Electronic Supplemental Information for:

Ammonium chloride-metal hydride based reaction cycle for vehicular applications

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Table S1. Predicted reaction pathways and calculated standard enthalpy of reaction for each of the systems studied.

Sample Reaction Path	Calculated $\Delta H°$ at 25°C/mol NH_4Cl of reaction (kJ/mol)	Theoretical reaction weight loss (%)		
		H_2	NH_3	Total
$NH_4Cl_{(s)} + NaH_{(s)} \rightarrow NaCl_{(s)} + H_{2(g)} + NH_{3(g)}$	−86.1	2.6	21.9	24.6
$NH_4Cl_{(s)} + NaH_{(s)} + PdCl_{2(s)} \rightarrow NaCl_{(s)} + H_{2(g)} + NH_{3(g)} + PdCl_{2(s)}$ (1mol% / 10 mol %)	−86.1	2.6/2.1	21.7/17.9	24.3/20.0
$NH_4Cl_{(s)} + NaNH_{2(s)} \rightarrow NaCl_{(s)} + 2NH_{3(g)}$	−64.6	0.0	36.8	36.8
$2NH_4Cl_{(s)} + MgH_{2(s)} \rightarrow MgCl_{2(s)} + 2H_{2(g)} + 2NH_{3(g)}$	−15.7	3.0	25.6	28.6
$NH_4Cl_{(s)} + LiH_{(s)} \rightarrow LiCl_{(s)} + H_{2(g)} + NH_{3(g)}$	−49.1	3.3	27.7	31.0
$NH_4Cl_{(s)} + LiNH_{2(s)} \rightarrow LiCl_{(s)} + H_{2(g)} + NH_{3(g)}$	−6.1	0.0	44.5	44.5
$2NH_4Cl_{(s)} + CaH_{2(s)} \rightarrow CaCl_{2(s)} + 2H_{2(g)} + 2NH_{3(g)}$	−40.6	2.7	22.8	25.5

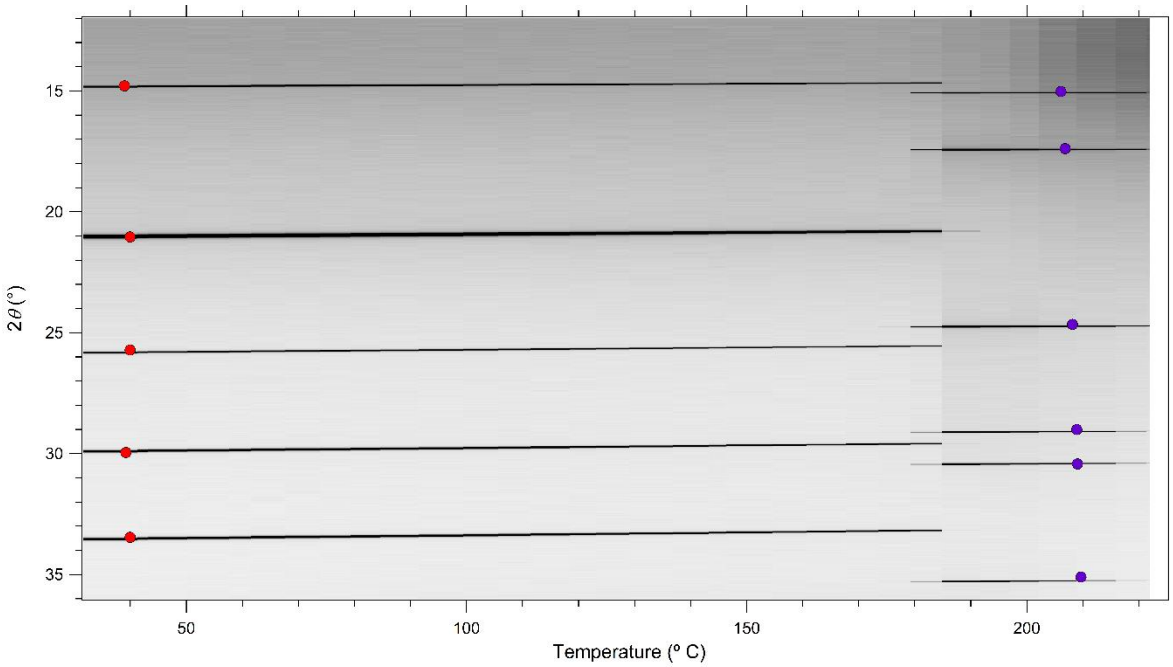

Fig. S1. In situ SR-XRD data for NH_4Cl. ● LT-NH_4Cl and ● HT-NH_4Cl. $\Delta T/t$ = 5 °C/min. λ = 1.0003896(1) Å.

