Electronic Supplementary Information for Dalton Transactions

Crystal structure of $Bi_{0.9}Sm_{0.1}Fe_{1-x}Mn_xO_3$ multiferroics

Stefan Saxin and Christopher S. Knee *

Department of Chemistry, University of Gothenburg, SE-412 96 Göteborg, Sweden

*corresponding author: knee@chem.gu.se
Tel. +46 31 786 9036

Supplementary Information

Rietveld fits

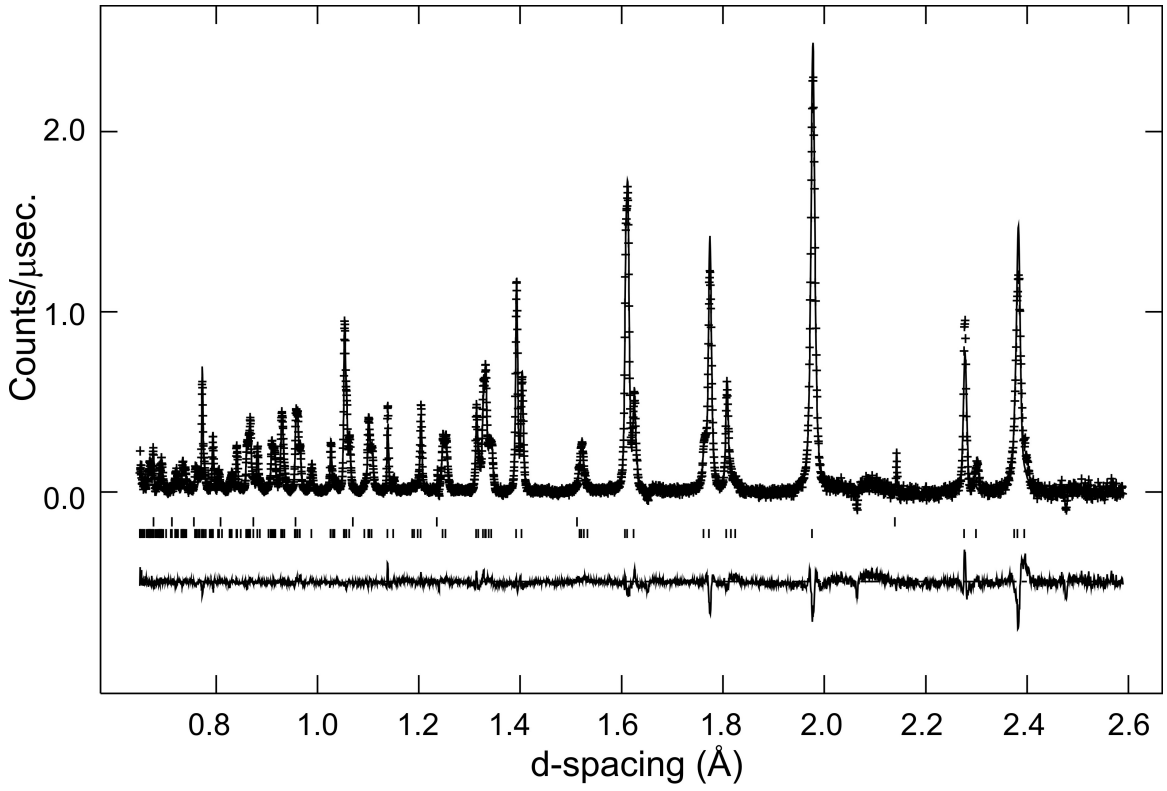

Figure S1. Rietveld fit achieved to the back scattering detector bank of HRPD for $Bi_{0.9}Sm_{0.1}FeO_3$ using a *R*3*c* model. Crosses are observed data points, upper line the calculated diffraction profile and lower line is the difference between observed and calculated intensities. Tick marks indicate allowed reflections from the perovskite phase (lower) and the vanadium sample holder (upper).

