Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supporting Information

## Synthesis, Structure and Dehydrogenation Mechanism of Calcium Amidoborane Hydrazinates

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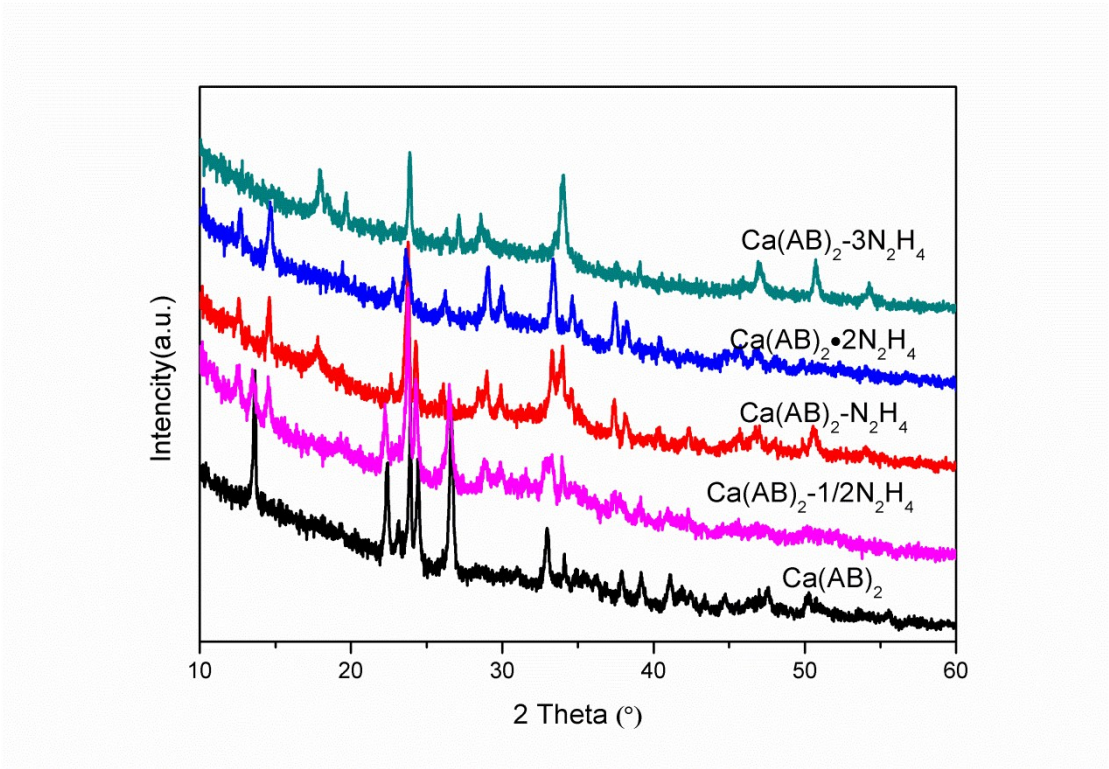


Fig. S1. XRD patterns of $Ca(NH_2BH_3)_2$, $Ca(NH_2BH_3)_2$-$1/2N_2H_4$, $Ca(NH_2BH_3)_2$-$N_2H_4$, $Ca(NH_2BH_3)_2 \cdot 2N_2H_4$, $Ca(NH_2BH_3)_2$-$3N_2H_4$.

