

Supporting Info

Synthesis and Thermal Stability of Perovskite Alkali Metal Strontium Borohydrides

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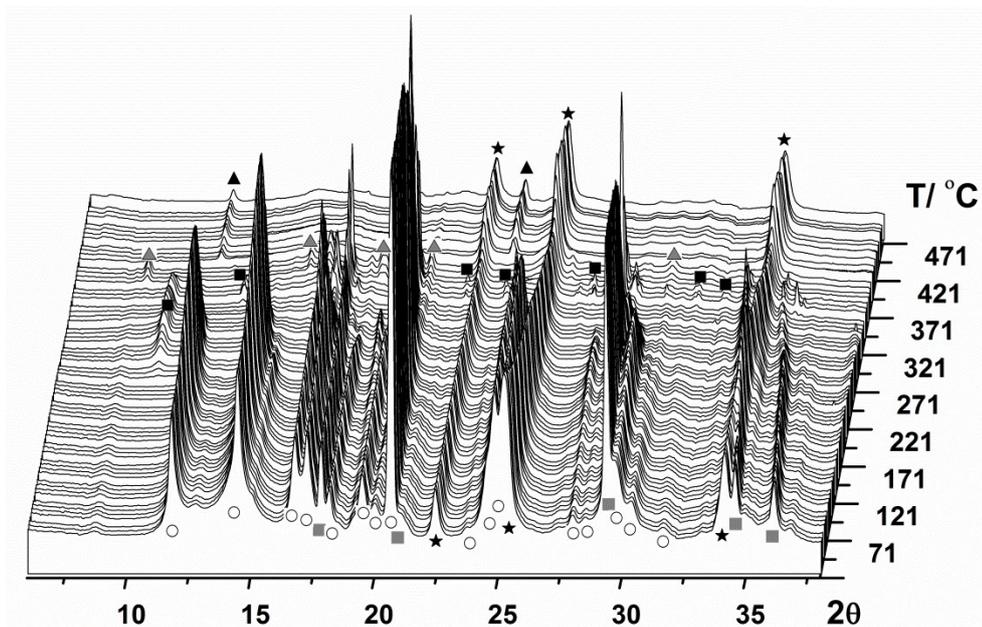


Figure S1. *In situ* SR-PXD data of the $\text{NaBH}_4\text{-Sr}(\text{BH}_4)_2$ (1:1) composite measured from RT to 500 °C ($\Delta T/\Delta t = 10$ °C/min, $p(\text{Ar}) = 1$ bar, $\lambda = 1.1037$ Å). Symbols: NaBH_4 (grey square), $\text{Sr}(\text{BH}_4)_2$ (white circle), WC (black five pointed star), Unknown 5 (black square), Unknown 6 (grey triangle), Unknown 7 (black triangle).

Initially, $\text{Sr}(\text{BH}_4)_2$, NaBH_4 and WC are present. Around 250 °C, intensity from $\text{Sr}(\text{BH}_4)_2$ decreases while new peaks belonging to 5 arises. Around 320 °C reflections from $\text{Sr}(\text{BH}_4)_2$ 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.

