Supporting information

Magnesium Borohydride Pyridine Derivatives as Electrolytes for All-Solid-State Batteries

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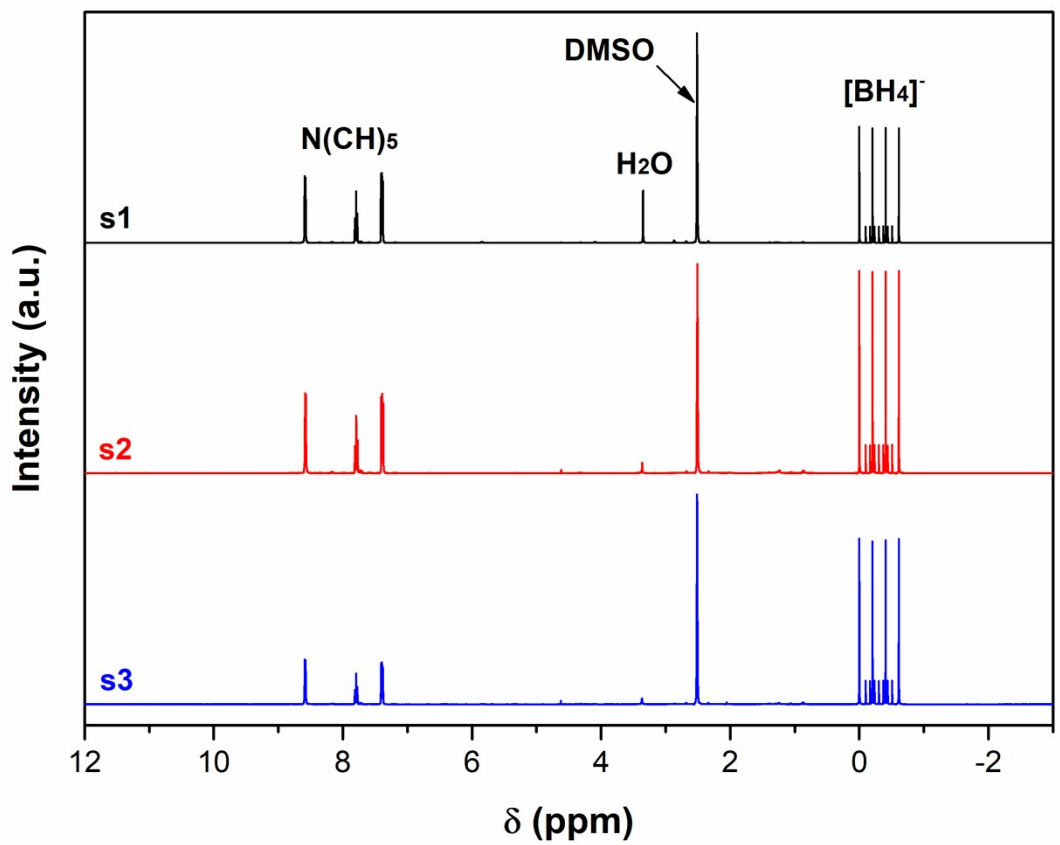

Figure S1. ^{1}H NMR spectra of **s1-s3**.

