Supporting Information

2-Aminoimidazole Borohydride as a Hydrogen Carrier

Yong Wu, Yue Qi, Jun Chen, He Fu, Jie Zheng* and Xingguo Li*

Beijing National Laboratory for Molecular Sciences (BNLMS), College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China

Supplementary figures

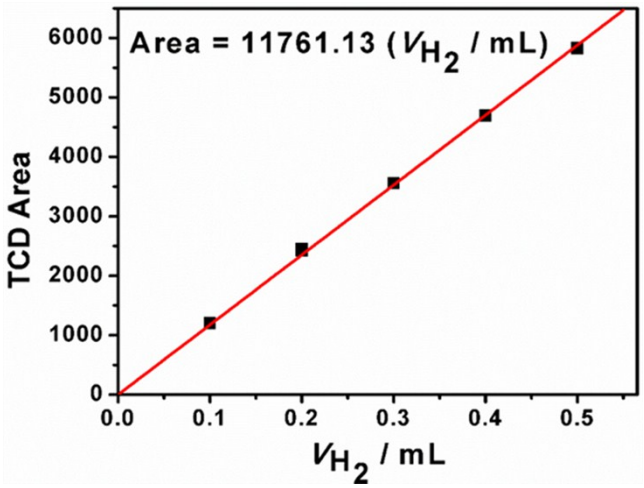

Fig. S1. The calibration curve for TCD measurement using H_2 as the standard material.

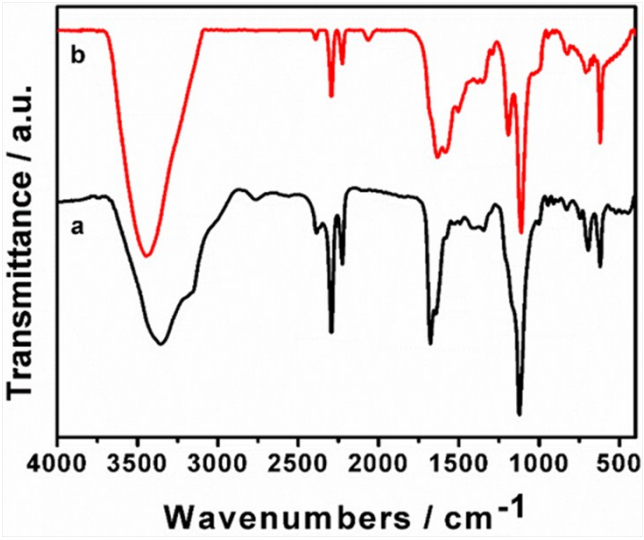

Fig. S2. FT-IR spectrum of (a) Im-NH_2-RT and (b) Im-NH_2-320.

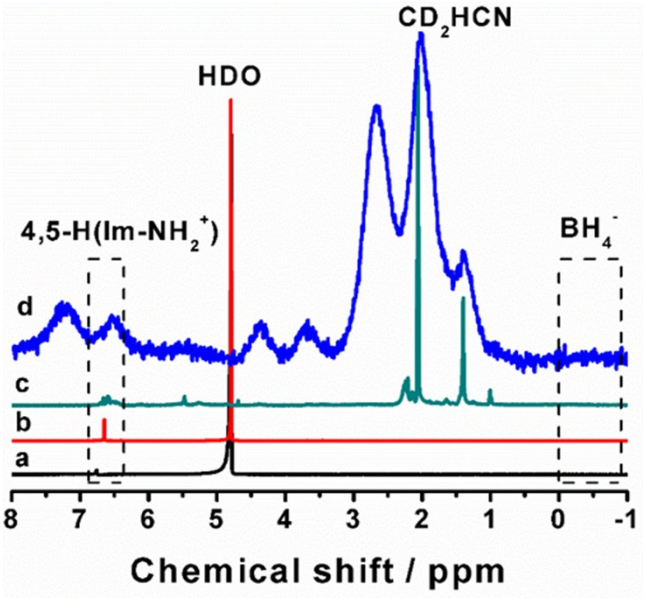

Fig. S3. ^{1}H NMR spectra of (a) $(Im\text{-}NH_2)_2SO_4$ (solvent: D_2O), (b)extraction from $Im\text{-}NH_2$-RT using IPA (solvent: D_2O), (c)extraction from $Im\text{-}NH_2$-RT using acetonitrile (solvent: d^3-acetonitrile), (d)extraction from $Im\text{-}NH_2$-RT using THF (solvent: d^3-acetonitrile). No signals of BH_4^- can be found in these extractions.