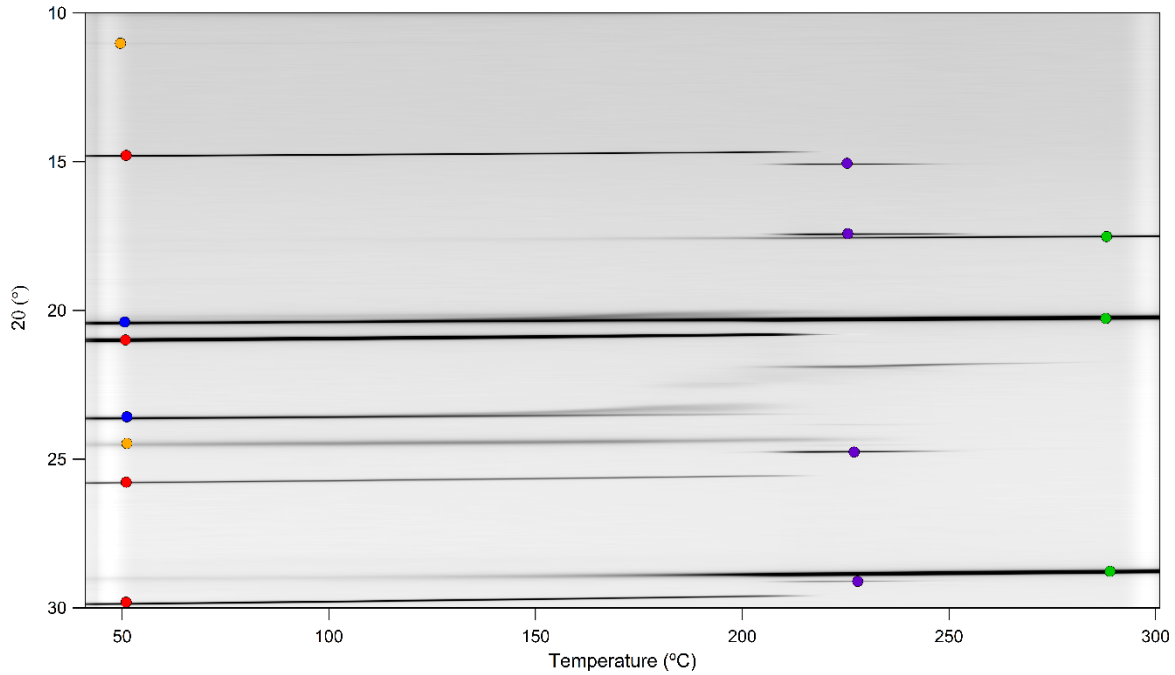

Fig. S2. In situ SR-XRD data for NH_4Cl + NaH. ● LT-NH_4Cl, ● NaH, ●NaOH, ● NaCl and ● HT-NH_4Cl. $\Delta T/t$ = 5 °C/min. λ = 1.0003896(1) Å.

