Supporting Information

Synthesis, Structure and Dehydrogenation Mechanism of Calcium Amidoborane Hydrazinates

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Fig. S1. XRD patterns of Ca(NH$_2$BH$_3$)$_2$, Ca(NH$_2$BH$_3$)$_2$-1/2N$_2$H$_4$, Ca(NH$_2$BH$_3$)$_2$-N$_2$H$_4$, Ca(NH$_2$BH$_3$)$_2$·2N$_2$H$_4$, Ca(NH$_2$BH$_3$)$_2$-3N$_2$H$_4$. 
Fig. S2. FTIR spectra of Ca(NH₂BH₃)₂, Ca(NH₂BH₃)₂-1/2N₂H₄, Ca(NH₂BH₃)₂-N₂H₄, Ca(NH₂BH₃)₂·2N₂H₄.
Fig. S3. $^{11}$B NMR of Ca(NH$_2$BH$_3$)$_2$, Ca(NH$_2$BH$_3$)$_2$-1/2N$_2$H$_4$, Ca(NH$_2$BH$_3$)$_2$-N$_2$H$_4$, Ca(NH$_2$BH$_3$)$_2$·2N$_2$H$_4$.

Fig. S4. MS profiles of the gaseous products of Ca(NH$_2$BH$_3$)$_2$, Ca(NH$_2$BH$_3$)$_2$-1/2N$_2$H$_4$, Ca(NH$_2$BH$_3$)$_2$-N$_2$H$_4$, Ca(NH$_2$BH$_3$)$_2$·2N$_2$H$_4$ after heating at 150°C.
Fig. S5. FTIR spectra of Ca(NH$_2$BH$_4$)$_2$·1/2N$_2$H$_4$ after heating at 80°C, 100°C, 150°C, 250°C and room temperature.

Fig. S6. TPD profiles of hydrogen desorption from Ca(NH$_2$BH$_4$)$_2$·1/2N$_2$H$_4$ at ramping rates of 2, 4, 6, and 8 K/ min, respectively.
Fig. S7. TPD profiles of hydrogen desorption from Ca(NH$_2$BH$_3$)$_2$ at ramping rates of 2, 4, 6, and 8 K/ min, respectively.

Fig. S8. FTIR spectra of Ca(NH$_2$BH$_3$)$_2$-1/2N$_2$H$_4$, Ca(NH$_2$BD$_3$)$_2$-1/2N$_2$H$_4$ and Ca(ND$_2$BH$_3$)$_2$-1/2N$_2$H$_4$. 
Fig. S9. XRD of Ca(NH$_2$BH$_3$)$_2$-1/2N$_2$H$_4$, Ca(NH$_2$BD$_3$)$_2$-1/2N$_2$H$_4$ and Ca(ND$_2$BH$_3$)$_2$-1/2N$_2$H$_4$. 