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Structural characterization of novel compounds in the M-B-C-N-H system (M=alkali metal) by means of Powder Neutron Diffraction

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Ammonia borane (NH3BH3, AB hereafter) possesses remarkable hydrogen gravimetric and volumetric capacities (19.6 wt% and 160 gH2/L, respectively) and it can release two thirds of its hydrogen atoms at moderate temperatures via a two-step decomposition process. However, the use of AB for solid-state hydrogen storage is limited by the concurrent release of volatile by-products (diborane, ammonia and borazine) and the exothermicity of the thermolysis reaction, which imposes serious difficulties to its reversible hydrogenation [1]. These drawbacks can be partially overcome by chemical substitution of H atoms in N-H groups of AB for Li or Na atoms, giving rise to the formation of the so-called alkali metal amidoboranes [2]. These compounds release pure hydrogen and present less exothermal hydrogen desorption enthalpies, showing a stabilization effect induced by alkali substitution. However, the reversible hydrogenation has not been achieved until now.

Ethane 1,2-di-amineborane (BH3NH2CH2CH2NH2BH3) (EDAB hereafter) is a chemical derivative of ammonia borane that has been recently considered as an interesting material for hydrogen storage applications [3]. EDAB releases ca. 10 wt% of hydrogen in a two-step process taking place at moderate temperatures. It does not desorb volatile by-products in addition to hydrogen and presents a higher thermal stability than AB. Structural properties of EDAB have been investigated in the 70Ł??s by means of X-ray diffraction (XRD) [4]. However, as far as we know, there are no neutron diffraction studies on this compound. We aim at synthesizing EDAB by using 11B and D isotopes in order to do neutron diffraction measurements in EDAB.

Next, we aim at investigating the structural properties of novel compounds in the M-B-C-N-H system (M=alkali metal) for hydrogen storage applications. These compounds will be prepared by reactive milling of EDAB (enriched with 11B and D) with alkali deuterides (LiD and NaD) under inert atmosphere. Preliminary XRD results show the formation of novel crystalline phases upon reactive milling of the base compounds. As far as we know, these compounds have not been previously reported in the literature. In this context, powder neutron diffraction constitutes a unique technique to characterize the structural properties of these novel compounds.

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