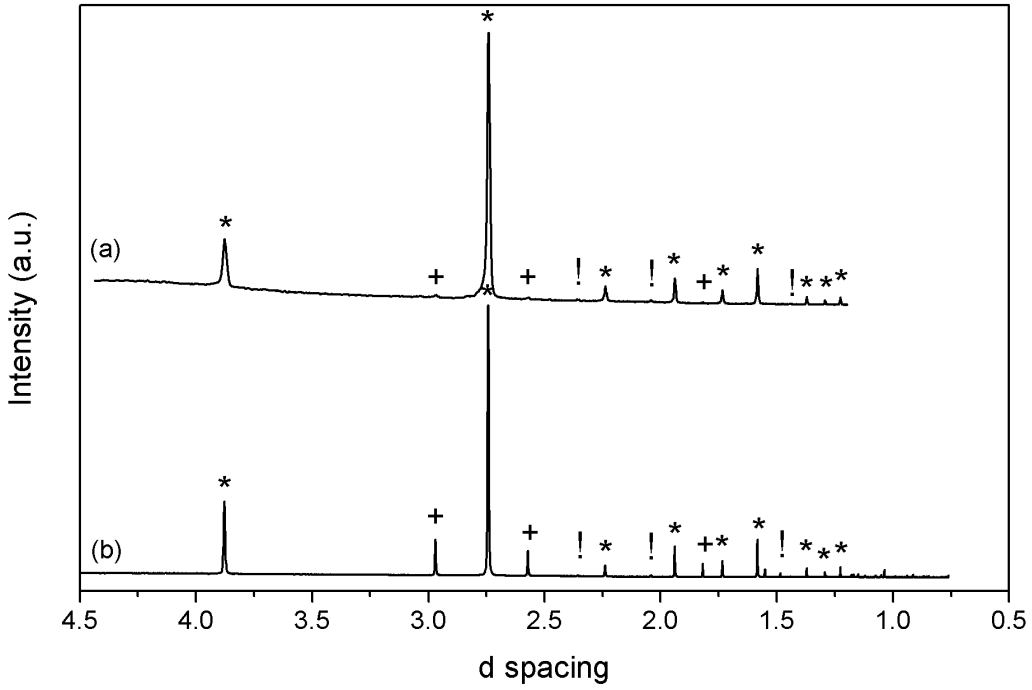

Fig. S3. XRD data for NH_4Cl + LiH collected at room temperature. (a) Data collected directly after ball milling on Bruker AXS D8 Advance Discover XRD System (λ = 1.5406 Å), (b) data collected 8 months after ball milling using Synchrotron radiation (λ = 1.0003896(1) Å). * = NH_4Cl, ! = LiH, + = LiCl.