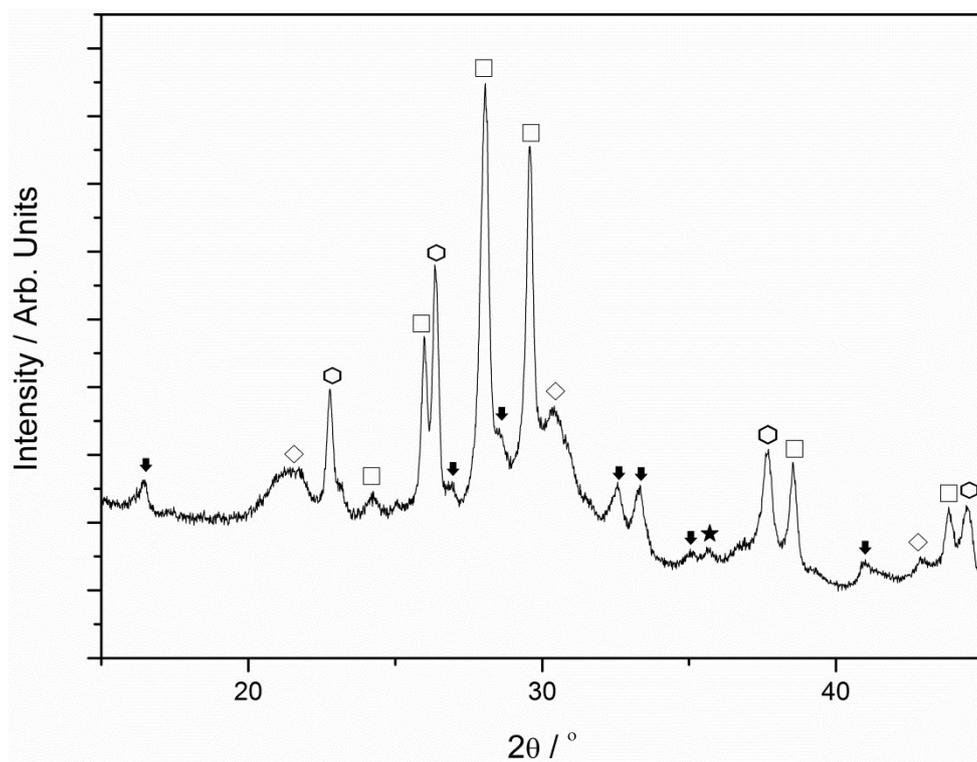


Figure S2. PXD pattern of $\text{KBH}_4 - \text{Sr}(\text{BH}_4)_2$ (1:1) after decomposition at $T = 550\text{ }^\circ\text{C}$ and $p(\text{H}_2) = 1$ bar ($\lambda = 1.54056\text{ \AA}$). Symbols: KBH_4 (white hexagon), SrH_2 (white square), SrB_6 (white diamond), WC (black five pointed star), Unknown **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 \AA).

