

Supporting information

In Situ X-ray Diffraction Studies on the De/re-hydrogenation Processes of the $K_2[Zn(NH_2)_4]\cdot 8LiH$ System

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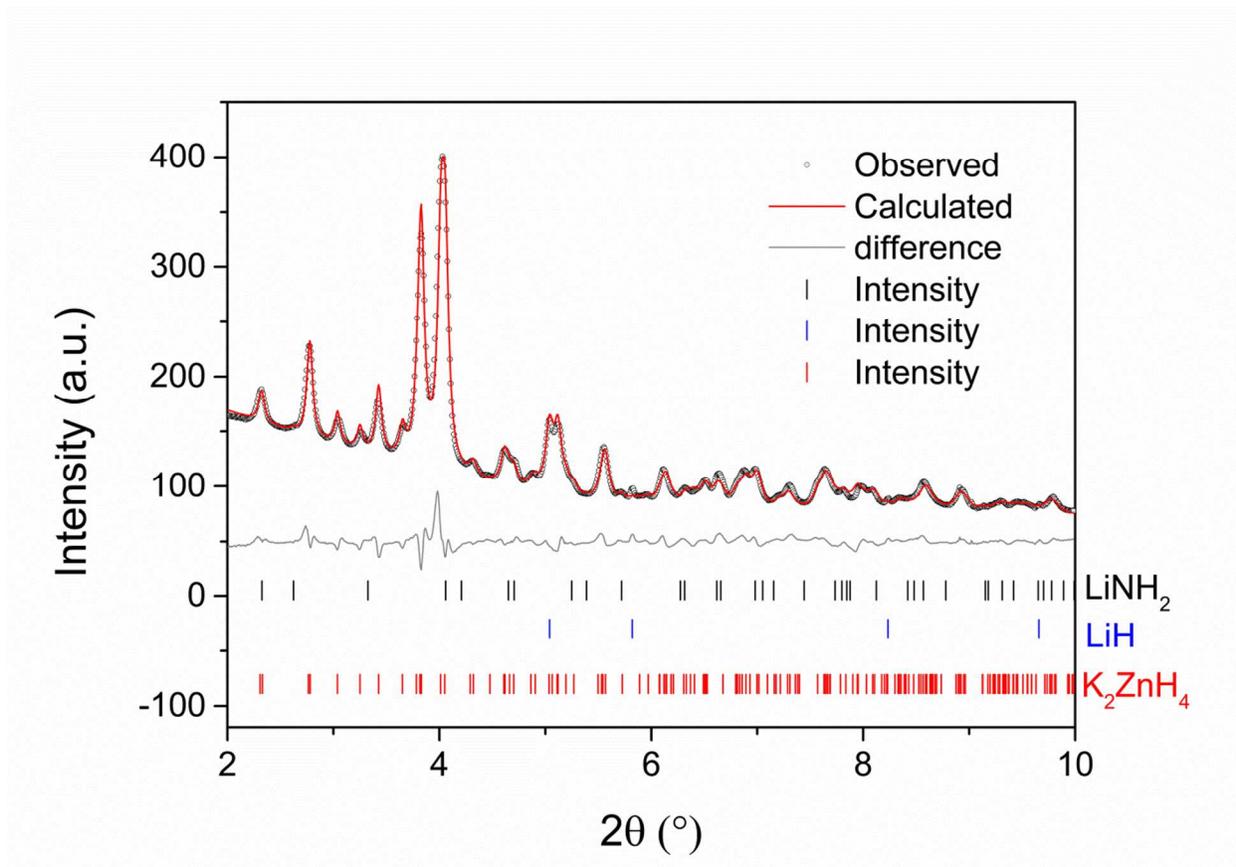


Figure S1. X-ray diffraction pattern (black dots) and Rietveld refinement (red line) of the as-ball milled $\text{K}_2[\text{Zn}(\text{NH}_2)_4]\cdot 8\text{LiH}$ ($4\text{LiNH}_2\cdot 4\text{LiH}\cdot \text{K}_2\text{ZnH}_4$) sample. Bragg reflections for each phase are indicated by the tick marks. The bottom line represents the difference curve ($I_{\text{obs}} - I_{\text{calc}}$). Weighted R-factor is $R_w(\%) = 3.05$. The refinement results show the weight contents of LiNH_2 , LiH and K_2ZnH_4 are ca. 33.53%, 10.28% and 56.19 %, respectively, which match well with the theoretical values (33.90% for LiNH_2 , 11.79% for LiH and 54.31 for K_2ZnH_4).