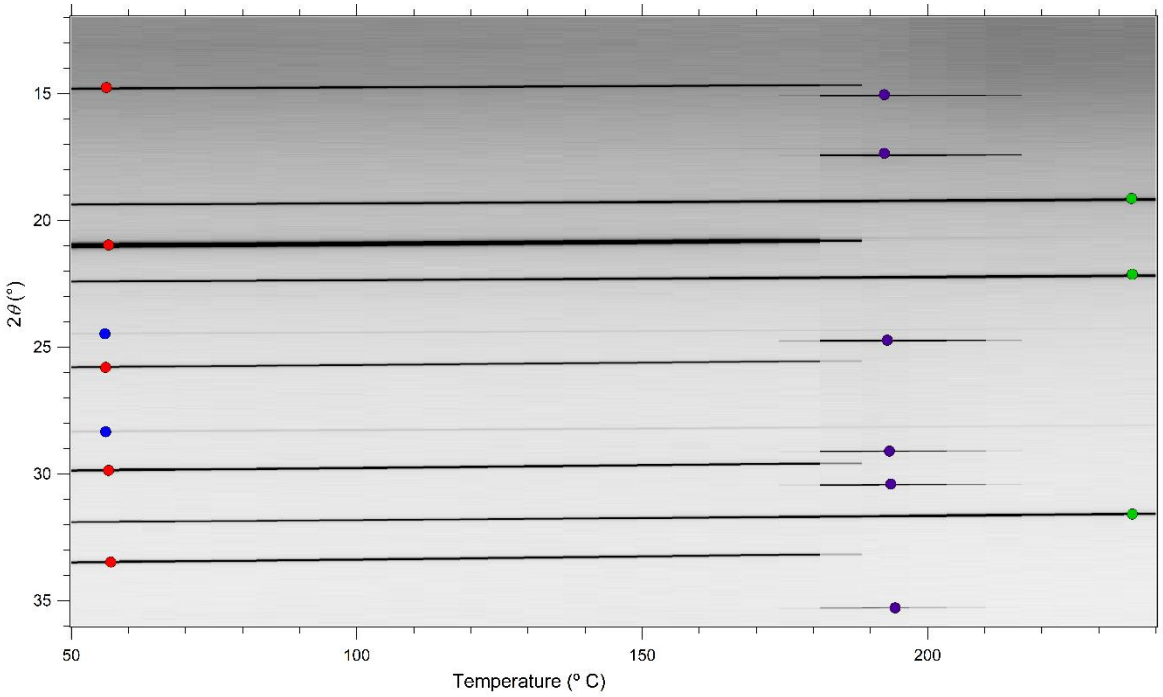

Fig. S4. In situ SR-XRD data for NH_4Cl + LiH. ● LT-NH_4Cl, ● LiH, ● LiCl and ● HT-NH_4Cl. $\Delta T/t$ = 5 °C/min. λ = 1.0003896(1) Å.

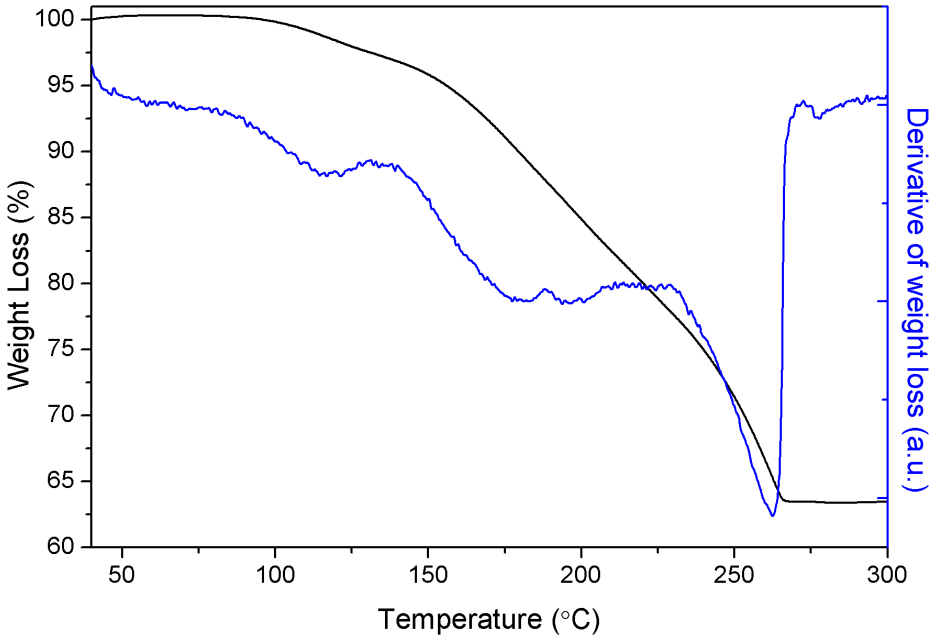

Fig. S5. TGA and first derivative of the TGA data for NH_4Cl + LiH. $\Delta T/t$ = 5 °C/min.