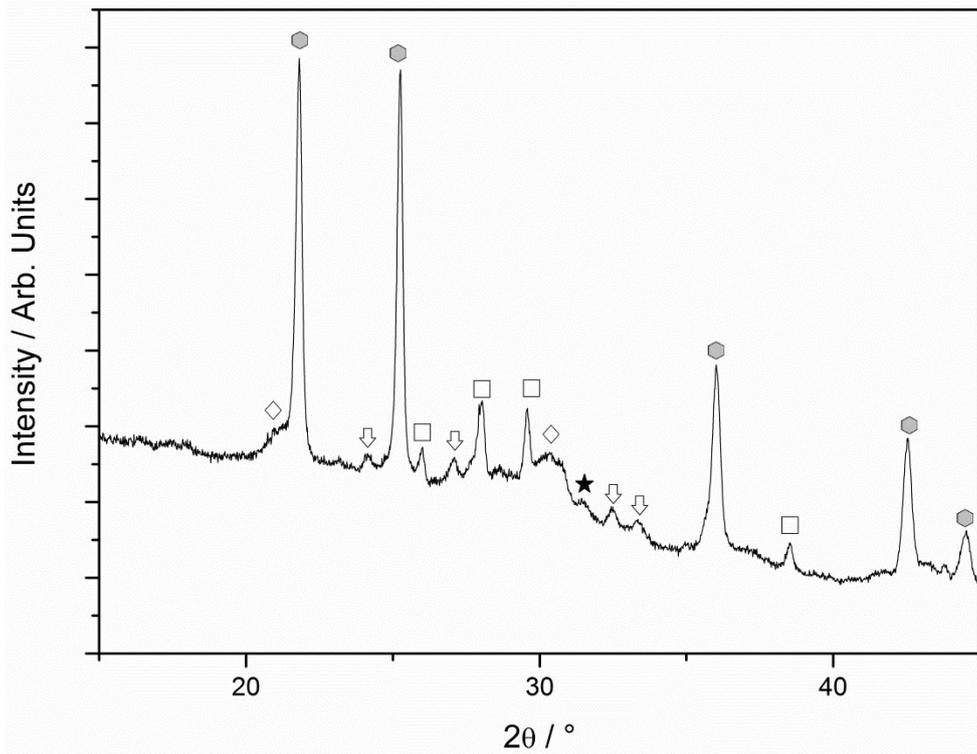


Figure S3. PXD pattern of $\text{RbBH}_4 - \text{Sr}(\text{BH}_4)_2$ (1:1) after decomposition at 550 °C $T = 550\text{ °C}$ and $p(\text{H}_2) = 1\text{ bar}$ ($\lambda = 1.54056\text{ \AA}$). Symbols: RbBH_4 (grey hexagon), SrH_2 (white square), SrB_6 (white diamond), WC (black five pointed star), Unknown **9** (white arrow).

An unknown (**9**) compound is present at $2\theta = 24.1, 27.1, 32.5$ and 33.3 ($d = 3.69, 3.29, 2.74$ and 2.68 \AA). 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.

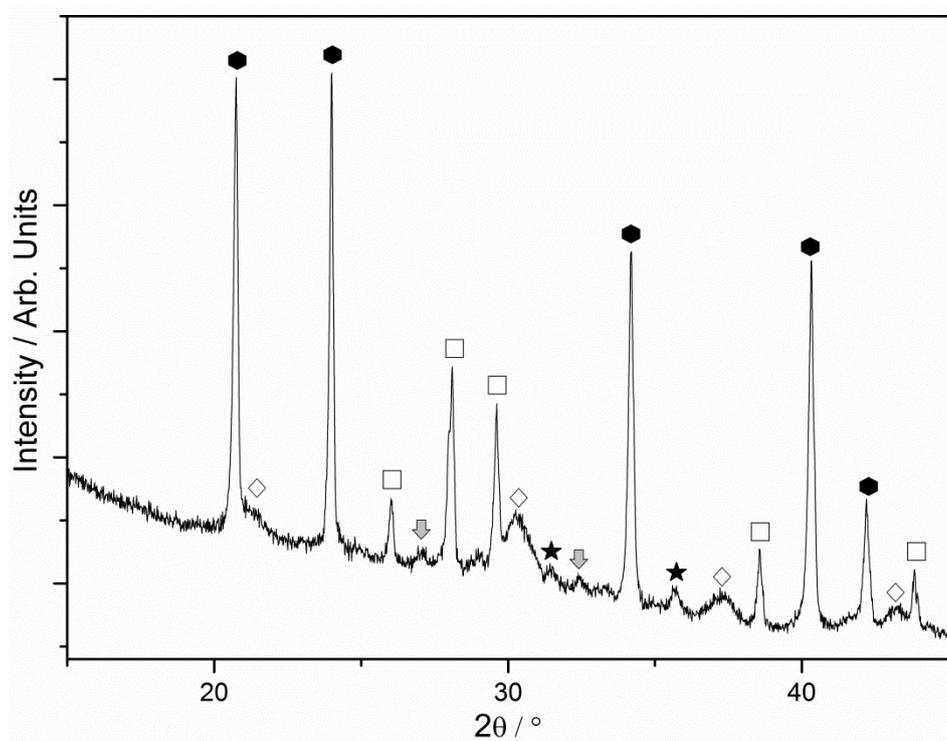


Figure S4. PXD pattern of $\text{CsBH}_4 - \text{Sr}(\text{BH}_4)_2$ (1:1) after decomposition at $T = 550\text{ °C}$ and $p(\text{H}_2) = 1\text{ bar}$ ($\lambda = 1.54056\text{ Å}$). Symbols: CsBH_4 (black hexagon), SrH_2 (white square), SrB_6 (white diamond), WC (black five pointed star), Unknown **10** (grey arrow).

