Supporting Information

2-Aminoimidazole Borohydride as a Hydrogen Carrier

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Supplementary figures

Fig. S1. The calibration curve for TCD measurement using H₂ as the standard material.

Fig. S2. FT-IR spectrum of (a) Im-NH₂-RT and (b) Im-NH₂-320.
Fig. S3. $^1$H NMR spectra of (a) (Im-NH$_2$)$_2$SO$_4$ (solvent: D$_2$O), (b) extraction from Im-NH$_2$-RT using IPA (solvent: D$_2$O), (c) extraction from Im-NH$_2$-RT using acetonitrile (solvent: d$_3$-acetonitrile), (d) extraction from Im-NH$_2$-RT using THF (solvent: d$_3$-acetonitrile). No signals of BH$_4^-$ can be found in these extractions.

Fig. S4. XRD pattern of Im-NH$_2$Cl.
Fig. S5. XRD pattern of Im-NH$_2$-RT(Cl).

Fig. S6. $^{11}$B NMR spectrum of Im-NH$_2$-RT(Cl). (solvent: d$_3$-acetonitrile).

Experimental details

Solid-state NMR
Solid-state NMR experiments were carried out on AVANCE III 400MHz WB solid-state NMR spectrometer using 4 mm high-speed spinning probes. The resonance frequencies were, respectively, 100.65 MHz for $^{13}$C (cross polarization, 400.25 MHz for $^1$H), and 128.41 MHz for $^{11}$B (magic angle spinning, one pulse). Typical acquisition parameters were pulse length 2000 µs ($^{13}$C, 2.3 µs for $^1$H) and 0.5 µs ($^{11}$B), delay 4s ($^{13}$C) and 1s ($^{11}$B), 1606 ($^{13}$C) and 214 ($^{11}$B) scans, respectively.

Synthesis of Im-NH$_2$Cl and Im-NH$_2$-RT(Cl)
0.5292 g (Im-NH$_2$)$_2$SO$_4$ and 0.4896 g BaCl$_2$·2H$_2$O were dissolved in 10 mL H$_2$O, respectively. Then they were mixed and stirred for 5 min. The precipitate was filtered and washed by 2 mL H$_2$O for three times. The solution was
dried and heated to 120 °C for 2 h. Some brown powders were obtained and characterized by XRD (Fig. S4). 59.8 mg Im-NH₂Cl and 18.9 mg NaBH₄ were solved in liquid ammonia in inert atmosphere. The homogenous solution was solidified using liquid nitrogen and then the ammonia was removed by dynamic vacuum at room temperature. Some powders were obtained and characterized by XRD (Fig. S5) and liquid NMR (Fig. S6).