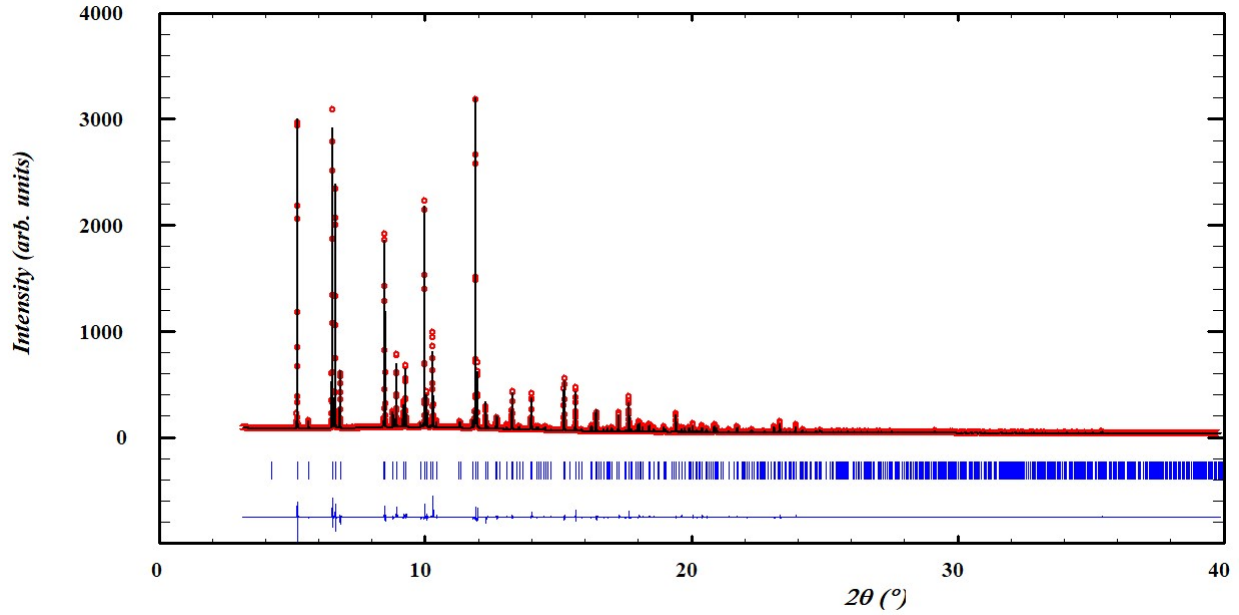

Figure S2. Rietveld refinement of $Mg(BH_4)_2 \cdot 3N(CH)_5$ (**s1**) from SR PXD data measured at T = 20 °C, λ = 0.70870 Å, showing experimental (red circles) and calculated (black line) PXD patterns, and a difference plot below (blue line). Final discrepancy factors: R_p = 2.51 %, R_{wp} = 2.19 % (not corrected for background), R_p = 11.2 %, R_{wp} = 18.2 % (conventional Rietveld R-factors), $R_{Bragg}(Mg(BH_4)_2 \cdot 3N(CH)_5)$ = 9.80 % and global χ^2 = 10.1.

