Supplementary data

Title: Crystallographic site swapping of La^{3+} ion in $BaA'LaTeO_6$ (A'=Na, K, Rb) double perovskite type compounds: A diffraction and photoluminescence evidence for the site swapping.

R. Phatak, S. K. Gupta, K. Krishnan, S. K. Sali, S. V. Godbole and A. Das*

** Corresponding Author:* ***sksali@barc.gov.in***

Figure 1 show the Rietveld refined XRD data for 20 atom % of Eu^{3+} doped in $BaRbLaTeO_6$ compound (i: e $BaRbLa_{0.8}Eu_{0.2}TeO_6$). The refined data showed the doped compound is pure and single phase. The refined cell parameters are a= 8.5757 (5) Å, V= 630.69 (4) $Å^3$. In Eu doped Rb compound there is decrease in the cell parameters compared to parent compound as expected by lanthanide contraction and Eu atom is located only at B site.

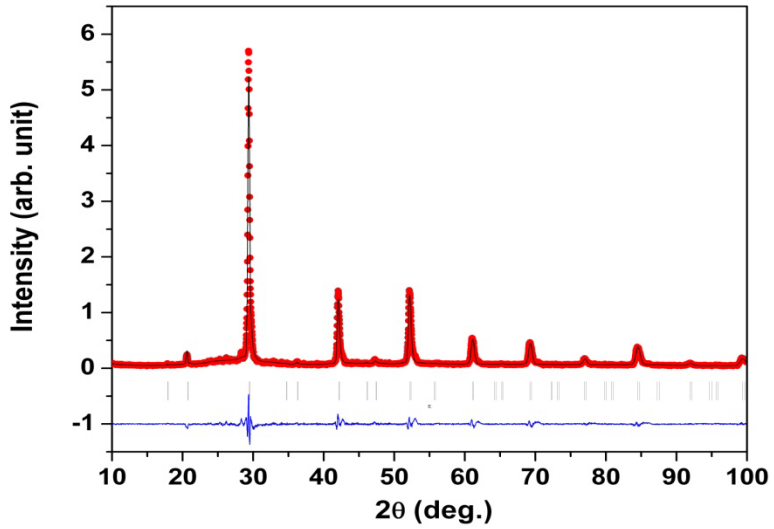

Figure 1. Rietveld refined X-ray diffraction pattern of 20 atom % Eu doped $BaRbLaTeO_6$ sample

Figure 2 show the Rietveld refined XRD data for 20 atom % of Eu^{3+} doped $BaLaNaTeO_6$ compound (i: e $BaLa_{0.8}Eu_{0.2}NaTeO_6$). The refined data showed that the doped compound is pure and single phase. Surprisingly it was noticed from the raw XRD data that the Eu doped sample has higher d values compared to parent compound $BaLaNaTeO_6$. This indicates that the Eu doped sample has marginally

higher unit cell parameters which are not expected because of the lanthanide contraction. The refined cell parameters are a= 5.8405(8) Å, b= 5.8449(5) Å, c= 8.2576(7) Å, β= 89.99(2)°, V= 281.89(5) $Å^3$.

Initially, the Eu atom was placed at La site, which gave poor fit for few reflections. Later the Eu and Na atom were equally distributed over both 'A' and 'B' sites in ABO_3 perovskite and occupancy was refined. Final converged distribution is $(BaLa_{0.8}Eu_{0.064}Na_{0.136})(Eu_{0.136}Na_{0.864}Te)O_6$. This refined distribution fits all the reflections and thus reducing the chi square value. At higher doping percent, Eu is expected to distribute over both A and B site because maximum co-ordination reported for Eu^{3+} ion is nine. But in the lower doping concentration of 6 atom % Eu which is used for carrying out photoluminescence measurements, Eu can be accommodated at A site. The increase in the volume of the cell in the Eu doped sample may be due to transfer of Na^+ ion from B site to A site and thus increasing its ionic size. It is also seen that in the doped sample the cell parameter beta reduces to 89.99 compared to 90.29 in parent compound, indicating pseudo cubic symmetry. Figure 2 shows the comparison of few reflections (2θ = 60 to 90°) for the parent and doped samples, where increase in the d-spacing and lowering of symmetry is clearly observed for doped sample.

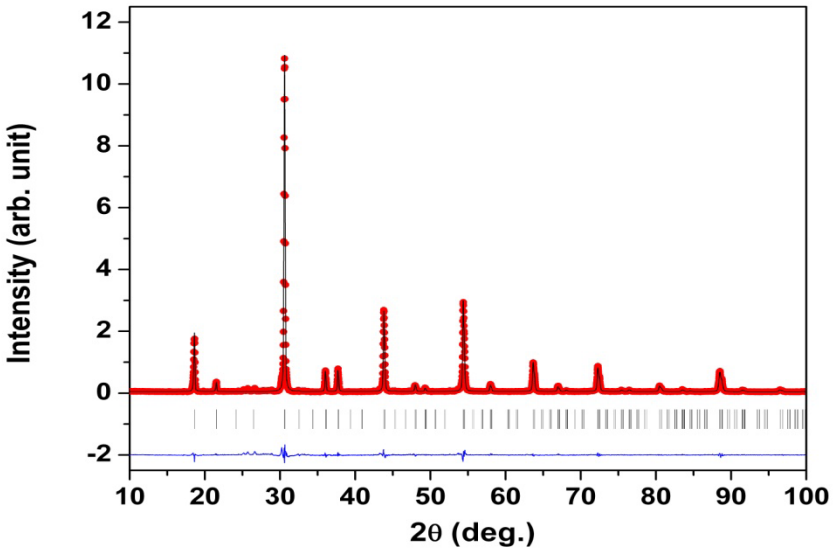

Figure 2. Rietveld refined X-ray diffraction pattern of 20 atom % Eu doped $BaLaNaTeO_6$ sample

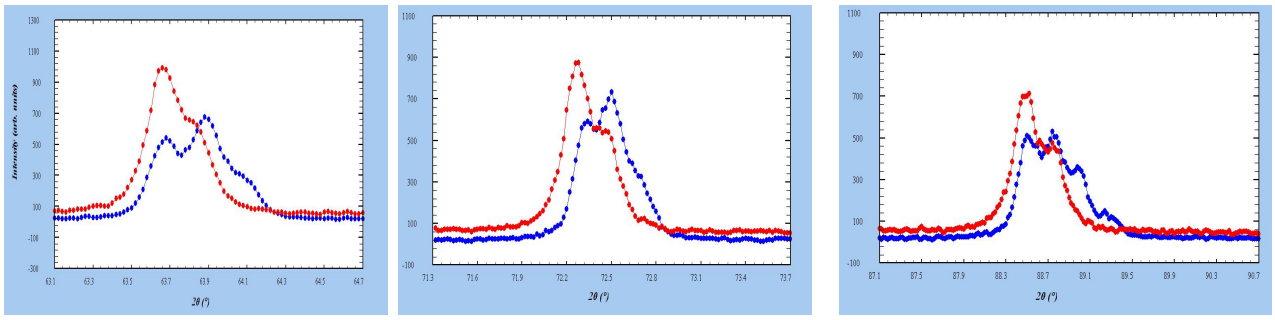

Figure 3. Comparison of few reflections in raw XRD data of BaLaNaTeO6 (Blue) and BaLa0.8Eu0.2NaTeO6 (Red)