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The Decomposition of α-$LiN_2H_3BH_3$: an Unexpected Hydrogen Release from a Homopolar Proton−Proton Pathway

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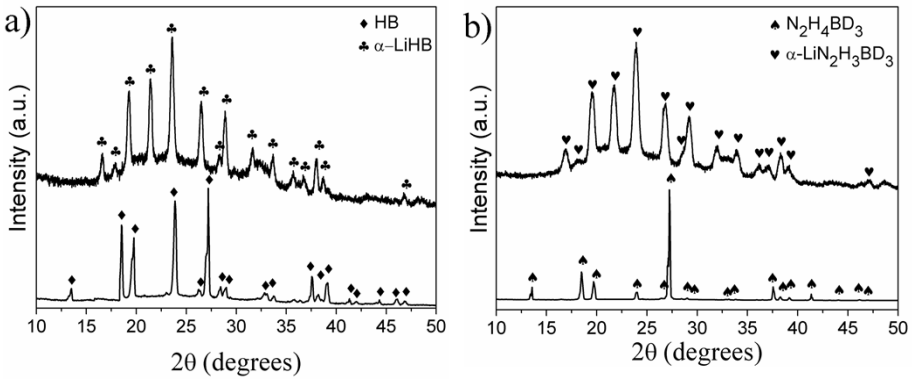

Fig. S1 XRD patterns of HB and α-$LiN_2H_3BH_3$ (a), $N_2H_3BD_3$ and α-$LiN_2H_3BD_3$ (b).

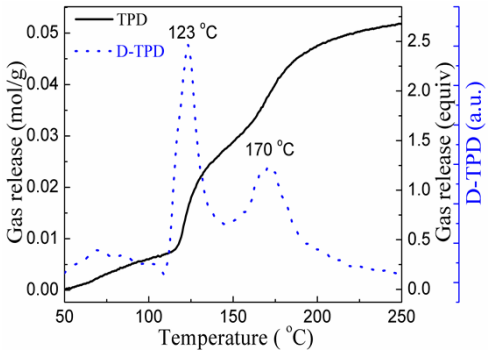

Fig. S2 Non-isothermal TPD curve and its differential curve (D-TPD) with a heating rate of 5 ^{o}C min^{-1} for the decomposition of α-LiHB.

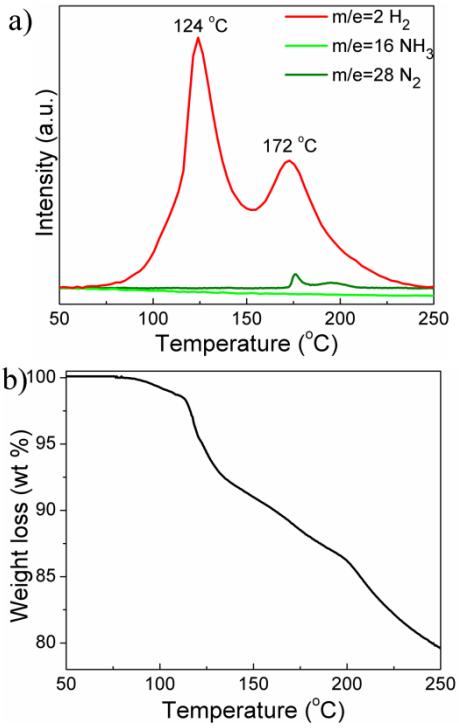

Fig. S3 a) MS and b) TG profiles of α-LiHB with a heating rate of 5 ^{o}C min^{-1} in argon.

The dehydrogenation properties of α-LiHB were investigated using Temperature-Programmed Desorption (TPD) and thermogravimetry analysis/mass spectroscopy (TG/MS) measurements with a heating rate of 5 ^{o}C min^{-1} as shown in Fig. S2 and S3. The TPD and TG/MS results are in good agreement with the previous reports.

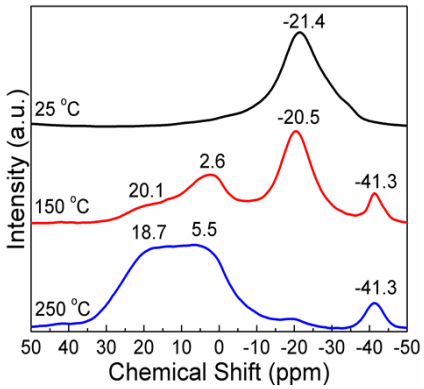

Fig. S4 ^{11}B NMR results for α-LiHB before and after heating to 150 °C and 250 °C.