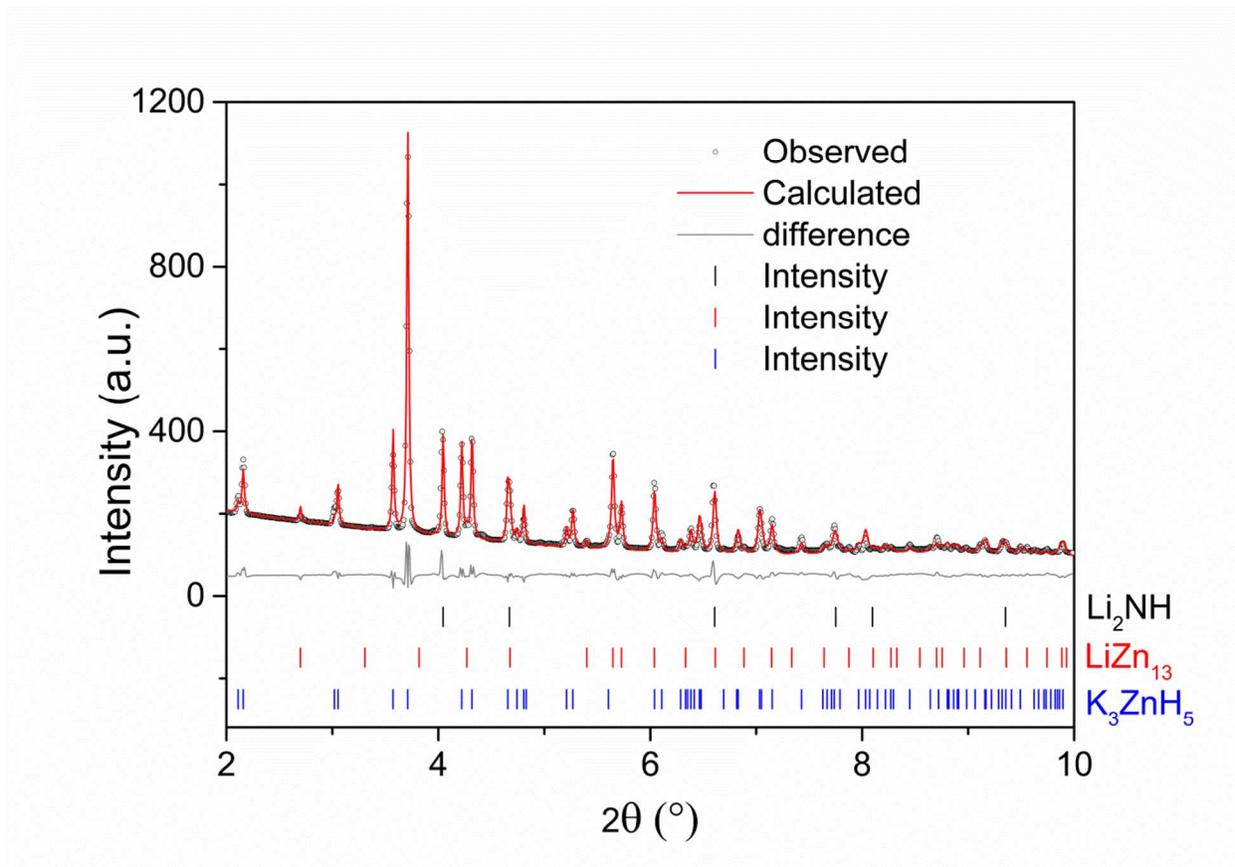


Figure S2. X-ray diffraction pattern (black dots) and Rietveld refinement (red line) of the $\text{K}_2[\text{Zn}(\text{NH}_2)_4]\cdot 8\text{LiH}$ sample after dehydrogenation to 316 °C. Bragg reflections for each phase are indicated by the tick marks. The bottom line represents the difference curve ($I_{\text{obs}} - I_{\text{calc}}$). The weighted R-factor is $R_w(\%) = 6.68$.