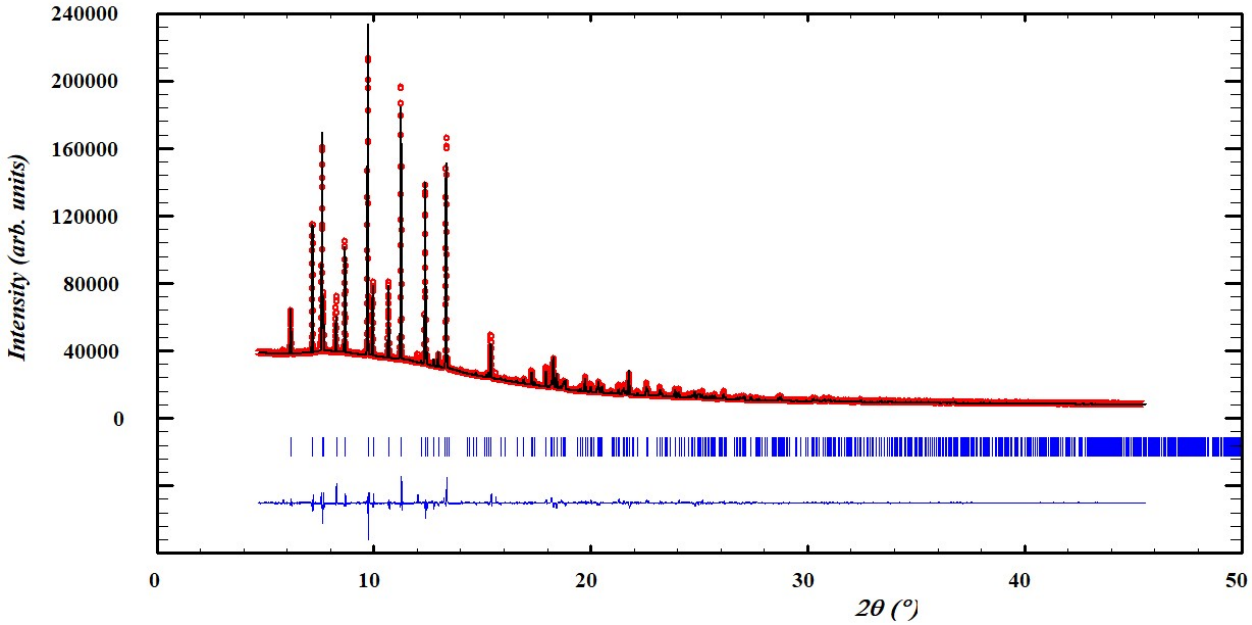

Figure S3. Rietveld refinement of $Mg(BH_4)_2 \cdot 2N(CH)_5$ (**s2**) from SR PXD data measured at T = 20 °C, λ = 0.826927 Å, showing experimental (red circles) and calculated (black line) PXD patterns, and a difference plot below (blue line). Final discrepancy factors: R_p = 1.60 %, R_{wp} = 2.74 % (not corrected for background), R_p = 20.4 %, R_{wp} = 14.2 % (conventional Rietveld R-factors), $R_{Bragg}(Mg(BH_4)_2 \cdot 2N(CH)_5)$ = 10.2 % and global χ^2 = 13.8.

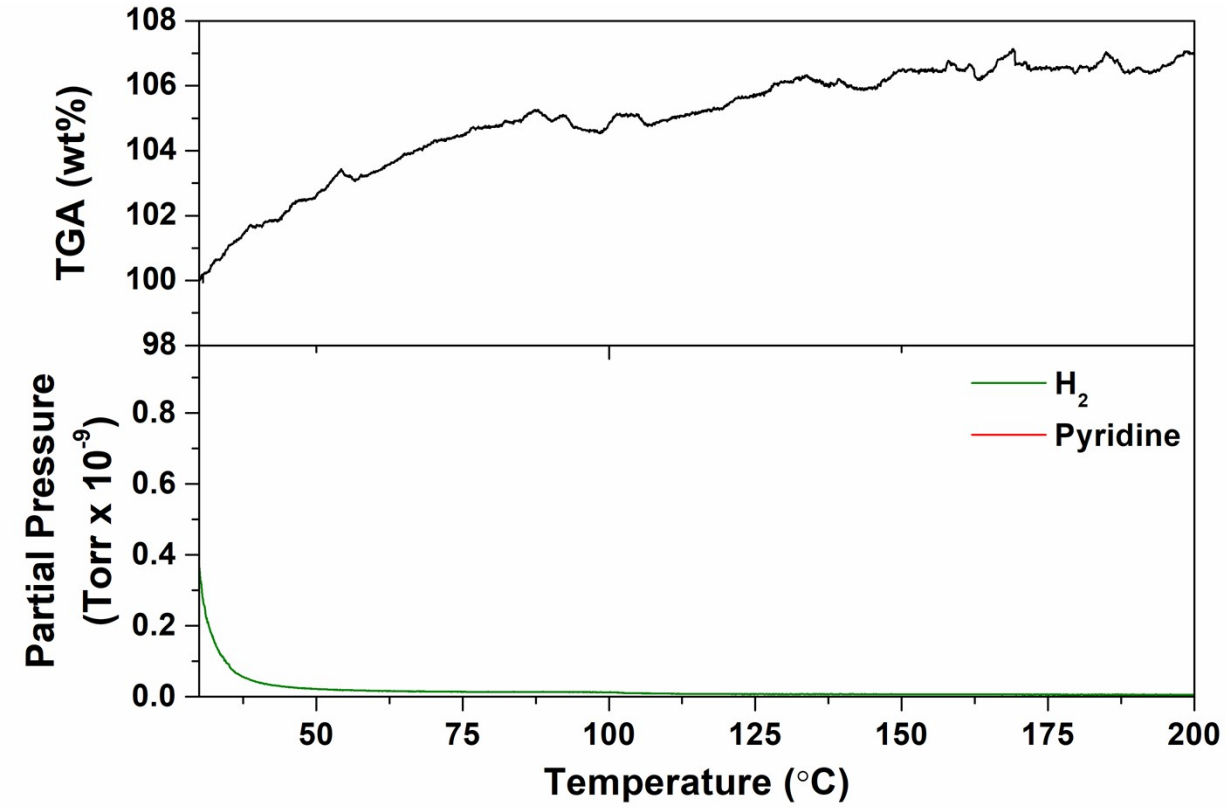

Figure S4. Thermal analysis (TG-MS) data of **s3** during heating with a heating rate of 0.5 °C/min. The apparent increasing weight% is an artifact from the instrument.

