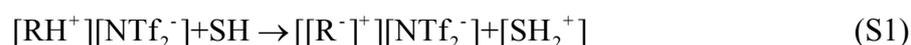


Protic ionic liquid [Bim][NTf₂] with strong hydrogen bond donating ability for highly efficient ammonia absorption

Supporting Information

1. Determination of dissociation constants pK_a

Dissociation equilibrium of the ILs can be described as the following process:



Where SH means a solvent, SH₂⁺ denotes a solvated proton, and RH⁺, [R⁻]⁺ represents the acid cation and the conjugate base of the cation of the IL. The dissociation constant of the ILs can be explained by:

$$K_a = \frac{[[\text{R}^-]^+][\text{NTf}_2^-][\text{SH}_2^+]}{[\text{RH}^+][\text{NTf}_2^-]} \quad (\text{S2})$$

There are mass and charge balance at any point of the titrations:

$$[[\text{RH}^+][\text{NTf}_2^-]]_{\text{total}} = [\text{NTf}_2^-] = [\text{RH}^+] + [[\text{R}^-]^+] \quad (\text{S3})$$

$$[\text{Na}^+] + [\text{SH}_2^+] + [\text{RH}^+] = [\text{S}^-] + [\text{NTf}_2^-] \quad (\text{S4})$$

[X] means the concentrations of the corresponding ions. For example, [[R⁻]⁺] means the concentration of [R⁻]⁺ in the solution during the titration and [[RH⁺][NTf₂⁻]]_{total} means the total concentration of the ILs. Therefore, from Eqs (S2), (S3), (S4), we

have

$$K_a = \frac{[\text{Na}^+] + [\text{SH}_2^+] - [\text{S}^-]}{[\text{S}^-] + [\text{NTf}_2^-] - [\text{Na}^+] - [\text{SH}_2^+]} * [\text{SH}_2^+] \quad (\text{S5})$$

When the pH value is lower than 7 during the titration, there is an assumption that the value of $[\text{S}^-]$ could be neglected and the equation becomes:

$$K_a = \frac{[\text{Na}^+] + [\text{SH}_2^+]}{[\text{NTf}_2^-] - [\text{Na}^+] - [\text{SH}_2^+]} * [\text{SH}_2^+] \quad (\text{S6})$$

Here in the Eq (S6), the only unknown parameter is the $[\text{SH}_2^+]$ and from the pH values, the activity concentration $a_{[\text{SH}_2^+]}$ could be calculated. To figure out the actual concentration of the $\{\text{SH}_2^+\}$, activity coefficient $f_{[\text{SH}_2^+]}$ needs to be known, as Eqs (S7), (S8), (S9) display.

$$[\text{SH}_2^+] = \frac{a_{[\text{SH}_2^+]}}{f_{[\text{SH}_2^+]}} \quad (\text{S7})$$

$$-\log f_{[\text{SH}_2^+]} = \frac{\frac{1}{2} Z^2 I^{1/2}}{1 + I^{1/2}} \quad (\text{S8})$$

$$I = \frac{1}{2} \sum Z^2 [X] \quad (\text{S9})$$

I above means the ionic strength of the solution and Z means the charge number of the ions. However, on account of high-concentration of KCl, the ionic strength of solution was almost the same during the whole titration and the variation could be neglected.

2. Fitting of the viscosities

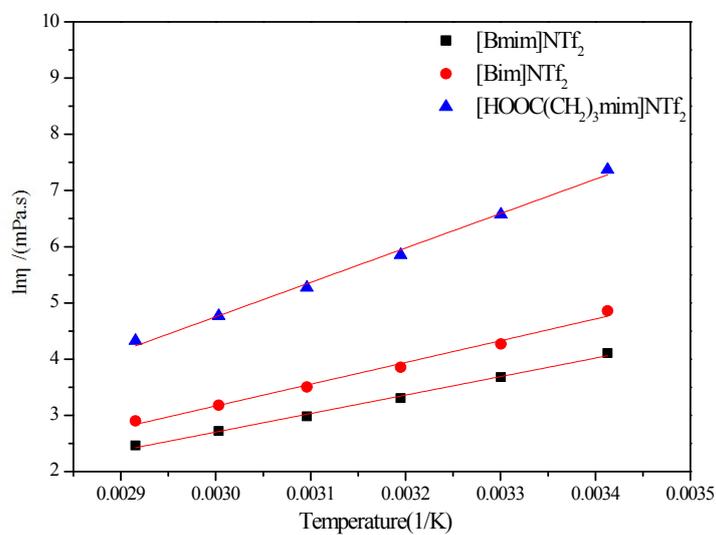


Figure S1. Semi-logarithmic Arrhenius-like plots.