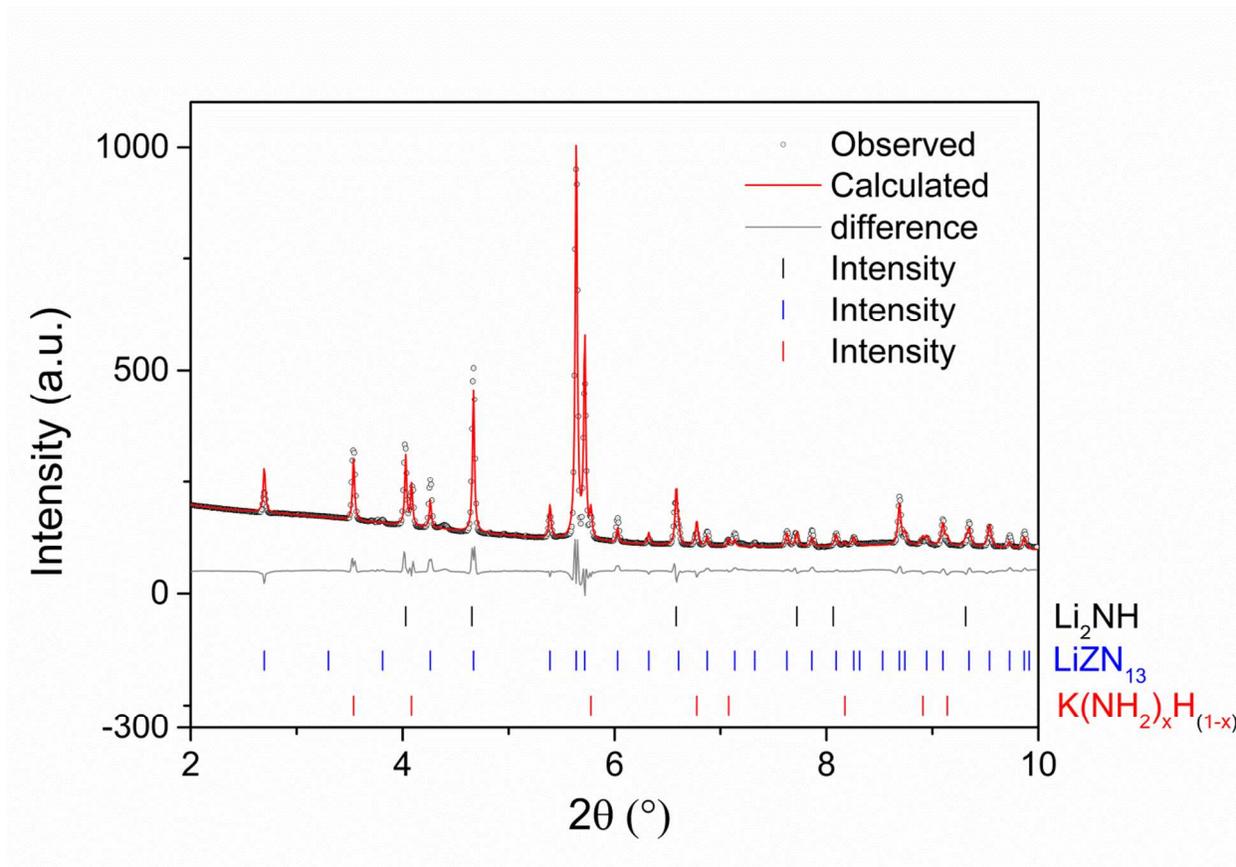


Figure S3. X-ray diffraction pattern (black dots) and Rietveld refinement (red line) of the $\text{K}_2[\text{Zn}(\text{NH}_2)_4]-8\text{LiH}$ sample dehydrogenated at 357 °C. Bragg reflections for each phase are indicated by the tick marks. The bottom line represents the difference curve ($I_{\text{obs}}-I_{\text{calc}}$) and the weighted R-factors is $R_w(\%)=6.91$.

