Supporting information

Investigation of the dynamics in $KSiH_3$ and new bi-anionic $K[SiH_3]_{1-x}[BH_4]_x$ complex hydrides by MAS-NMR spectroscopy

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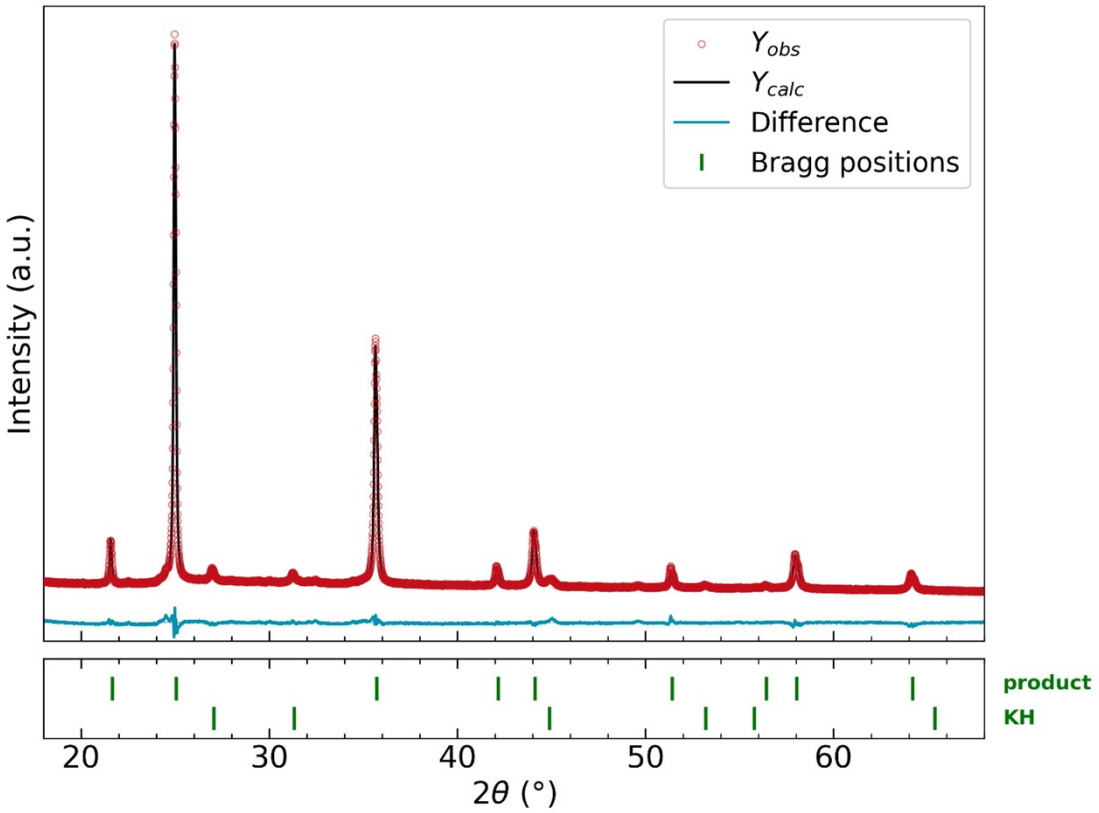