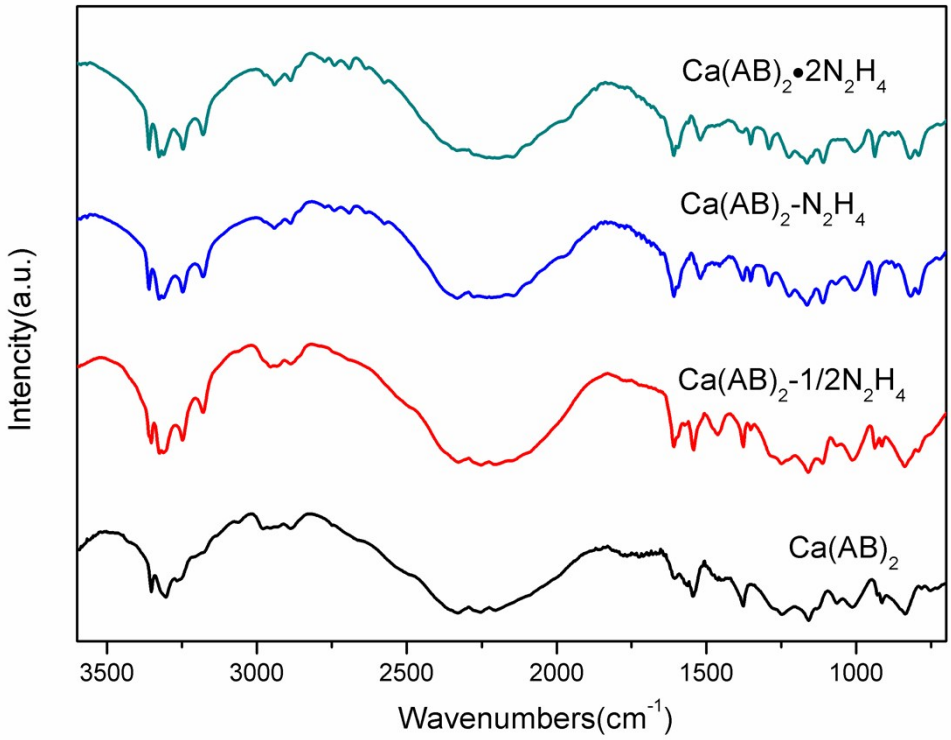


Fig. S2. FTIR spectra of $Ca(NH_2BH_3)_2$, $Ca(NH_2BH_3)_2$-$1/2N_2H_4$, $Ca(NH_2BH_3)_2$-$N_2H_4$, $Ca(NH_2BH_3)_2 \cdot 2N_2H_4$.

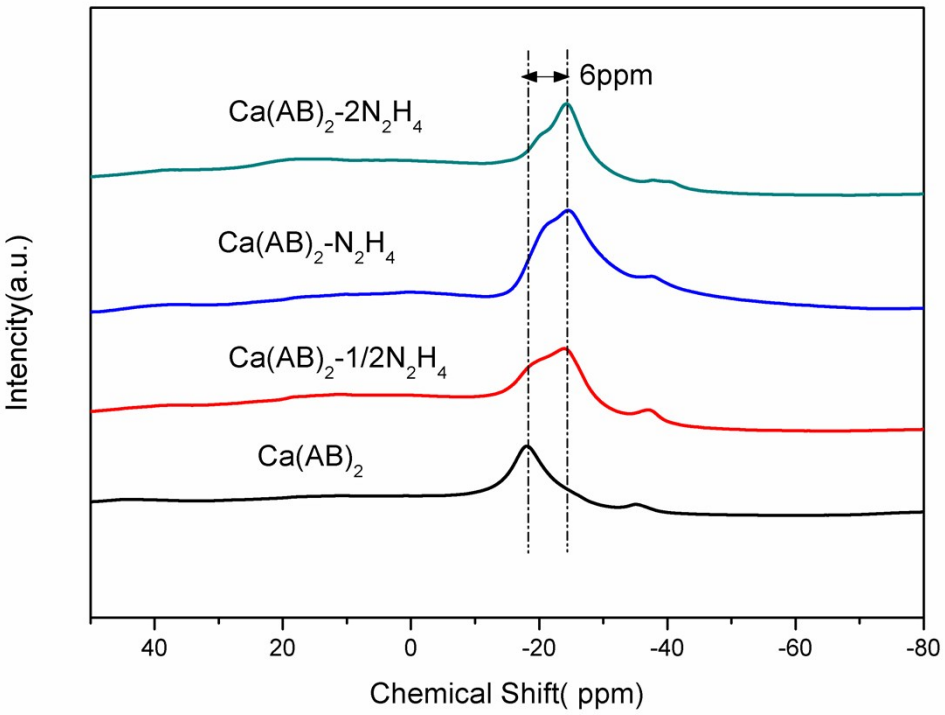


Fig. S3. $^{11}B$ NMR of $Ca(NH_2BH_3)_2$, $Ca(NH_2BH_3)_2$-$1/2N_2H_4$, $Ca(NH_2BH_3)_2$-$N_2H_4$, $Ca(NH_2BH_3)_2 \cdot 2N_2H_4$.