An unknown (**10**) compound is present at $2\theta = 27.0$ and 32.4° ($d = 3.29$ and 2.76).

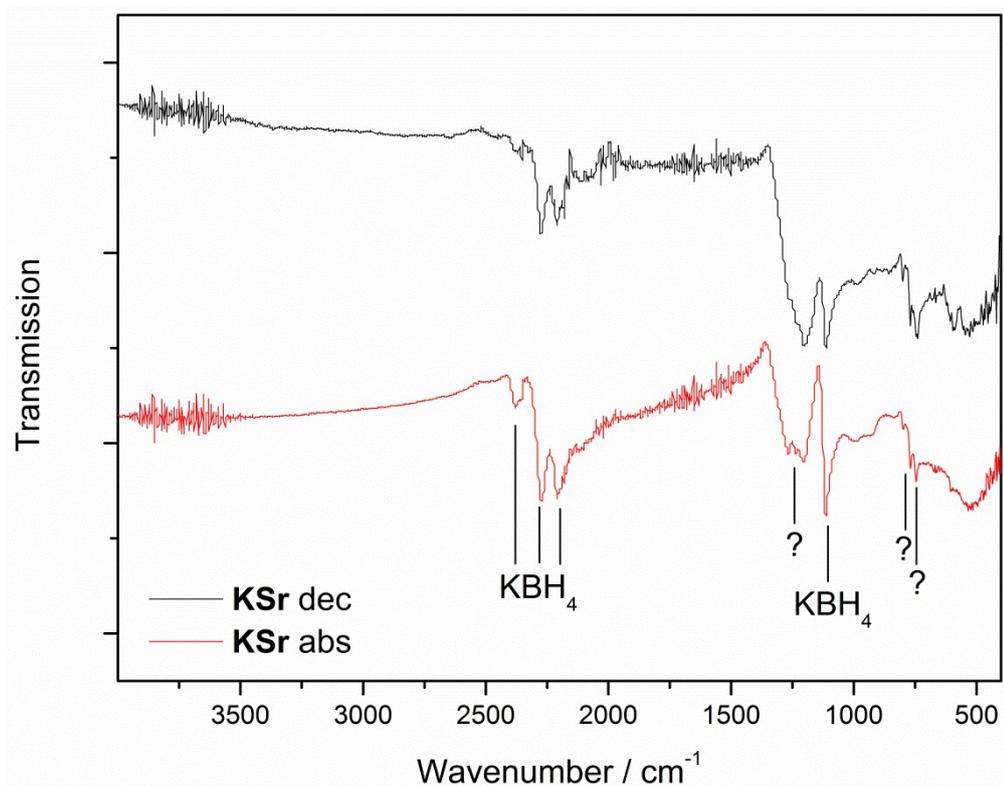


Figure S5. FT-IR of $\text{KBH}_4 - \text{Sr}(\text{BH}_4)_2$ (1:1) after decomposition at 550 °C (black curve) and hydrogenation at 350 °C and $p(\text{H}_2) = 100$ bar (red curve).

