

The Rietveld Refinement of The Rare Earth Orthoborates

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Borate containing compounds have long been the subject of interest over many decades, motivated by their extraordinary optical properties [1]. The structural description of some rare earth-activated orthoborates corresponding to the empirical formula LnBO_3 (Ln= La, Nd, Sm, and Eu) were reinvestigated using solid state wet reactions by Mahiou's group [2]. The rare-earth borates are characterized by a high structural flexibility caused in the linkage planar/nonplanar BO_3 - groups and BO_4 -tetrahedra, which can occur as isolated or condensed fundamental building units [3].

In the present research, we prepared LnBO_3 (Ln=Y, La, Nd, Sm, Eu, Gd, Dy, Ho, Er, Tm, Yb, Lu) powder samples by using with Ln_2O_3 and H_3BO_3 (ratio=1:2) at 900 °C for 10 hour and 1000 °C for 5 hour heatings were applied in muffle furnace. Then, their XRD patterns at 700, 900, 1000 °C were investigated. For GdBO_3 , space group was found to be $P6_3/mmc$ and the unit cell parameters were found as $a=3.83302(9)$, and $c=8.9084(3)$ Å. The R values were found as $R_{\text{exp}}=2.87$, $R_{\text{wp}}=10.65$, $\text{GOF}=13.73$. Finally, their pure lanthanide orthoborate phases and crystal structure analysis were performed by Rietveld Analysis using High Score Plus.

References:

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