# Ternary borides in the Li-Ni-B system: synthesis, crystal structure and magnetic properties

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Syntheses using precursors with drastically different reactivity is a challenge. Borides are the examples of such synthetic targets, where synthesis is hampered by the inertness and high melting point of elemental boron. Although challenging to synthesize, borides exhibit interesting functionality and useful properties [1-2]. We are interested in strongly anisotropic transition metal (T) borides where the magnetic exchange between transition metal spins will be realized in T-B frameworks separated from each other by alkali metal cations. Because of the synthetic difficulties associated with the preparation of these compounds from highly reactive and volatile alkali metal and refractory and inert boron and transition metal, only few ternary compounds have been reported. For synthesis of those compounds the prolonged annealing (over 3 months) and the use of significant excess of alkali metals were previously proposed [3-5]. We have developed a fast and facile synthetic route towards alkali-transition borides using alkali metal hydrides, which were successfully implemented for preparation of different classes of ternary compounds [6]. Using this method, "$Li_{1.2}Ni_{2.5}B_2$" can be prepared within 24 hours, which is considerably faster comparing to the preparation method described in literature (3 months annealing) [3]. The structure and composition of this boride has been re-determined by means of single crystal X-ray diffraction. This allowed for the accurate determination of structural features, including splitting of Ni sites and partially occupied boron atomic positions, as well as correct composition as $LiNi_3B_{1.8}$. The hydride synthesis route has been further applied for the preparation of two previously reported ternary Li-Ni-B phases, as well as a new ternary $Li_{1.3}NiB$ phase, whose structure has not been previously reported. The crystal structure, characterization by STEM and $^{7}Li$ and $^{11}B$ solid-state NMR, as well as magnetic properties of the ternary Li-Ni-B borides will be discussed.

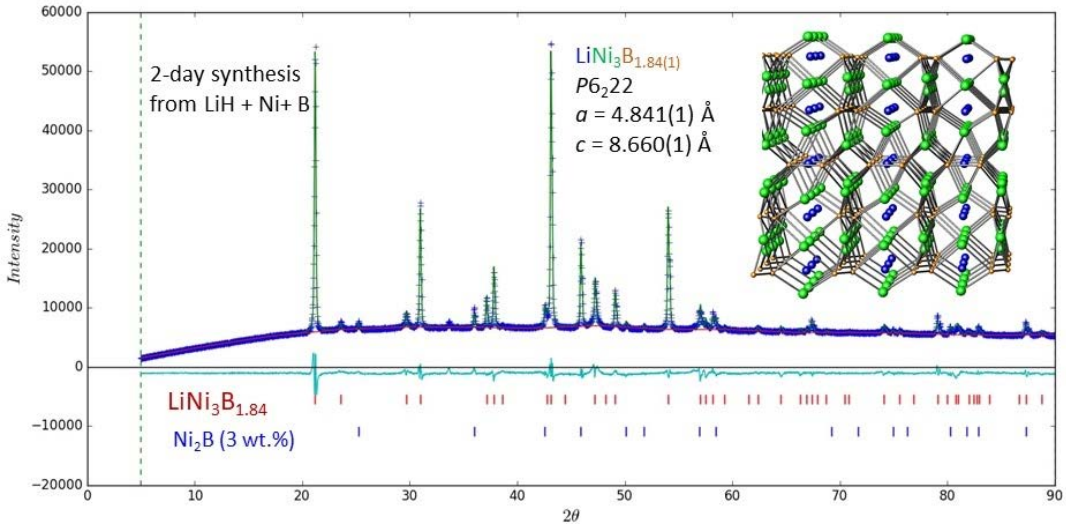


**Figure 1**. X-ray powder diffraction pattern of "$Li_{1.2}Ni_{2.5}B_2$" sample obtained after 2 days annealing of LiH + Ni + B mixture and Rietveld fit showing that target phase is a major phase with only minor content of $Ni_2B$ impurity. Insert: crystal structure of $LiNi_3B_{1.8}$; Li – blue, B – orange, Ni - green.

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