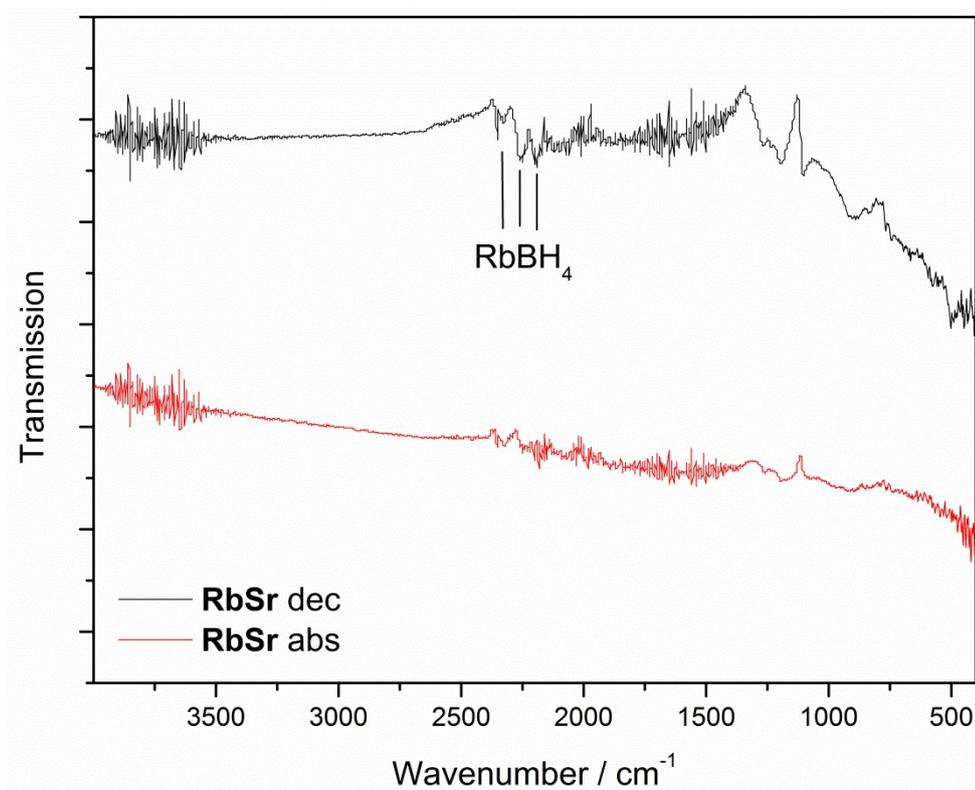


Figure S6. FT-IR of $\text{RbBH}_4 - \text{Sr}(\text{BH}_4)_2$ (1:1) after decomposition at 550 °C (black curve) and hydrogenation at 350 °C at $p(\text{H}_2) = 100$ bar (red curve).

