Supporting Info

Synthesis and Thermal Stability of Perovskite Alkali Metal Strontium Borohydrides

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**Figure S1.** *In situ* SR-PXD data of the NaBH$_4$–Sr(BH$_4$)$_2$ (1:1) composite measured from RT to 500 °C (\(\Delta T/\Delta t = 10 \, ^\circ\text{C}/\text{min}, p(\text{Ar}) = 1 \, \text{bar}, \lambda = 1.1037 \, \text{\AA}\)). Symbols: NaBH$_4$ (grey square), Sr(BH$_4$)$_2$ (white circle), WC (black five pointed star), Unknown 5 (black square), Unknown 6 (grey triangle), Unknown 7 (black triangle).

Initially, Sr(BH$_4$)$_2$, NaBH$_4$ and WC are present. Around 250 °C, intensity from Sr(BH$_4$)$_2$ decreases while new peaks belonging to 5 arises. Around 320 °C reflections from Sr(BH$_4$)$_2$ disappear while Bragg peaks from 5 disappear at 360 °C. No diffraction from SrB$_6$ or SrH$_2$ is identified. Instead, Bragg peaks belonging to 6 appear between 360 and 400 °C when finally reflections from 7 shows up and is present until the end of the measurement.
Figure S2. PXD pattern of KBH$_4$ – Sr(BH$_4$)$_2$ (1:1) after decomposition at $T = 550$ °C and $p$(H$_2$) = 1 bar ($\lambda = 1.54056$ Å). Symbols: KBH$_4$ (white hexagon), SrH$_2$ (white square), SrB$_6$ (white diamond), WC (black five pointed star), Unknown 8 (black arrow).

An unknown (8) compound is present at $2\theta = 16.4, 26.9, 28.5, 32.6, 33.3, 35.0$ and 41.0° ($d = 5.38, 3.31, 3.12, 2.74, 2.69, 2.55$ and 2.19 Å).
Figure S3. PXD pattern of RbBH$_4$–Sr(BH$_4$)$_2$ (1:1) after decomposition at 550 °C $T = 550$ °C and $p$(H$_2$) = 1 bar ($\lambda = 1.54056$ Å). Symbols: RbBH$_4$ (grey hexagon), SrH$_2$ (white square), SrB$_6$ (white diamond), WC (black five pointed star), Unknown 9 (white arrow).

An unknown (9) compound is present at 20 = 24.1, 27.1, 32.5 and 33.3 ($d = 3.69, 3.29, 2.74$ and 2.68 Å). The reflections at $d = 2.74$ and 2.68 are similar to those unknown in KSr, hence the unknown compound probably contains Sr. However, it has not been possible to identify the compound.
Figure S4. PXD pattern of CsBH$_4$ – Sr(BH$_4$)$_2$ (1:1) after decomposition at $T = 550 \, ^\circ\text{C}$ and $p(\text{H}_2) = 1 \, \text{bar}$ ($\lambda = 1.54056 \, \text{Å}$). Symbols: CsBH$_4$ (black hexagon), SrH$_2$ (white square), SrB$_6$ (white diamond), WC (black five pointed star), Unknown 10 (grey arrow).

An unknown (10) compound is present at $2\theta = 27.0$ and $32.4^\circ$ ($d = 3.29$ and 2.76).
Figure S5. FT-IR of KBH$_4$ – Sr(BH$_4$)$_2$ (1:1) after decomposition at 550 °C (black curve) and hydrogenation at 350 °C and $p$(H$_2$) = 100 bar (red curve).
Figure S6. FT-IR of RbBH$_4$ – Sr(BH$_4$)$_2$ (1:1) after decomposition at 550 °C (black curve) and hydrogenation at 350 °C at $p$(H$_2$) = 100 bar (red curve).
**Figure S7.** FT-IR of CsBH$_4$ – Sr(BH$_4$)$_2$ (1:1) after decomposition at 550 °C (black curve) and hydrogenation at 350 °C at $p$(H$_2$) = 100 bar (red curve).
Figure S8. Sieverts measurement of $\text{KBH}_4 - \text{Sr(BH}_4\text{)}_2$ (1:1) showing the two desorptions conducted in the temperature range $\text{RT} - 550 \degree \text{C}$ ($\Delta T/\Delta t = 3 \degree \text{C}/\text{min}$ and $p(\text{H}_2) = 1 \text{ bar}$).
Figure S9. Sieverts measurement of RbBH$_4$ – Sr(BH$_4$)$_2$ (1:1) showing the two desorptions conducted in the temperature range RT – 550 °C ($\Delta T/\Delta t = 3$ °C/min and $p$(H$_2$) = 1 bar).
Figure S10. Sieverts measurement of CsBH$_4$ – Sr(BH$_4$)$_2$ (1:1) showing the two desorptions conducted in the temperature range RT – 550 °C ($\Delta T/\Delta t = 3$ °C/min and $p$(H$_2$) = 1 bar).