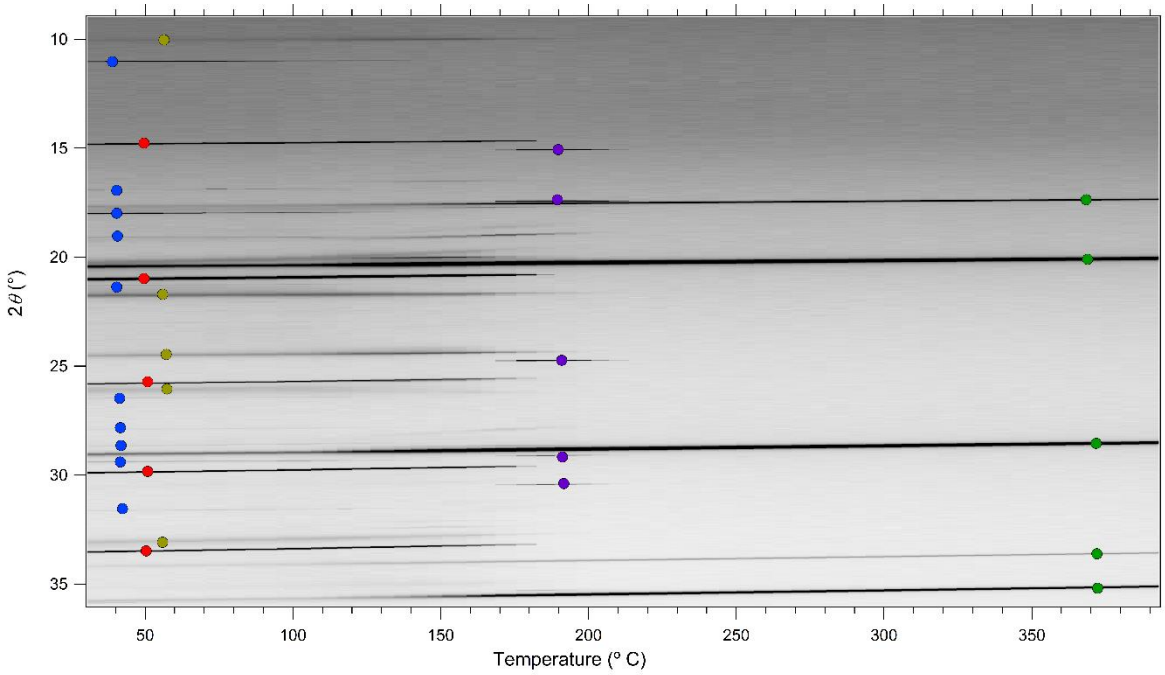

Fig. S6. In situ SR-XRD data for NH_4Cl + $NaNH_2$. ● LT-NH_4Cl, ● $NaNH_2$, ● NaCl, ●NaOH, and ● HT-NH_4Cl. ΔT/t = 5 °C/min. λ = 1.0003896(1) Å.

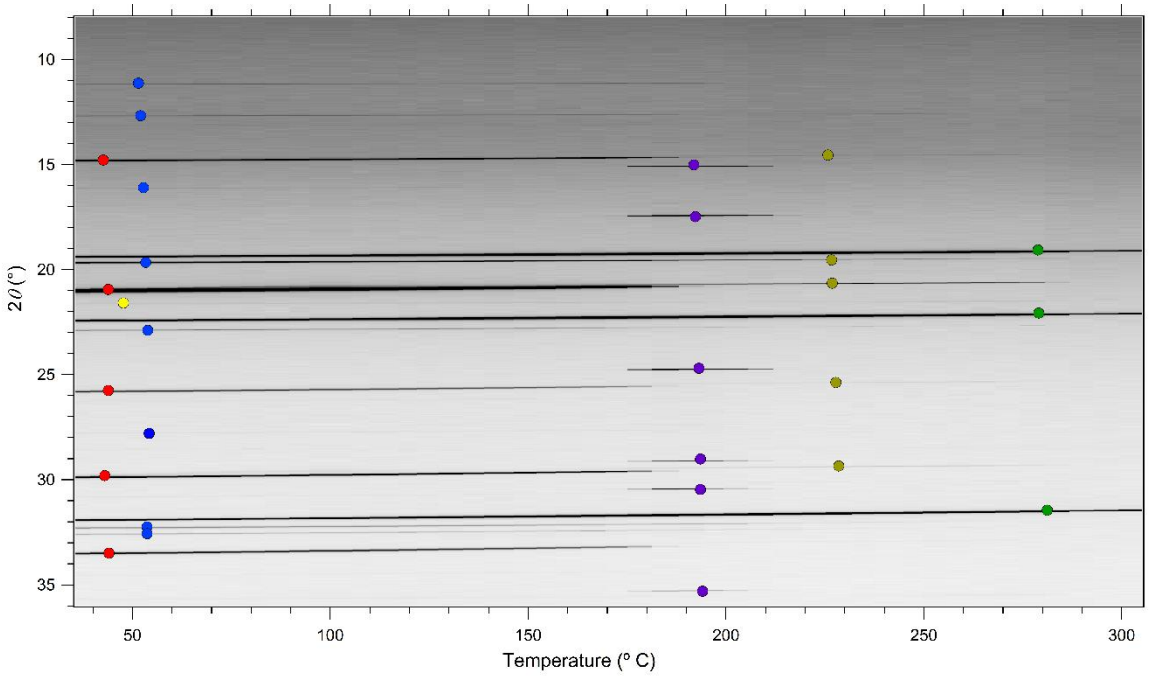

Fig. S7. In situ SR-XRD data for NH_4Cl + $LiNH_2$. ● LT-NH_4Cl, ● $LiNH_2$, ● Li_2O, ● LiCl, ● HT-NH_4Cl and ●unknown. ΔT/t = 5 °C/min. λ = 1.0003896(1) Å.