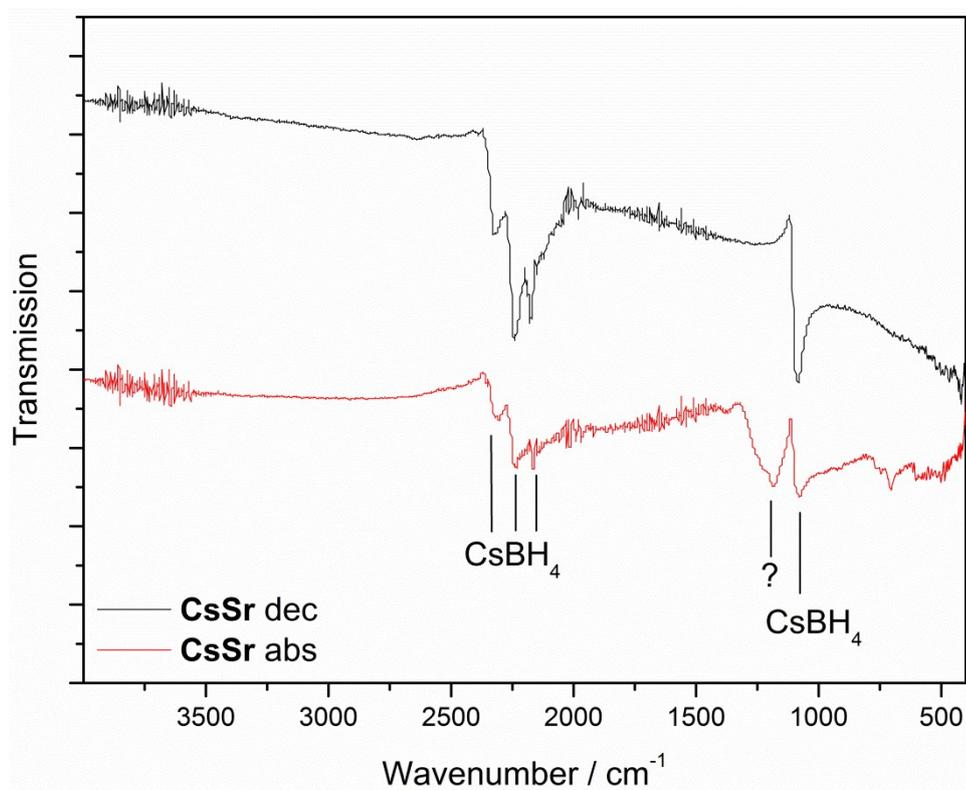


Figure S7. FT-IR of CsBH₄ – Sr(BH₄)₂ (1:1) after decomposition at 550 °C (black curve) and hydrogenation at 350 °C at $p(\text{H}_2) = 100$ bar (red curve).

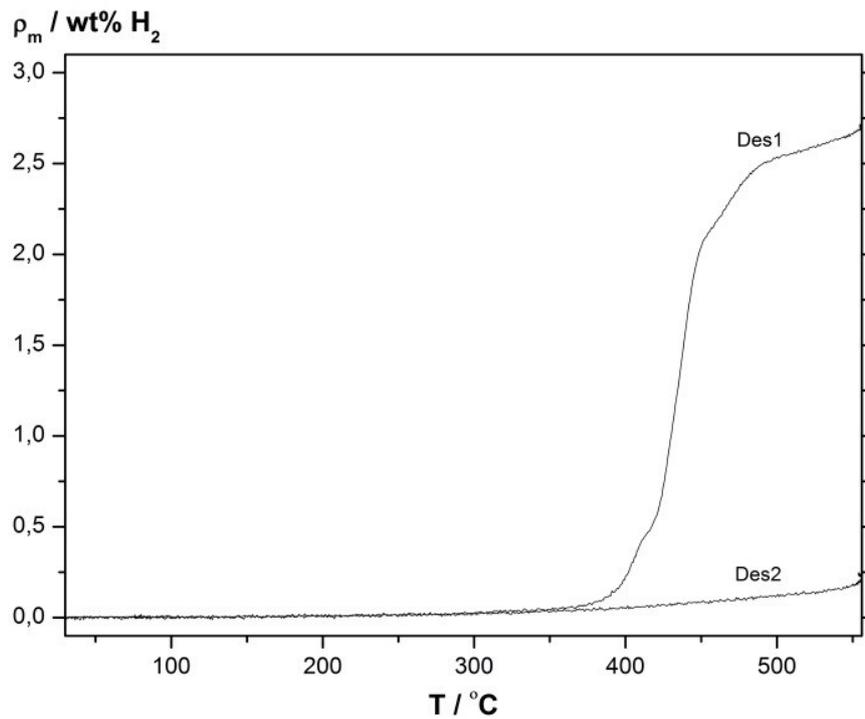


Figure S8. Sieverts measurement of $\text{KBH}_4 - \text{Sr}(\text{BH}_4)_2$ (1:1) showing the two desorptions conducted in the temperature range RT – 550 $^\circ\text{C}$ ($\Delta T/\Delta t = 3$ $^\circ\text{C}/\text{min}$ and $p(\text{H}_2) = 1$ bar).