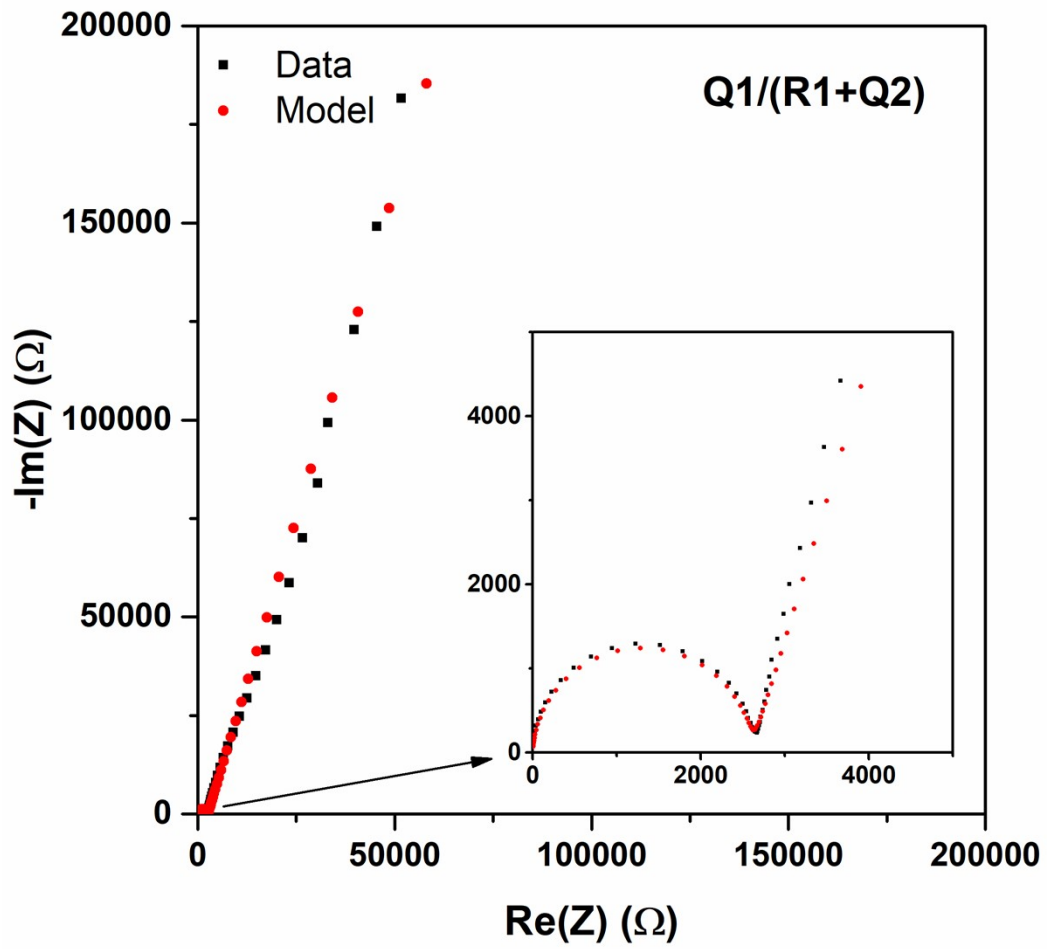

Figure S5. Fitting of the Nyquist data of $Mg(BH_4)_2 \cdot 3N(CH)_5$ (**s1**) at room temperature after stabilization.