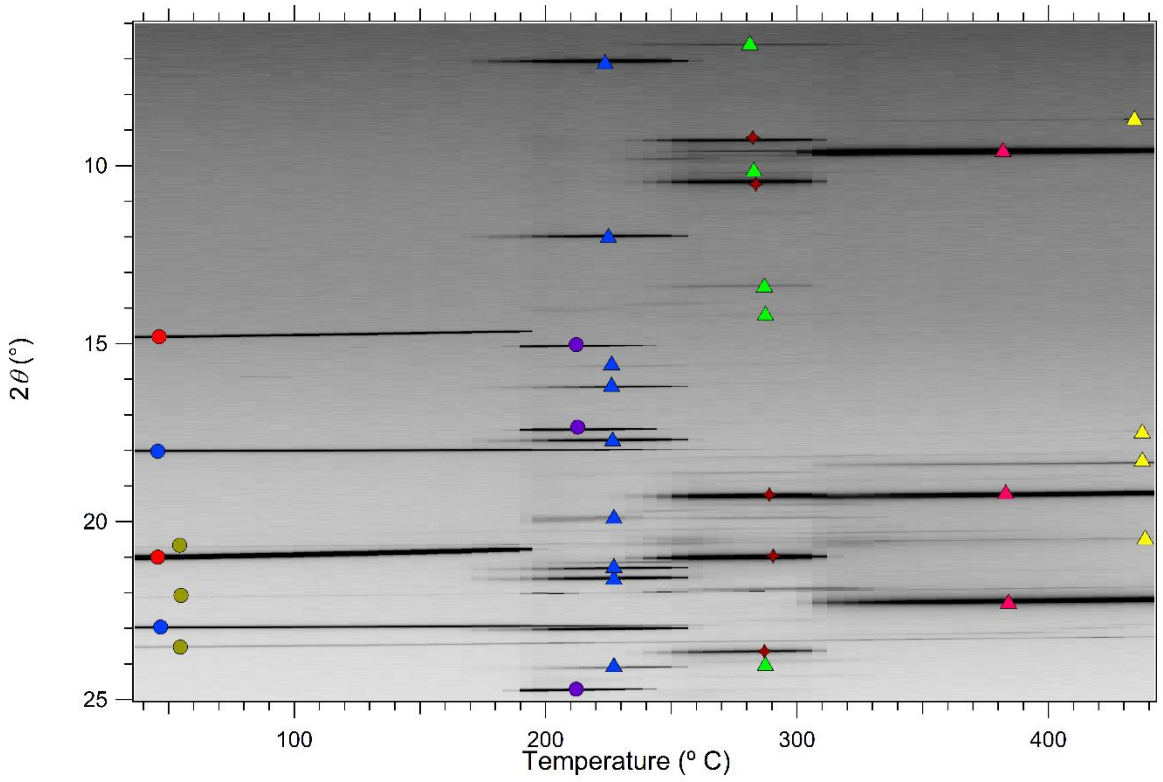

Fig. S8. In situ SR-XRD data for NH_4Cl + MgH_2. ● LT-NH_4Cl, ● MgH_2, ● Mg, ▲$(NH_4)_2MgCl_4$, ● HT-NH_4Cl, ✦ unknown, ▲ unknown, ▲ unknown and ▲$MgCl_2$. ΔT/t = 5 °C/min. λ = 1.0003896(1) Å.

