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Synthesis and characterization of amide-borohydrides: New complex light hydrides for potential hydrogen storage

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Abstract

The reactions $x\text{LiNH}_2 + (1-x)\text{LiBH}_4$ and $x\text{NaNH}_2 + (1-x)\text{NaBH}_4$ have been investigated and new phases identified. The lithium amide-borohydride system is dominated by a body centred cubic compound of formula $\text{Li}_4\text{BH}_4(\text{NH}_2)_3$. In the sodium system, a new hydride of approximate composition $\text{Na}_2\text{BH}_4\text{NH}_2$ has been identified with a primitive cubic structure and lattice parameter $a \approx 4.7 \text{ \AA}$. The desorption of gases from the two amide-borohydrides on heating followed a similar pattern with the relative proportions of H_2 and NH_3 released depending critically on the experimental set-up: in the IGA, ammonia release occurred in two steps – beginning at 60 and 260 °C for $\text{Li}_4\text{BH}_4(\text{NH}_2)_3$ – the second of which was accompanied by hydrogen release; in the TPD system the main desorption product was hydrogen again at 260 °C for $\text{Li}_4\text{BH}_4(\text{NH}_2)_3$ accompanied by around 5% ammonia.

We hypothesize that the BH_4^- anion can play a similar role to LiH in the $\text{LiNH}_2 + \text{LiH}$ system, where ammonia release is suppressed in favour of hydrogen. The reaction $x\text{LiNH}_2 + (1-x)\text{LiAlH}_4$ did not result in the production of any new phases but TPD experiments show that hydrogen is released from the mixture $2\text{LiNH}_2 + \text{LiAlH}_4$, over a wide temperature range. We conclude that mixed complex hydrides may provide a means of tuning the dehydrogenation and rehydrogenation reactions to make viable storage systems.



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Keywords

Hydrogen storage materials; Chemical synthesis; Amide; Borohydride; Temperature programmed desorption

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