Electronic Supplementary Information

Hydrogen storage and ionic mobility in amide–halide systems

Paul A. Anderson,* Philip A. Chater, David R. Hewett and Peter R. Slater

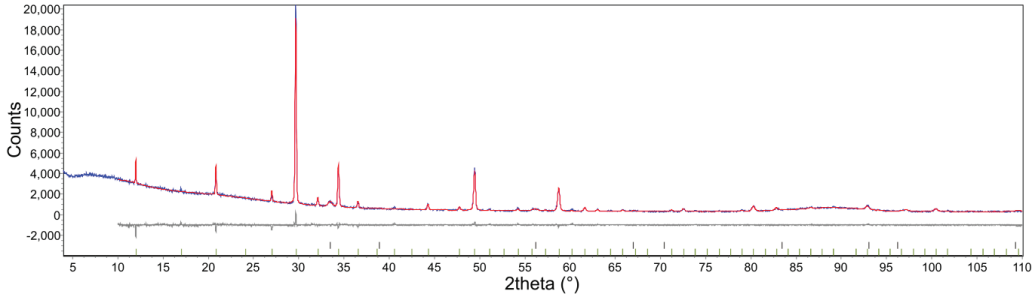

Fig. S1 Preliminary Rietveld plot for $Li_4(NH_2)_3Cl$. Tick marks indicate peak positions due to $Li_4(NH_2)_3Cl$ (green) and Li_2O (black).

Table S1 Results of preliminary Rietveld refinement of $Li_4(NH_2)_3Cl$.[†]

Atom	Wyckoff Position	*x*	*y*	*z*
Cl	8a	0.8715(9)	*x*	*x*
N	24c	0.1347(8)	0.8931(4)	0.1250(5)
Li1	8a	0.0105(17)	*x*	*x*
Li2	12b	0.2196(8)	0	0.25
Li3	12b	0.7991(17)	0	0.25

[†]Space group $I2_13$, a = 10.41353(8) Å, V = 1131.69(8) Å^3. R_{wp} 5.171, R_{exp} 3.412, χ^2 1.516.

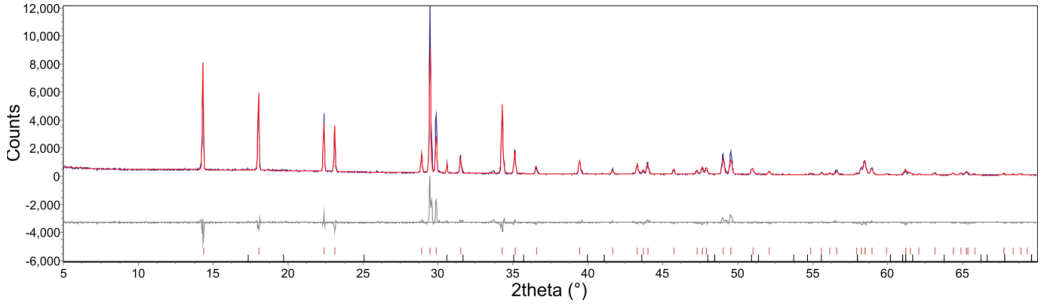

Fig. S2 Preliminary Rietveld plot of N and Br positions in $Li_7(NH_2)_6Br$. Tick marks indicate peak positions due to $Li_7(NH_2)_6Br$ (red) and $LiNH_2$ (black).

Table S2 Preliminary Results of Rietveld refinement of the anion lattice in $Li_7(NH_2)_6Br$.[‡]

Atom	Wyckoff Position	*x*	*y*	*z*
Br	3a	0	0	0
N	18f	0.1931(10)	0.2346(10)	0.6539(11)

[‡]Space group $R\bar{3}$, a = 9.8213(4) Å, c = 8.9595(4) Å, V = 748.43(7) Å^3.
R_{wp} 14.759, R_{exp} 5.194, χ^2 2.841.