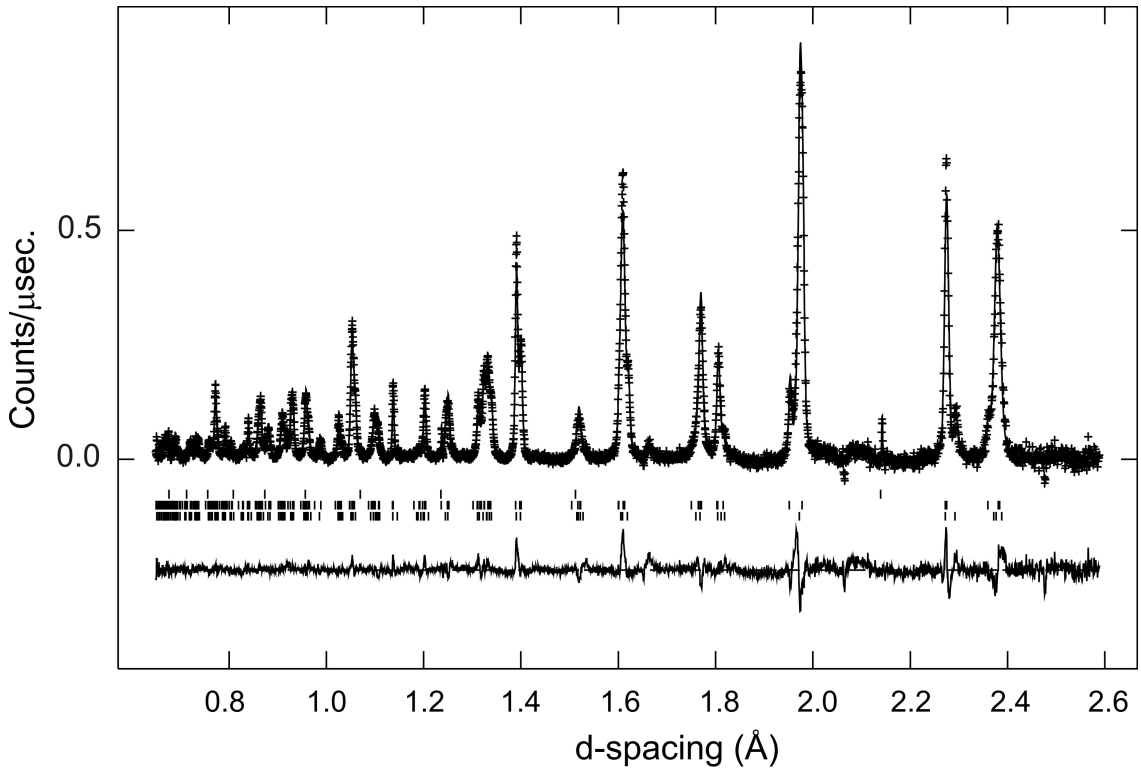

Figure S2. Rietveld fit achieved to the back scattering detector bank of HRPD for bi-phasic $Bi_{0.9}Sm_{0.1}Fe_{0.85}Mn_{0.15}O_3$. Crosses are observed data points, upper line the calculated diffraction profile and lower line is the difference between observed and calculated intensities. Tick marks indicate position of allowed reflections from the perovskite *R*3*c* (bottom) and *Imma* (middle) structural models, and from the vanadium sample holder (top).

Table S1. Goodness of fit parameters obtained from Le Bail extractions for $Bi_{0.9}Sm_{0.1}Fe_{0.70}Mn_{0.30}O_3$. The cell constants, 8 background, and 2 profile parameters were allowed to vary. On the basis of this analysis the *Imma* model was selected for the full Rietveld analysis as presented in the article.

Model	*Imma*	*Pnma*	$Pn2_1a$	*Pbam*	*I*4/*mcm*
a (Å) ≈	5.58	5.58	5.58	5.58	5.58
b (Å) ≈	7.79	7.79	7.79	11.16	5.58
c (Å) ≈	5.59	5.59	5.59	7.79	7.79
χ^2	4.45	6.29	6.27	6.31	12.22
R_{wp} (%)	5.83	6.93	6.92	6.94	9.66
R_p (%)	5.94	6.57	6.55	7.17	8.75