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ARTICLE

Guanidinium octahydrotriborate: An ionic liquid with a high hydrogen capacity

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Supplementary materials:



Fig. S1 Powder XRD pattern of the precipitate from the reaction between C(NH₂)₃Cl and NaB₃H₈ in THF.



Fig. S2 Low temperature DSC curves of guanidinium octahydrotriborate (with NaCl).



Fig. S3 Guanidinium octahydrotriborate in THF in different concentrations. From left to right: 10 mol/L, 1 mol/L, 0.6 mol/L, 0.4 mol/L, and 0.2 mol/L.



Fig. S4 DTA curve of guanidinium octahydrotriborate (with NaCl).



Fig. S5 Solution ¹¹B NMR spectra of guanidinium octahydrotriborate in THF (black); guanidinium octahydrotriborate heated at 100 °C: for 0.5 h (red), and for 95 h (blue).



Fig. S6 MS spectra of the gas release from different concentrations of guanidinium octahydrotriborate in THF: (a) 0.1 mol/L; (b) 0.5 mol/L; (c) 1 mol/L.



Fig. S7 Solid state cross-polarization MAS ¹³C NMR spectra of the 4 D products, the 6.5 D products, and the 6.5 D products samples after evacuation at 120 °C.



Fig. S8 FTIR spectra of the 4 D (blue) and 6.5 D (black) products.



Fig. S9 TPD-MS measurements of the 6.5 D products upon further heating up to 480 °C.



Fig. S10 Solid state MAS cross-polarization (left) and one-pulse (right) ¹¹B NMR of the dehydrogenation products from different concentrations of guanidinium octahydrotriborate.



Fig. S11 Solid state MAS cross-polarization ¹³C NMR of the dehydrogenation products from different concentrations of guanidinium octahydrotriborate.



Fig. S12 Solid state MAS one-pulse ¹¹B NMR of the products from 0.1 mol/L guanidinium octahydrotriborate at 100 °C after 6.5 H₂ was released (black) and from the decomposition of the as-prepared guanidinium octahydrotriborate at 85 °C (red).



Fig. S13 Solid state MAS cross-polarization ¹³C NMR of the products from 0.1 mol/L guanidinium octahydrotriborate at 100 °C after 6.5 H₂ was released (black) and from the decomposition of the as-prepared guanidinium octahydrotriborate at 85 °C (red).