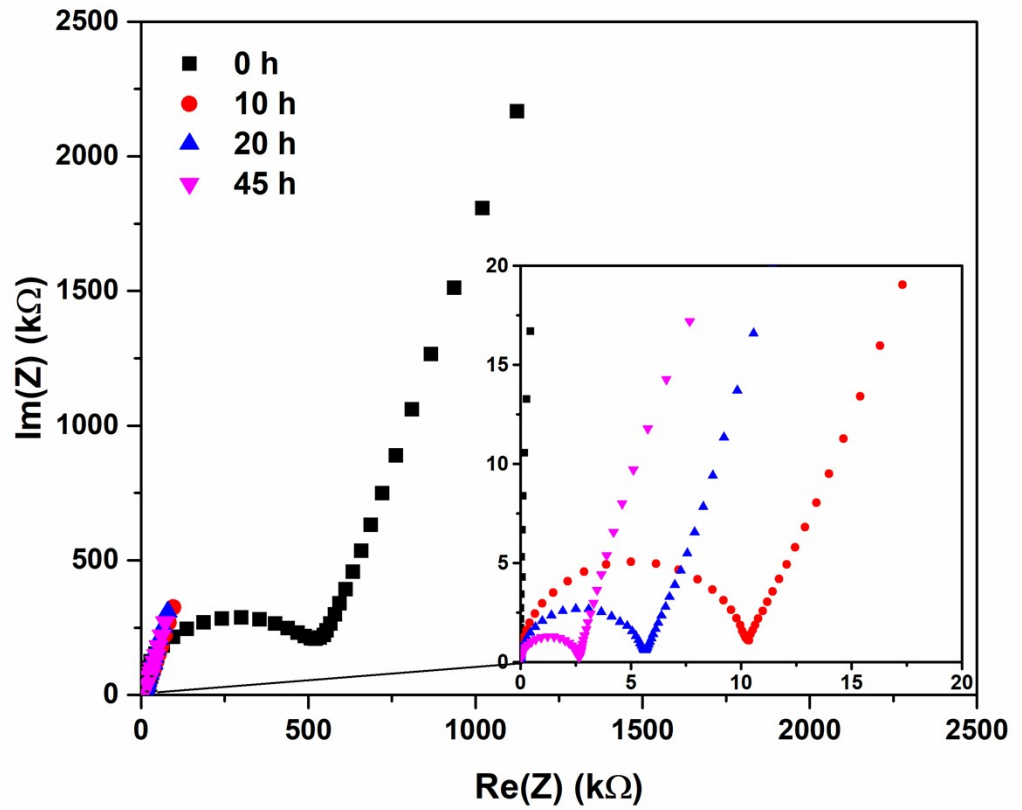

Figure S6. Nyquist plots of $Mg(BH_4)_2 \cdot 3N(CH)_5$ (**s1**) from electrochemical impedance spectroscopy measurements during stabilization at room temperature in intervals of 1 h.

