The Decomposition of $\alpha$-LiN$_2$H$_3$BH$_3$: an Unexpected Hydrogen Release from a Homopolar Proton–Proton Pathway

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Fig. S1 XRD patterns of HB and α-LiN$_2$H$_3$BH$_3$ (a), N$_2$H$_3$BD$_3$ and α-LiN$_2$H$_3$BD$_3$ (b).
**Fig. S2** Non-isothermal TPD curve and its differential curve (D-TPD) with a heating rate of 5 °C min\(^{-1}\) for the decomposition of α-LiHB.
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 °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 $\alpha$-LiHB before and after heating to 150 °C and 250 °C.