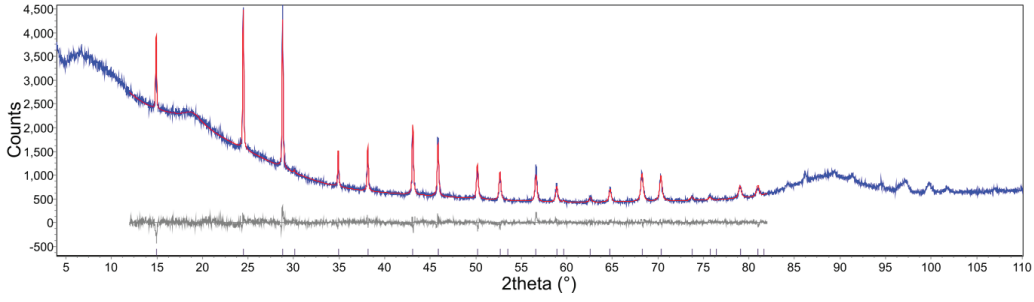

Fig. S3 Preliminary Rietveld plot for $Li_5(NH)_2I$. Tick marks indicate peak positions due to $Li_5(NH)_2I$.

Table S3 Results of preliminary Rietveld refinement of $Li_5(NH)_2I$.[§]

Atom	Wyckoff Position	*x*	*y*	*z*
I	8a	0.125	0.125	0.125
N	16d	0.5	0.5	0.5
Li	48f	0.383(5)	0.125	0.125

[§]Space group $Fd\bar{3}m$ (origin choice 2), a = 10.27203(12) Å, V = 1083.85(4) Å^3.
R_{wp} 4.053, R_{exp} 3.223, χ^2 1.258.

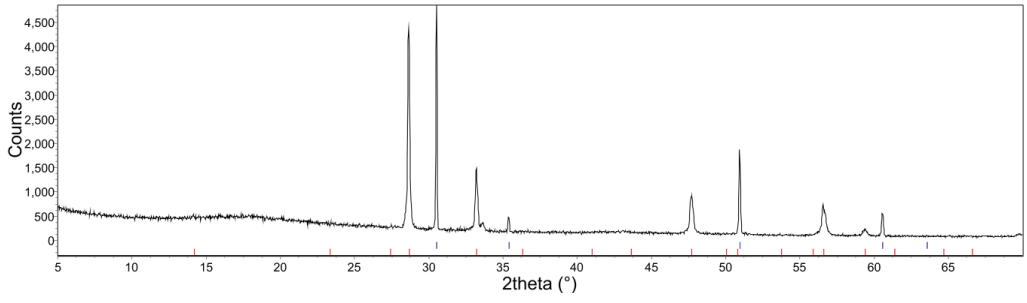

Fig. S4 Powder X-ray diffraction pattern of $Li_6Mg_{0.5}(NH_2)_6Br$ + 6LiH after TPD–MS experiment. Tick marks indicate peaks due to $Fm\bar{3}m$, a = 5.06552(12) Å (blue) and $Fd\bar{3}m$, a = 10.7739(4) Å (red) phases.

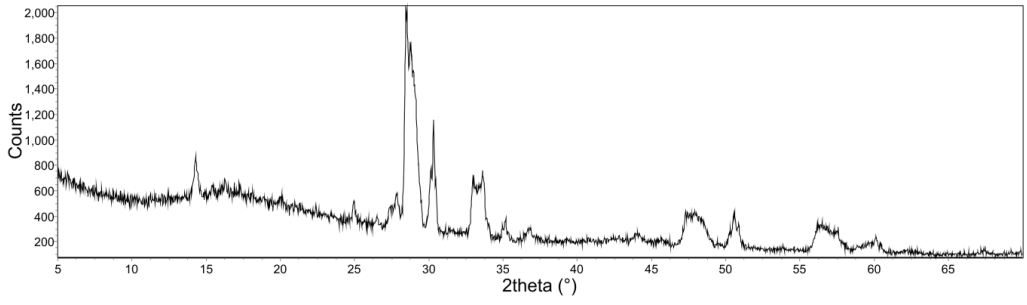

Fig. S5 Powder X-ray diffraction pattern of $Li_7(NH_2)_6Br$ + 6LiH after TPD–MS experiment.

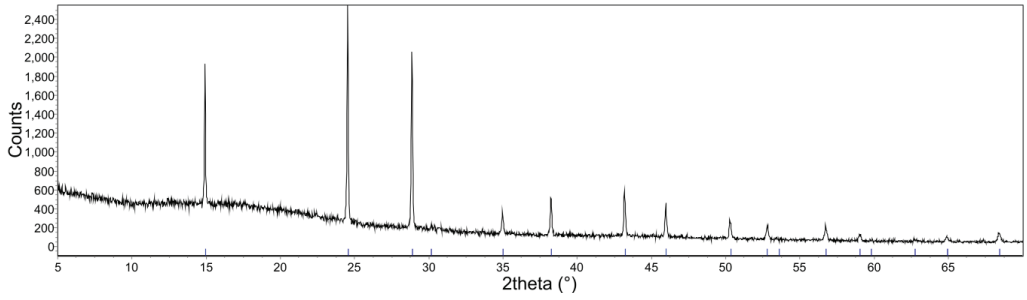

Fig. S6 Powder X-ray diffraction pattern of $3LiNH_2{\cdot}LiI$ + 3LiH after TPD–MS experiment. Tick marks indicate peaks due to $Li_5(NH)_2I$.