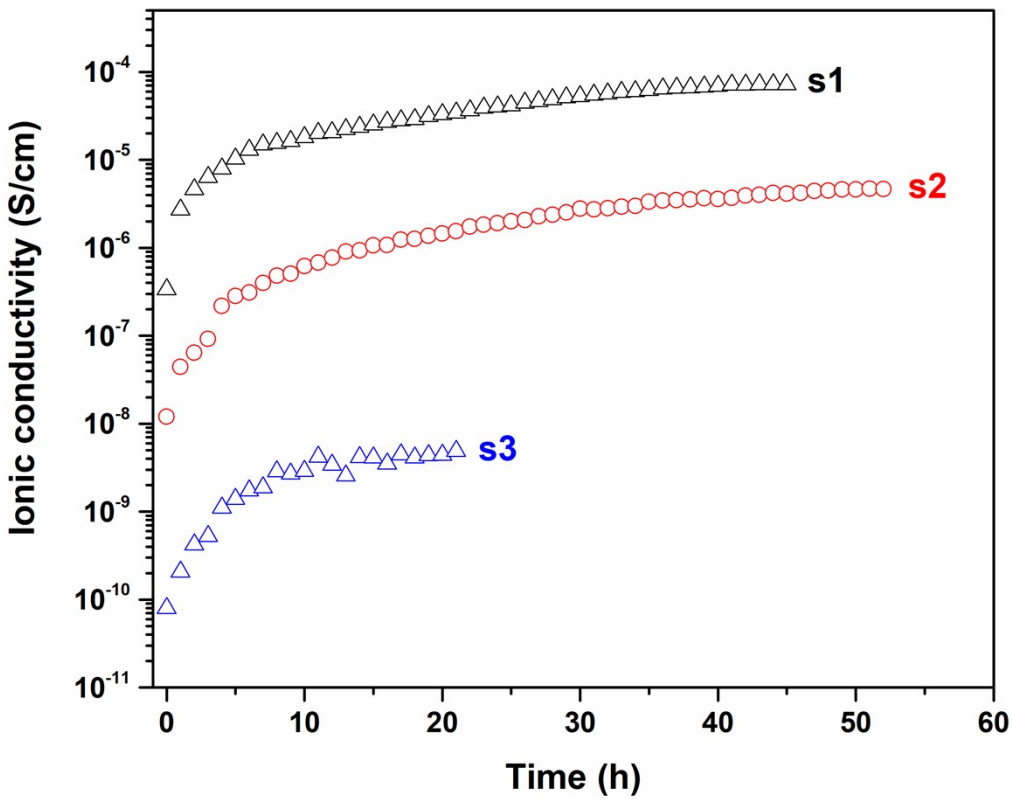

Figure S7. Time-evolution of the ionic conductivity of **s1-s3** measured by electrochemical impedance spectroscopy at room temperature in intervals of 1 h.

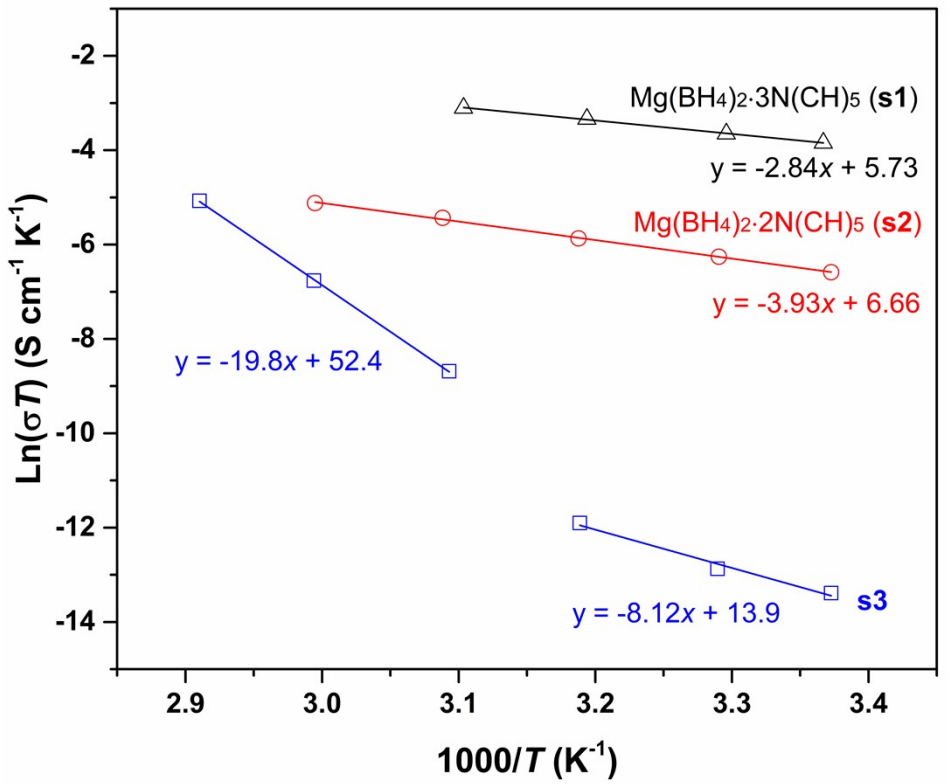

Figure S8. Arrhenius plot of ln(σ*T*) vs 1000/*T* to evaluate the activation energy.