction was carried out using a PANalytical Empyrean diffractometer (Cu $K_{\alpha 1}$ radiation source). Diffraction patterns were collected over the 2θ range $3 \leq 2\theta \leq 70$ °C and a collection time of 1 hour. Analysis using Rietveld refinement methods of the resulting diffraction patterns was carried out with the GSAS software package and EXPGUI interface.

The Rietveld refinement models used were the $P2_1am$ model for $0 < x \leq 0.5$ and the parent $P4/mmm$ model for $x > 0.5$. For the $x > 0.5$ compositions we acknowledge that although the unit cells are *metrically* tetragonal, within the resolution of our instrumentation, the true symmetry is likely to be the $Amm2$ model reported for $CsLaNb_2O_7$. This approximation has negligible influence on the lattice parameters reported here, which are intended only to demonstrate that a continuous solid solution exists, and that the composition $CsBi_{0.6}La_{0.4}Nb_2O_7$ targeted here is validated experimentally, in the absence of precise chemical analysis.

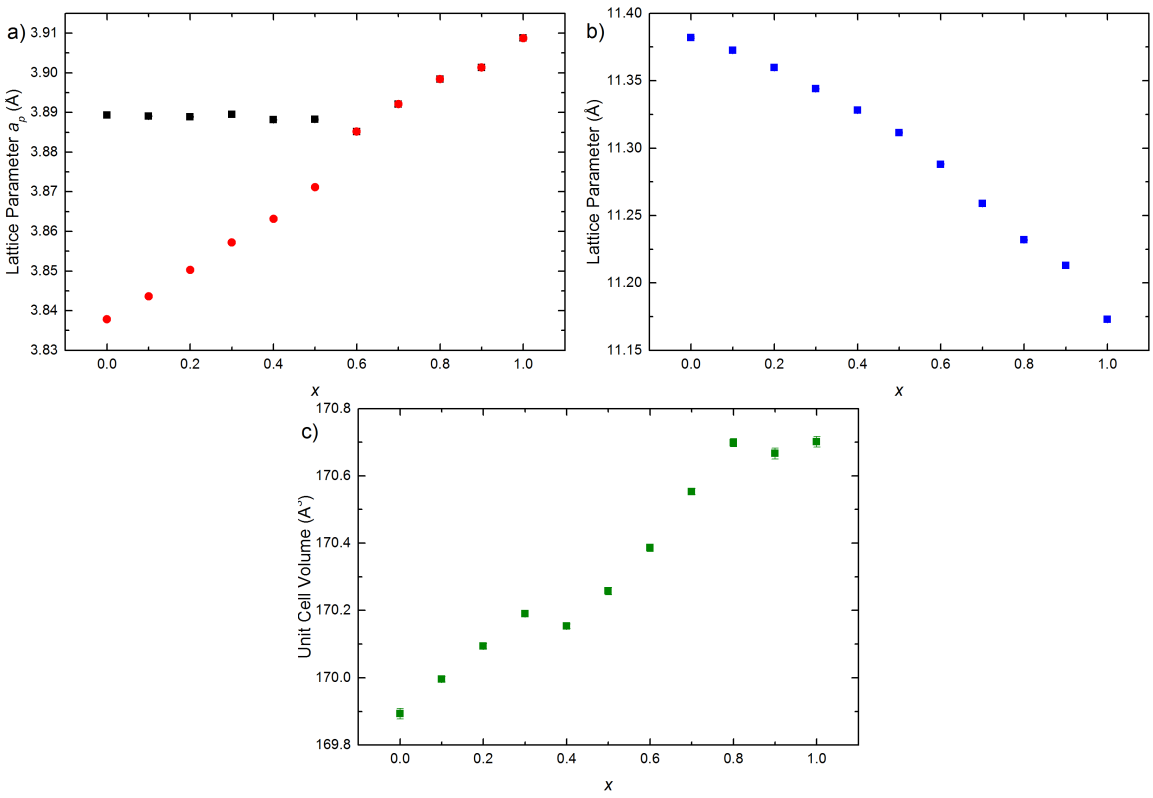

Figure S1: a) normalised *a* (black squares) and *b* (red circles) lattice parameters obtained for varying values of *x* across the solid solution $CsBi_{1-x}La_xNb_2O_7$, b) *c* lattice parameter for varying values of *x* and c) (normalized) unit cell volume for varying values of *x*.