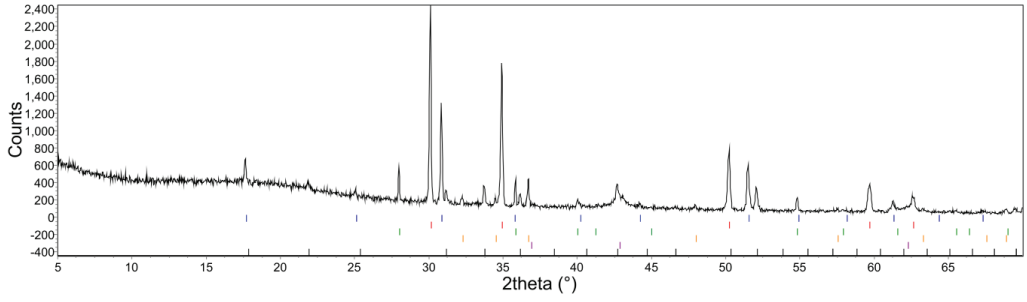

Fig. S7 Powder X-ray diffraction pattern of $2Li_3Mg_{0.5}(NH_2)_3Cl$ + $3MgH_2$ after TPD-MS experiment. Tick marks indicate peaks due to β-$Li_2Mg(NH)_2$ (blue), LiCl (red), MgH_2 (green), Mg (orange), MgO (purple) and Mg_3N_2 (black).

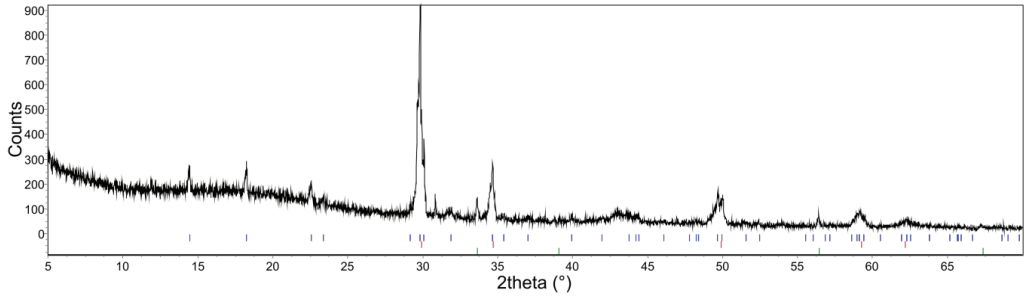

Fig. S8 Powder X-ray diffraction pattern of $3Li_2NH{\cdot}½MgCl_2$ after hydrogenation at 300°C, 100 bar H_2. Tick marks indicate peaks due to a rhombohedral $Li_4(NH_2)_3Cl$-like phase (blue), LiCl (red) and Li_2O (green).

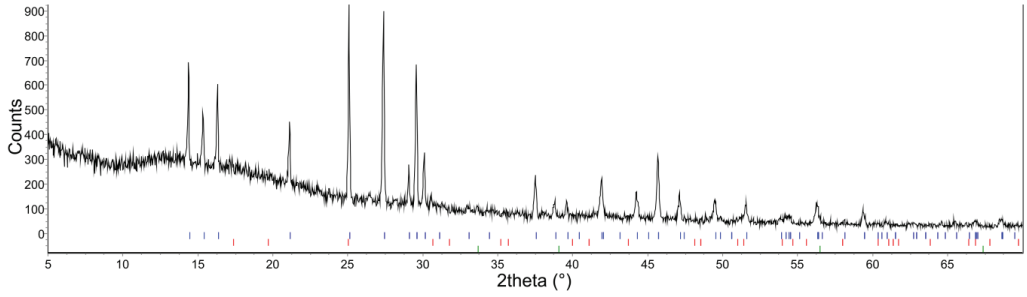

Fig. S9 Powder X-ray diffraction pattern of $3Li_2NH{\cdot}LiI$ after hydrogenation at 300°C, 100 bar H_2. Tick marks indicate peaks due to $Li_3(NH_2)_2I$ (blue), $LiNH_2$ (red) and Li_2O (green).