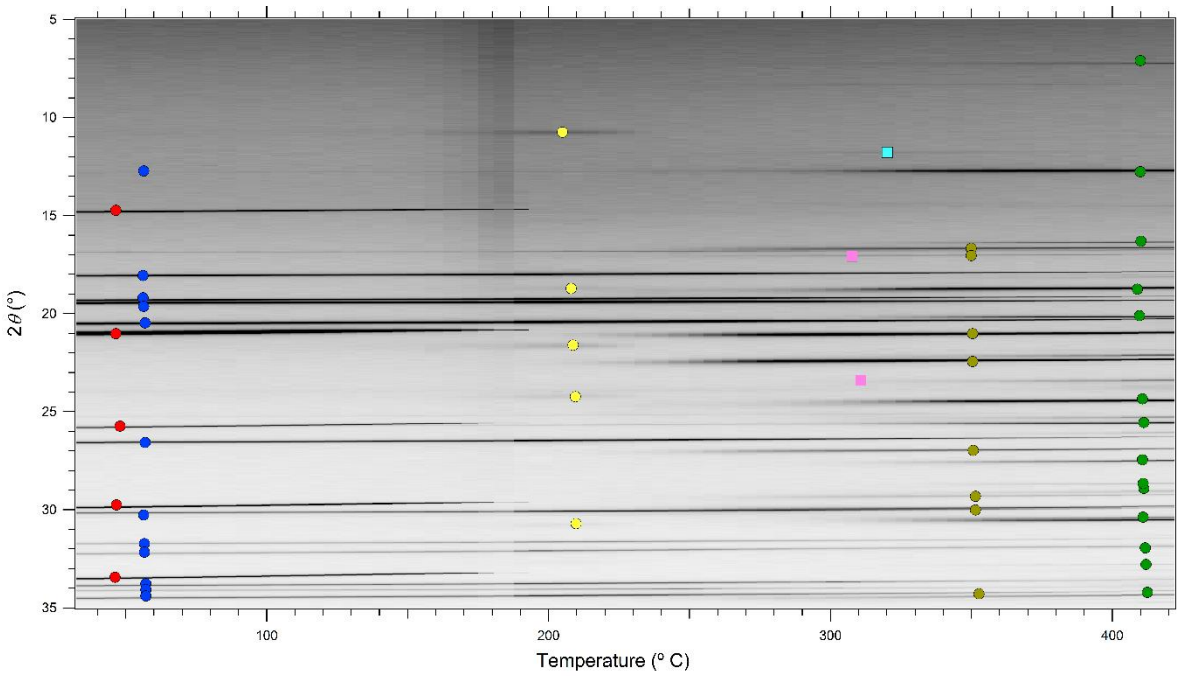

Fig. S9. In situ SR-XRD data for $NH_4Cl + CaH_2$. ● LT-NH_4Cl, ● CaH_2, ▲ NH_4CaCl_3, ■ unknown, ■ unknown, ● CaHCl and ● $CaCl_2$. ΔT/t = 5 °C/min. λ = 1.0003896(1) Å.