Figure S1. Rietveld refinement of $K[SiH_3]_{0.75}[BH_4]_{0.25}$

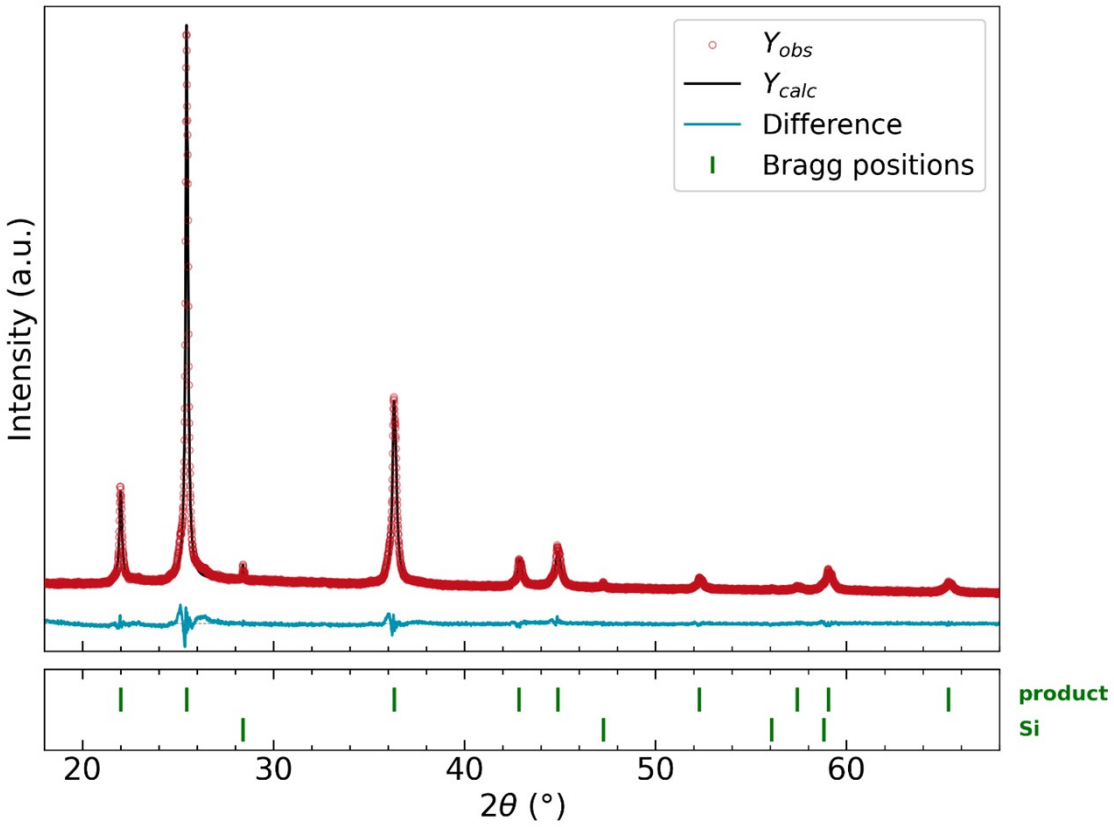

Figure S2. Rietveld refinement of $K[SiH_3]_{0.5}[BH_4]_{0.5}$

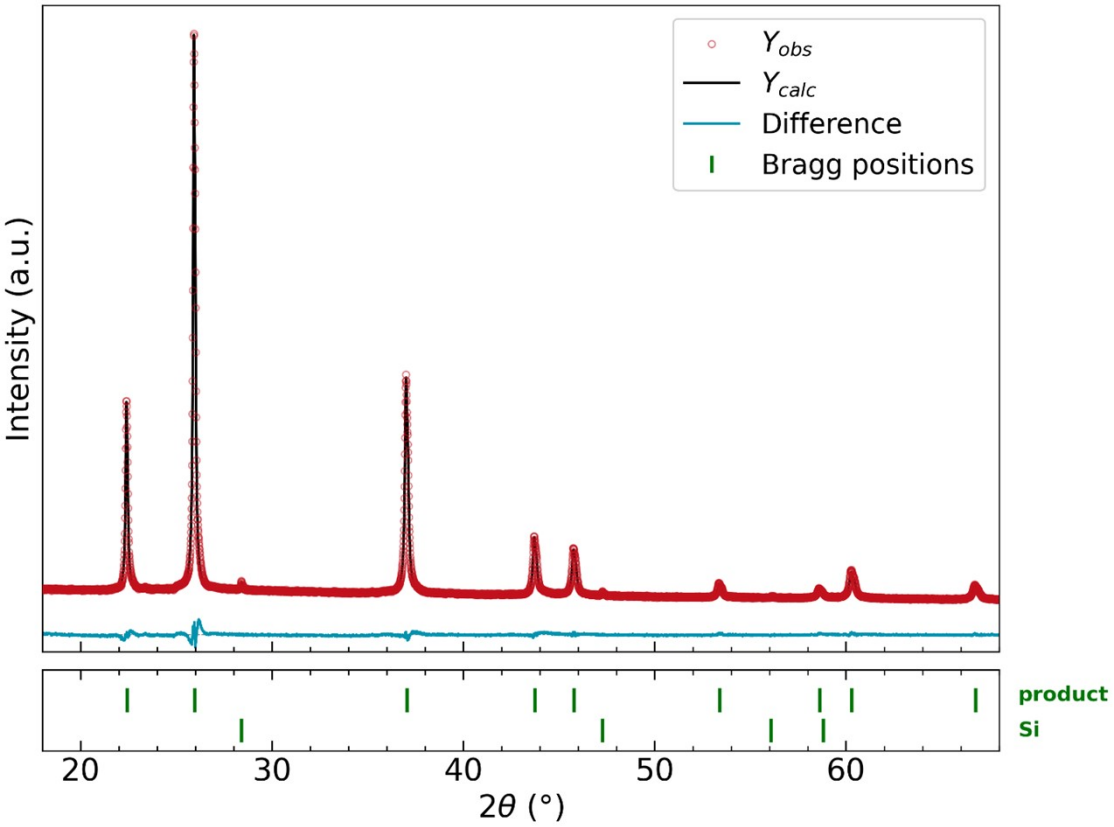

Figure S3. Rietveld refinement of $K[SiH_3]_{0.25}[BH_4]_{0.75}$

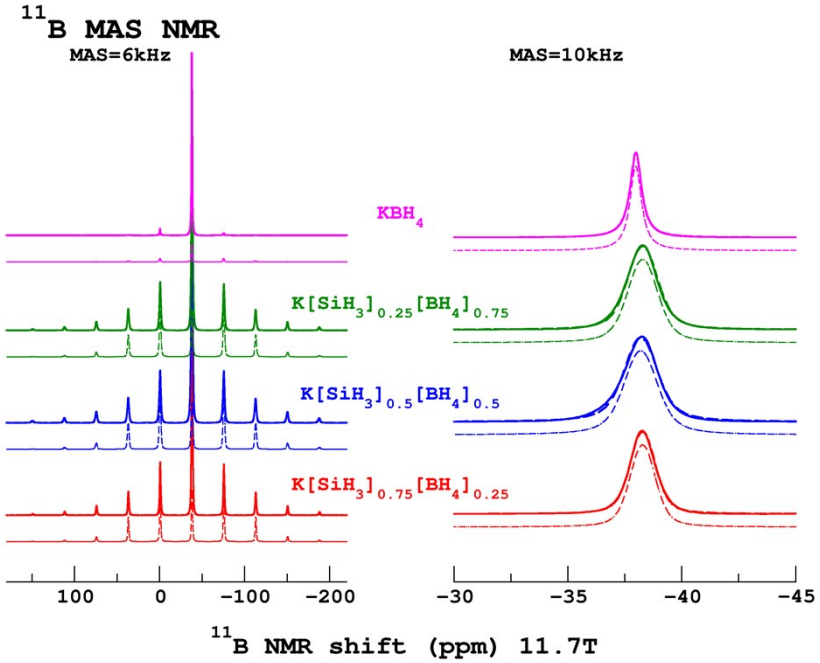

Figure S4. ^{11}B MAS NMR spectra acquired at 6 kHz and 12.5 kHz of $K[SiH_3]_{0.75}[BH4]_{0.25}$ (red), $K[SiH_3]_{0.5}[BH4]_{0.5}$ (blue), $K[SiH_3]_{0.25}[BH4]_{0.75}$ (green), and KBH_4 (magenta). The dashed lines represent the simulation spectra used to extract the NMR parameters (cf. Table 2 in the main text).