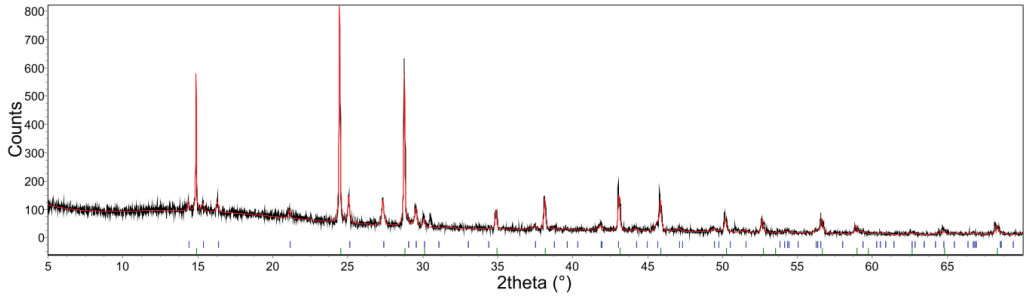

Fig. S10 Observed (black) and calculated (red) powder X-ray diffraction pattern of $3Li_2NH{\cdot}LiI$ after hydrogenation at 200°C, 100 bar H_2, for 1 hour. Tick marks indicate peaks due to $Li_3(NH_2)_2I$ (blue, ~24.4 wt%) and $Li_5(NH)_2I$ (green, ~75.6 wt%).

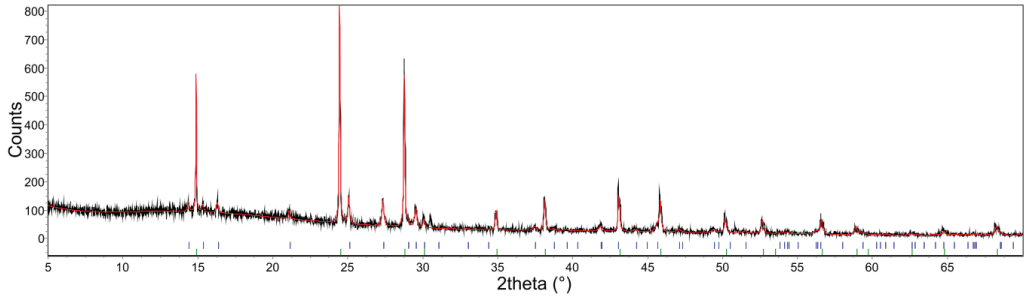

Fig. S11 Observed (black) and calculated (red) powder X-ray diffraction pattern of $3Li_2NH{\cdot}½MgI_2$ after hydrogenation at 200°C, 100 bar H_2, for 1 hour. Tick marks indicate peaks due to $Li_2Mg_{0.5}(NH_2)_2I$ (blue, ~30.4 wt%) and $Li_4Mg_{0.5}(NH)_2I$ (green, ~69.6 wt%).

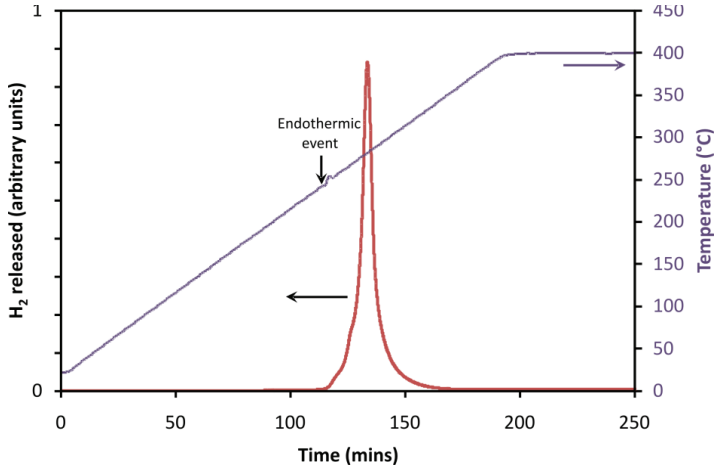

Fig. S12 TPD–MS data for $Li_6Mg_{0.5}(NH_2)_6Br + 3MgH_2$ showing an endothermic event in the temperature trace immediately prior to hydrogen release.