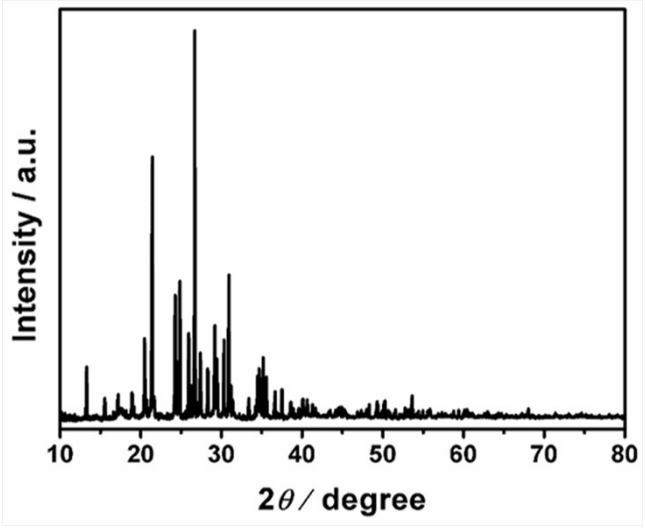

Fig. S4. XRD pattern of $Im\text{-}NH_2Cl$.

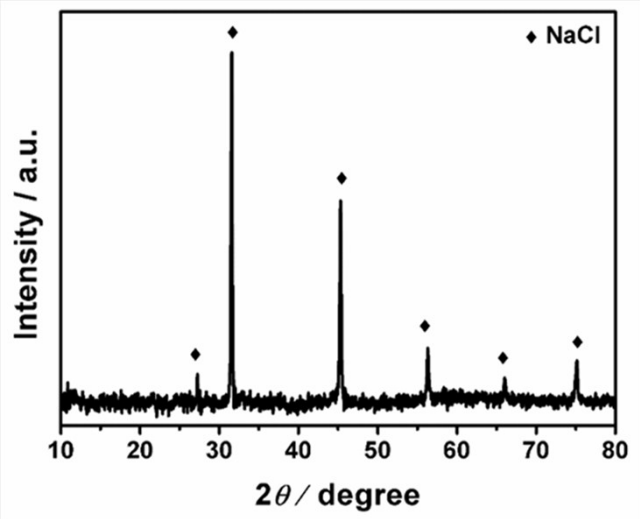

Fig. S5. XRD pattern of Im-NH_2-RT(Cl).

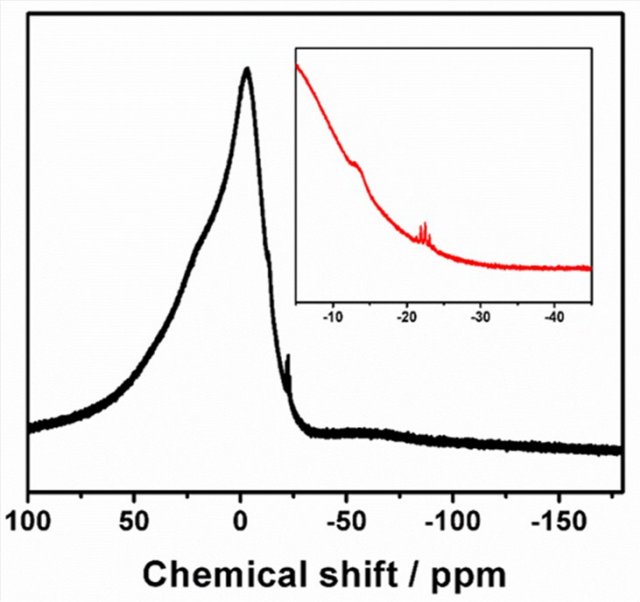

Fig. S6. ^{11}B NMR spectrum of Im-NH_2-RT(Cl). (solvent: d^3-acetonitrile).

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_2Cl and Im-NH_2-RT(Cl)

0.5292 g (Im-NH_2)$_2SO_4$ and 0.4896 g $BaCl_2 \cdot 2H_2O$ were dissolved in 10 mL H_2O, respectively. Then they were mixed and stirred for 5 min. The precipitate was filtered and washed by 2 mL H_2O for three times. The solution was

dried and heated to 120 ℃ for 2 h. Some brown powders were obtained and characterized by XRD (Fig. S4).

59.8 mg Im-NH_2Cl and 18.9 mg $NaBH_4$ 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).