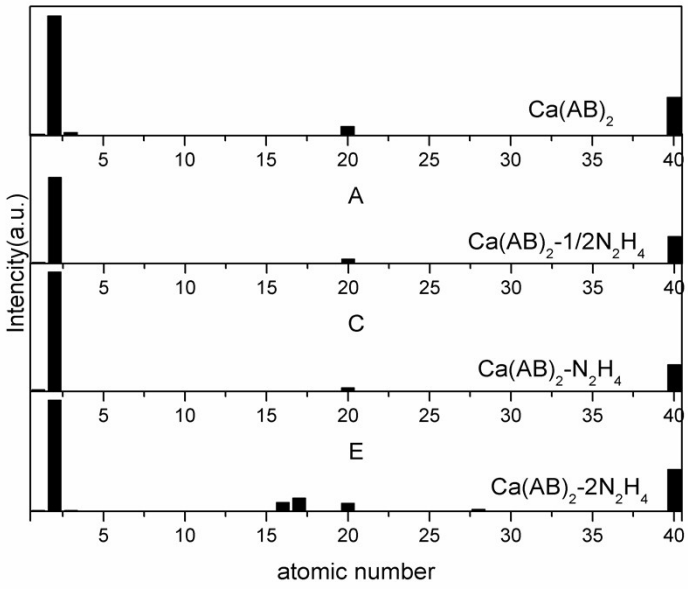


Fig. S4. MS profiles of the gaseous products of $Ca(NH_2BH_3)_2$, $Ca(NH_2BH_3)_2$-$1/2N_2H_4$, $Ca(NH_2BH_3)_2$-$N_2H_4$, $Ca(NH_2BH_3)_2 \cdot 2N_2H_4$ after heating at 150°C.

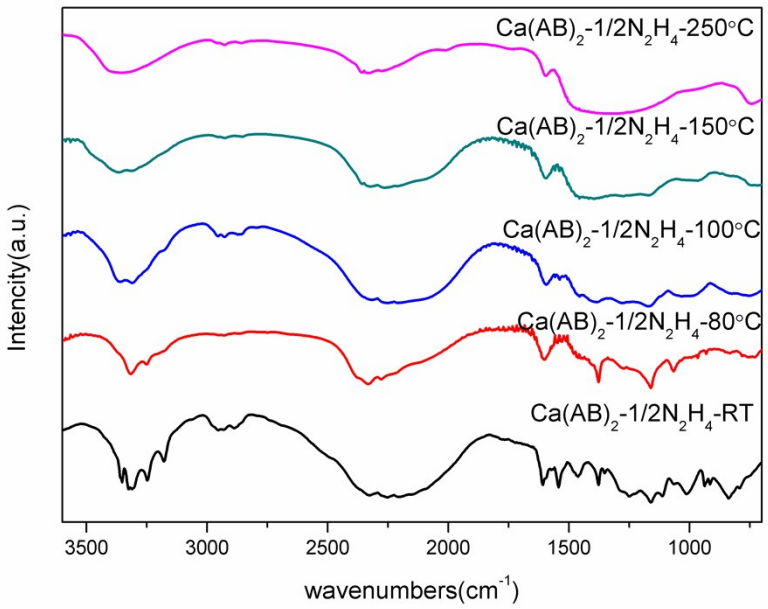


Fig. S5. FTIR spectra of $Ca(NH_2BH_3)_2$-$1/2N_2H_4$ after heating at 80°C, 100°C, 150°C, 250°C and room temperature.