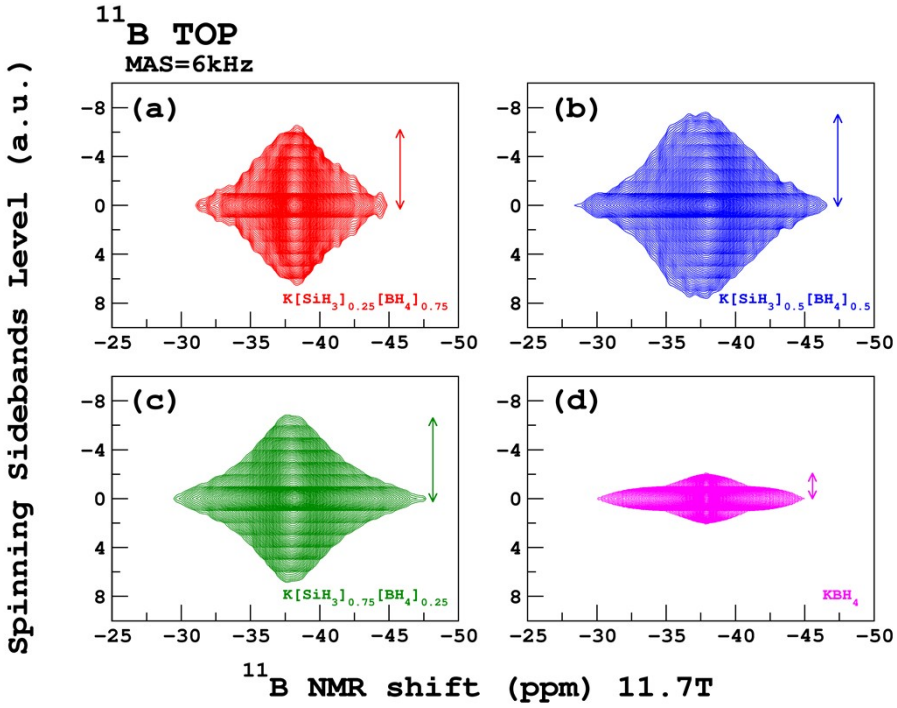

Figure S5. (a-d) ^{11}B Two-Dimensional One Pulse (TOP) spectra reconstructed from MAS-NMR spectra acquired at a spinning frequency of 6 kHz.