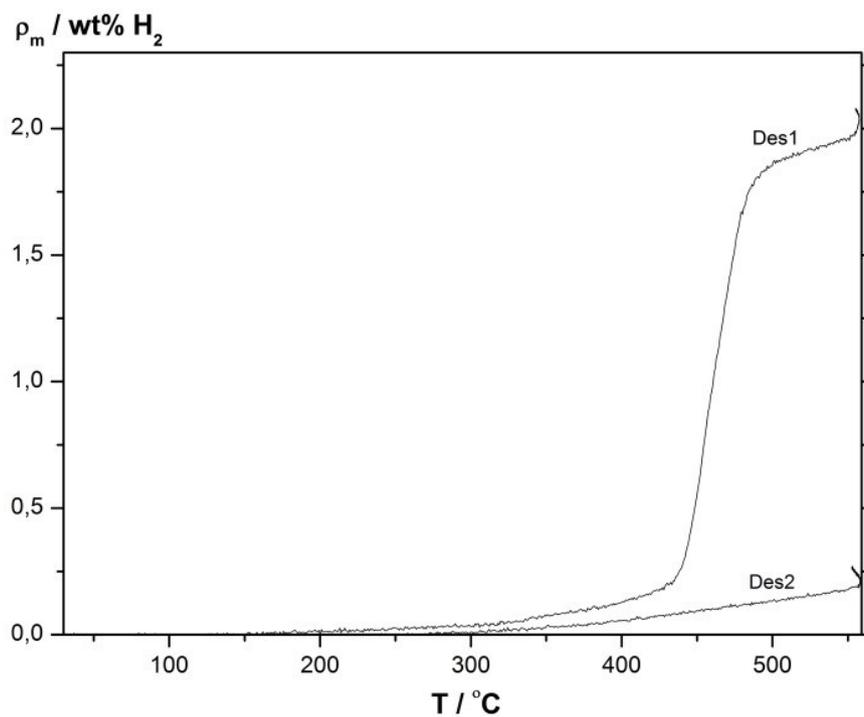


Figure S9. Sieverts measurement of $\text{RbBH}_4 - \text{Sr}(\text{BH}_4)_2$ (1:1) showing the two desorptions conducted in the temperature range RT – 550 °C ($\Delta T/\Delta t = 3$ °C/min and $p(\text{H}_2) = 1$ bar).

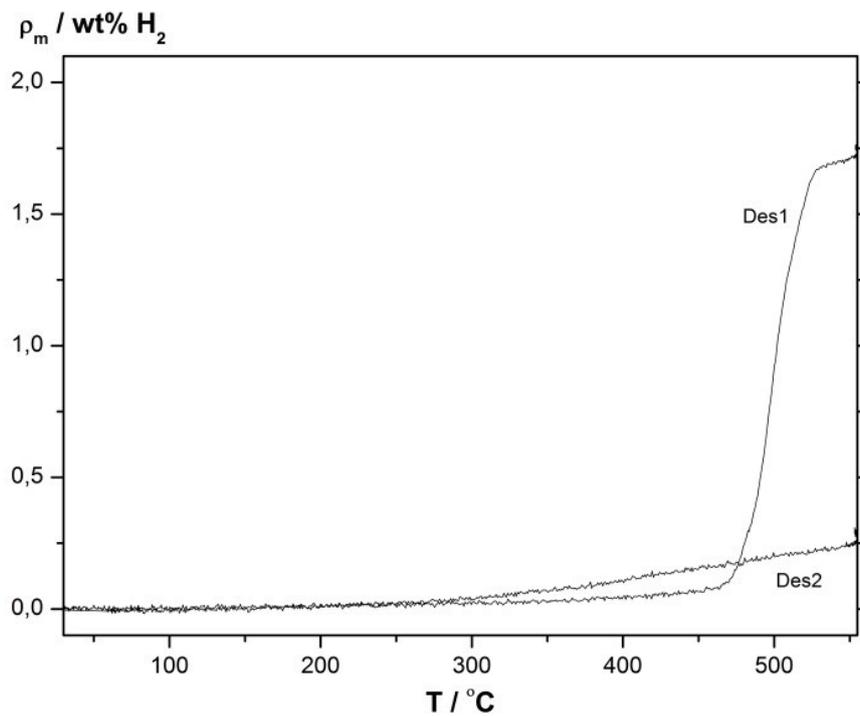


Figure S10. Sieverts measurement of $\text{CsBH}_4 - \text{Sr}(\text{BH}_4)_2$ (1:1) showing the two desorptions conducted in the temperature range RT – 550 °C ($\Delta T/\Delta t = 3$ °C/min and $p(\text{H}_2) = 1$ bar).