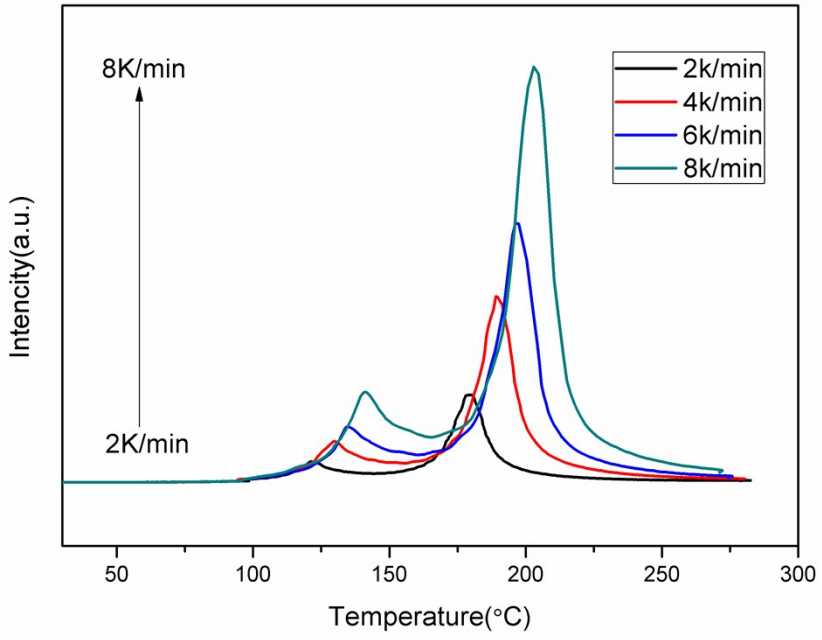


Fig. S6. TPD profiles of hydrogen desorption from $Ca(NH_2BH_3)_2$-$1/2N_2H_4$ at ramping rates of 2, 4, 6, and 8 K/ min, respectively.

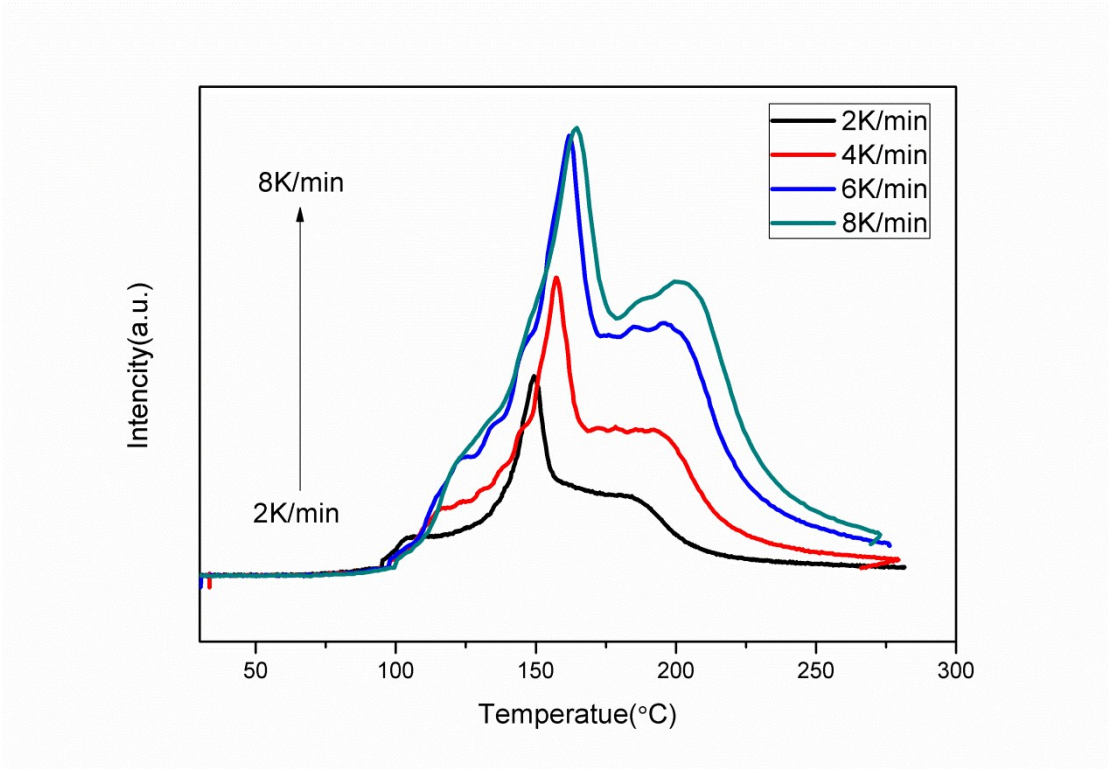


Fig. S7. TPD profiles of hydrogen desorption from $Ca(NH_2BH_3)_2$ at ramping rates of 2, 4, 6, and 8 K/ min, respectively.