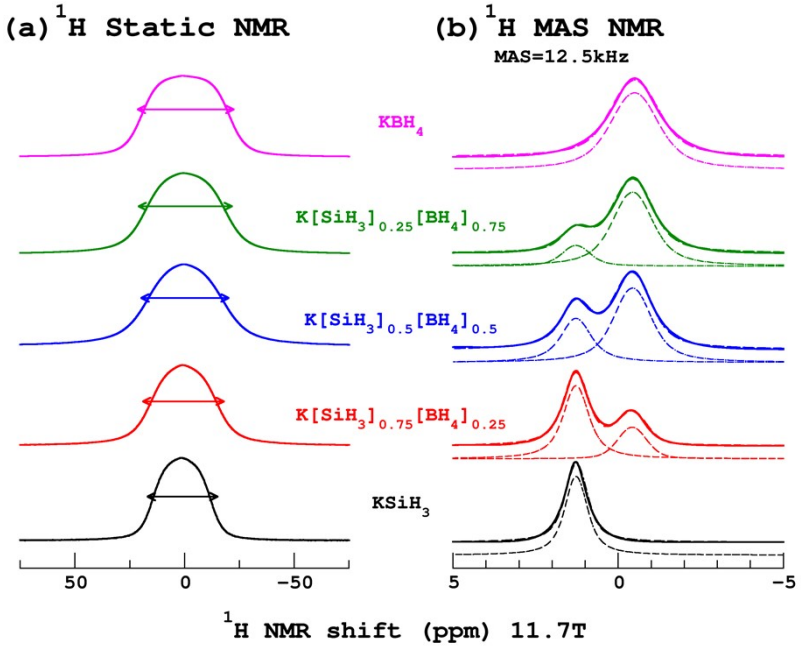

Figure S6. (a) ^{1}H static and (b) ^{1}H MAS NMR spectra of $KSiH_3$ (black), $K[SiH_3]_{0.75}[BH_4]_{0.25}$ (red), $K[SiH_3]_{0.5}[BH_4]_{0.5}$ (blue), $K[SiH_3]_{0.25}[BH_4]_{0.75}$ (green), and KBH_4 (magenta). The arrows indicate the FWHM values of static spectra, and the dashed lines represent the simulations.

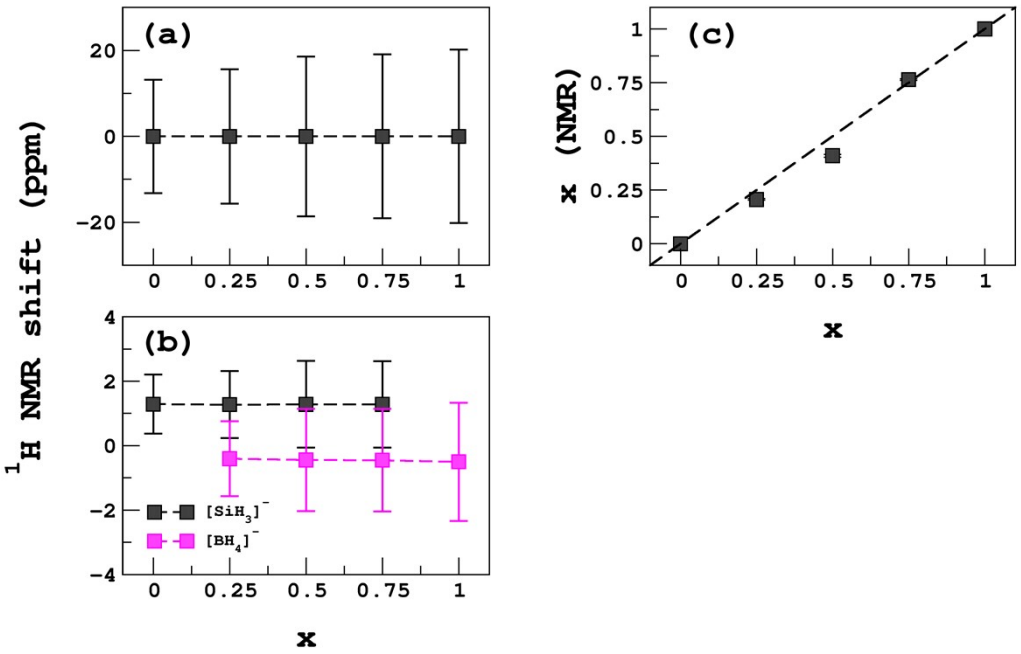

Figure S7. (a-b) the evolution of chemical of shift of ^{1}H chemical shift of ^{1}H in static and MAS NMR, respectively, with error bar corresponding to the FWHM. (c) Experimental x values calculated from NMR versus theoretical x.