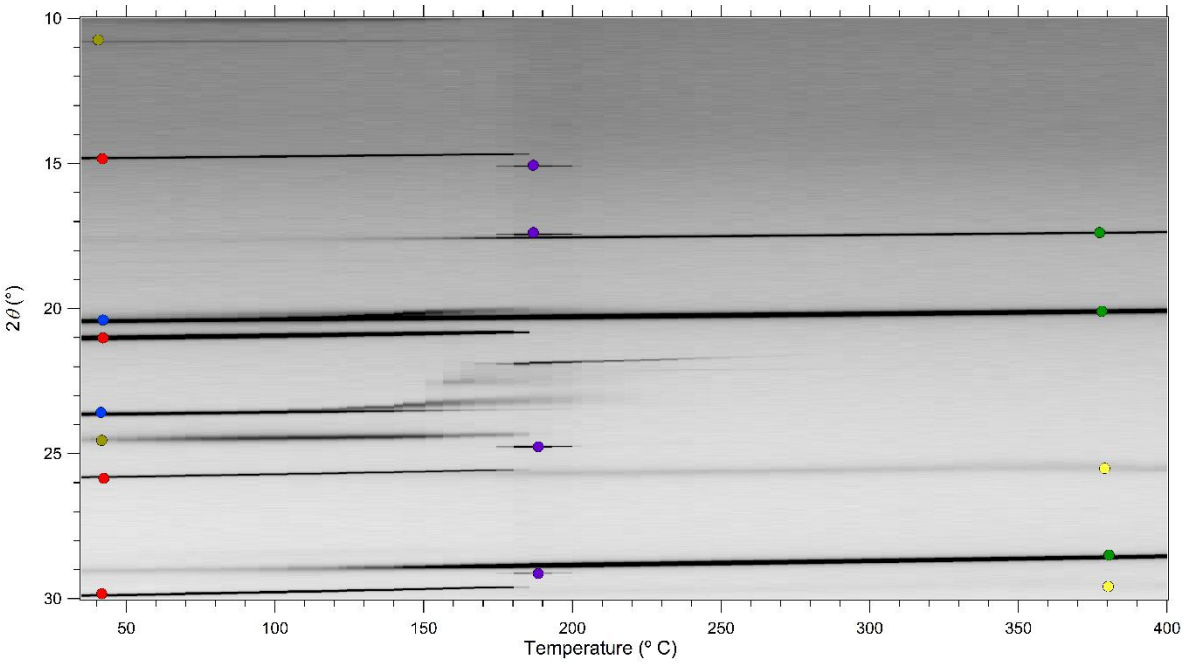

Fig. S10. In situ SR-XRD data for $NH_4Cl + NaH + PdCl_2$ (1 mol%). ● LT-NH_4Cl, ● NaH, ● NaOH, ● NaCl, ● Pd and ● HT-NH_4Cl. ΔT/t = 5 °C/min. λ = 1.0003896(1) Å.

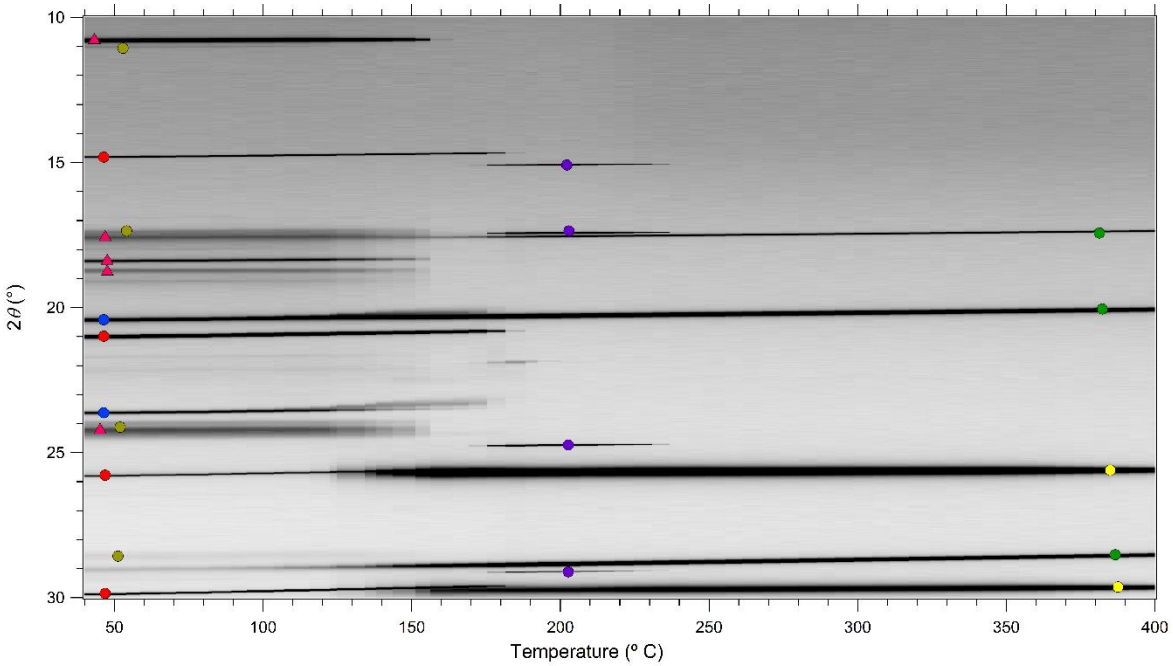

Fig. S11. In situ SR-XRD data for NH_4Cl + NaH + $PdCl_2$ (10 mol%). ● LT-NH_4Cl, ● NaH, ●NaOH, ● NaCl, ▲$PdCl_2$, ● Pd and ● HT-NH_4Cl. ΔT/t = 5 °C/min. λ = 1.0003896(1) Å.