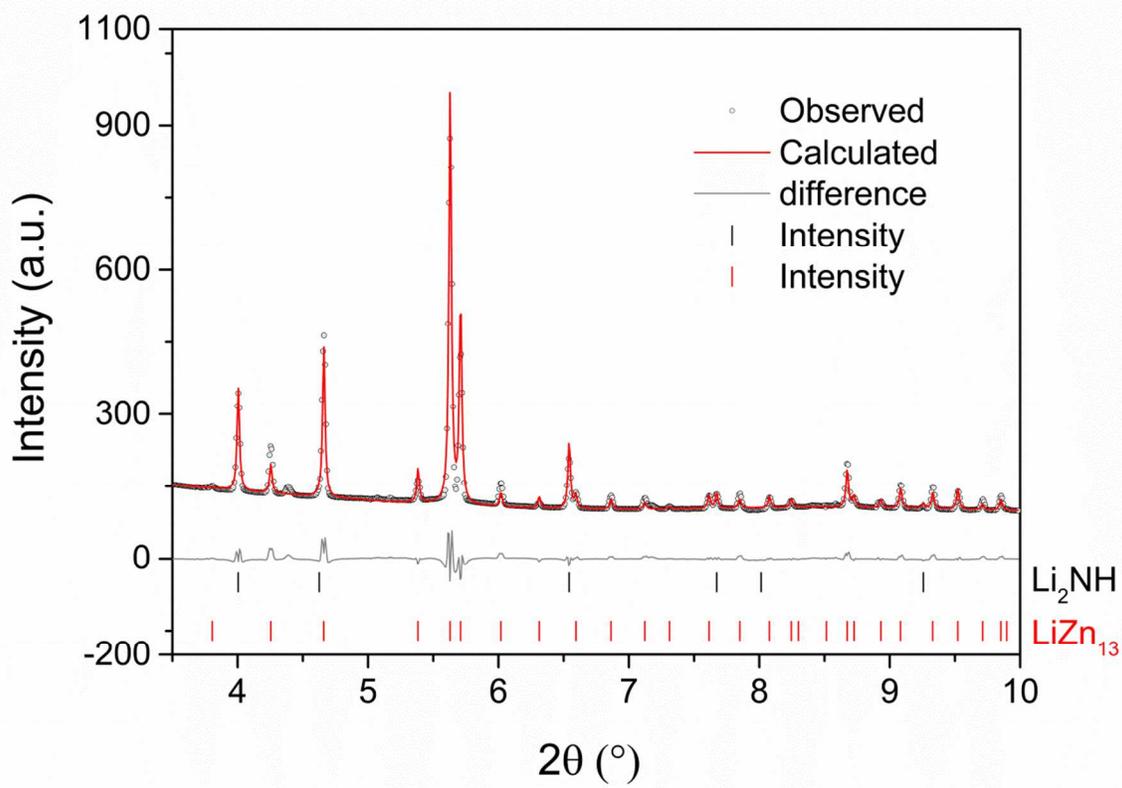


Figure S4. X-ray diffraction pattern (black dots) and Rietveld refinement (red line) of the $\text{K}_2[\text{Zn}(\text{NH}_2)_4]\cdot 8\text{LiH}$ sample after dehydrogenation at 400°C . Bragg reflections for each phase are indicated by the tick marks. The bottom line represents the difference curve ($I_{\text{obs}} - I_{\text{calc}}$). The weighted R-factor is $R_w(\%) = 6.61$.