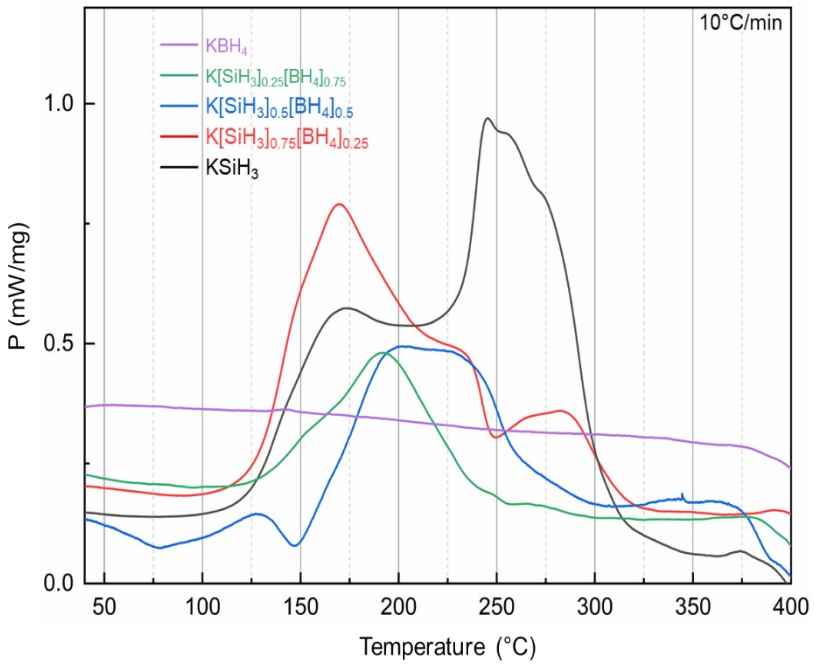

Figure S8. Differential scanning calorimetry of KBH_4, $KSiH_3$ and $K[SiH_3]_{1-x}[BH_4]_x$ with x = 0.25, 0.5, 0.75.

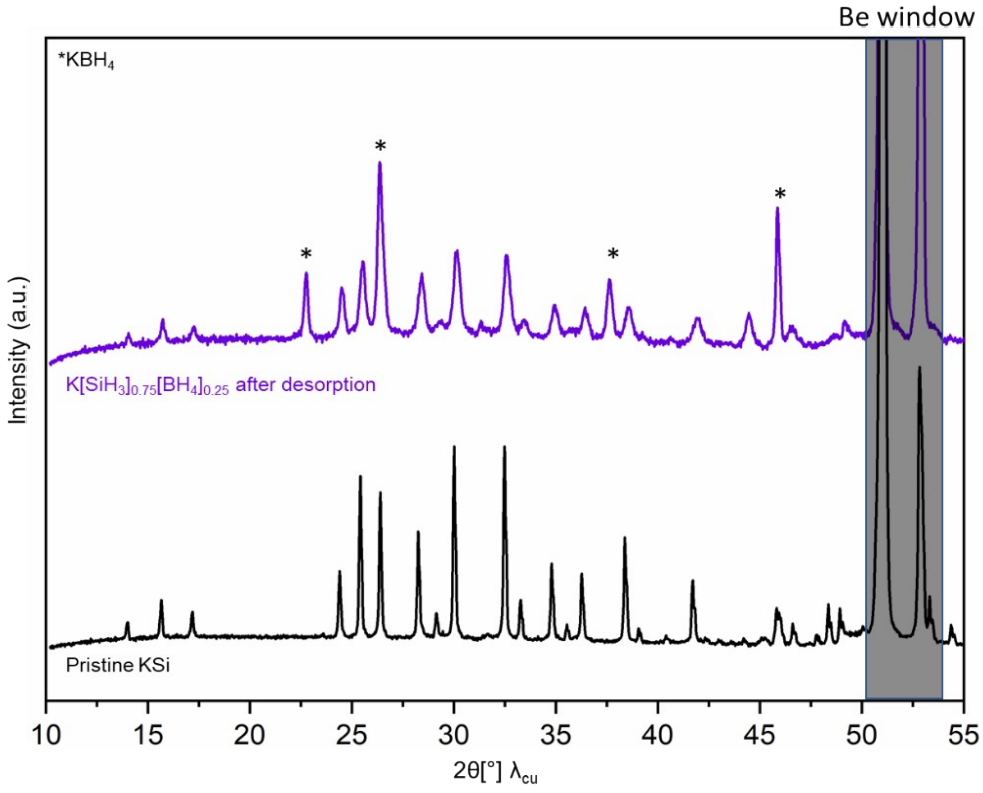

Figure S9. XRD patterns of $K[SiH_3]_{0,75}[BH_4]_{0,25}$ after desorption at 240°C and pristine KSi as reference.