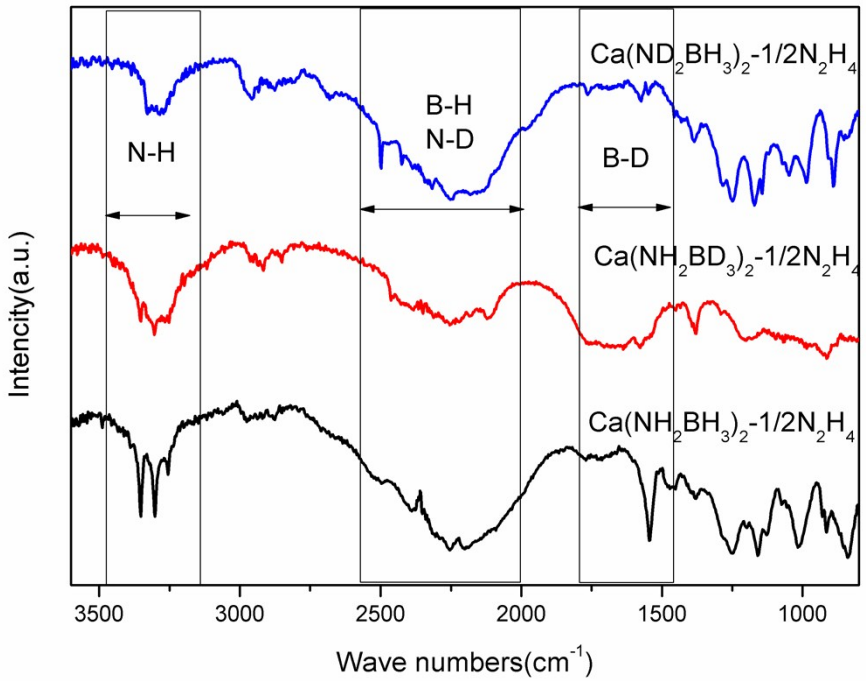


Fig. S8. FTIR spectra of $Ca(NH_2BH_3)_2$-$1/2N_2H_4$, $Ca(NH_2BD_3)_2$-$1/2N_2H_4$ and $Ca(ND_2BH_3)2$-$1/2N_2H_4$.

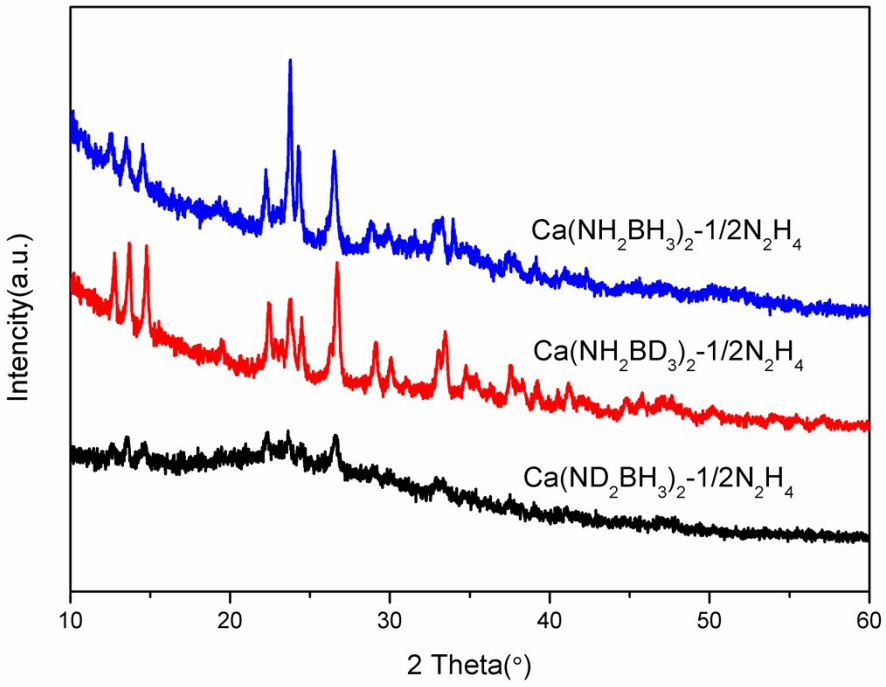


Fig. S9. XRD of $Ca(NH_2BH_3)_2$-$1/2N_2H_4$, $Ca(NH_2BD_3)_2$-$1/2N_2H_4$ and $Ca(ND_2BH_3)_2$-$1/2N_2H_4$.