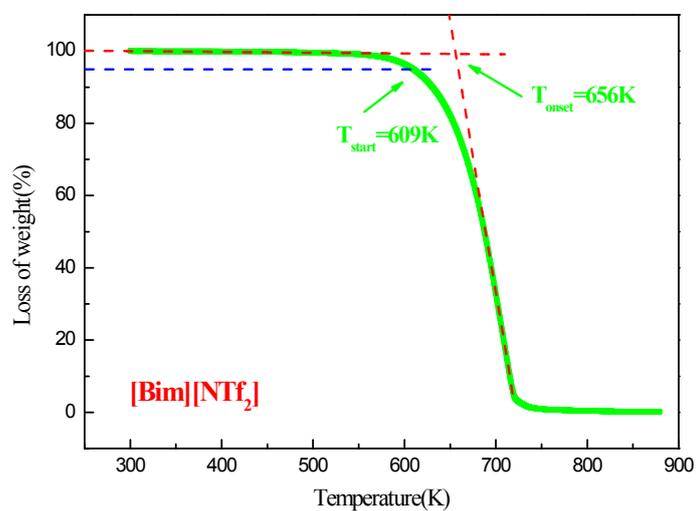


Figure S2. Thermogravimetric analysis of decomposition of [Bim][NTf₂] as a function of temperature.

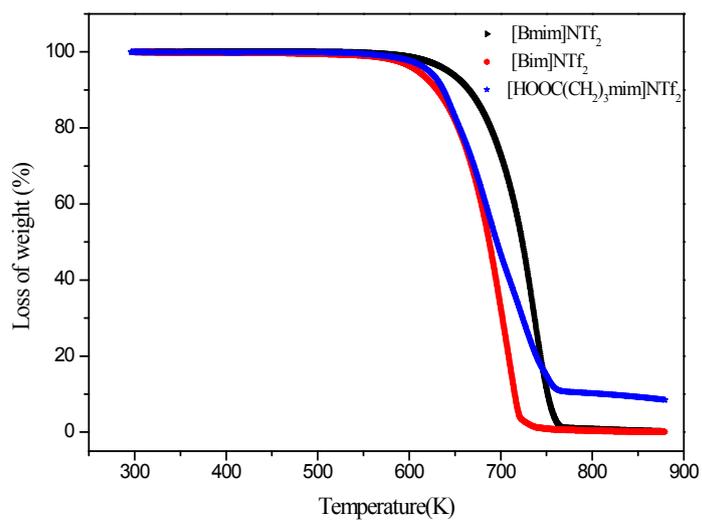


Figure S3. TGA trace of ILs at a heating rate of 10 K/min in the N₂ atmosphere

Table S1. Onset and start temperatures for thermal decomposition of the ILs

ILs	T _{onset} /K	T _{start} /K ^[B]
BmimNTf ₂	687	643
BimNTf ₂	656	609
[HOOC(CH ₂) ₃ mim]NTf ₂	637	621

[B]: temperature with 5% weight loss

3. Reliability of our apparatus

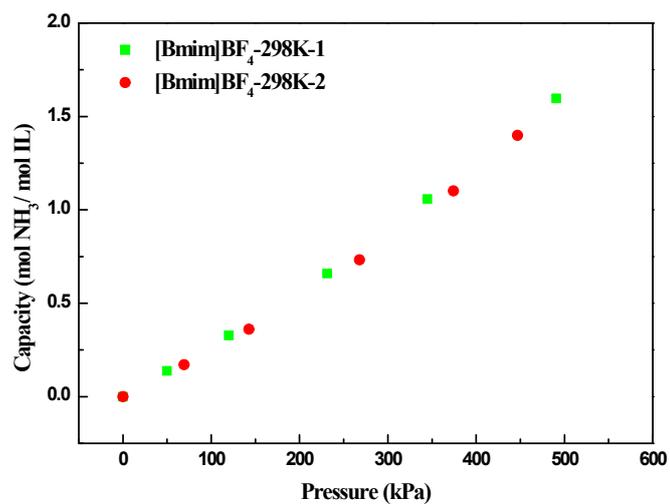


Figure S4. Reliability check of the apparatus using [Bmim][BF₄]

4. ¹H-NMR spectra of the ILs and [Bim][NTf₂] with different concentrations of NH₃

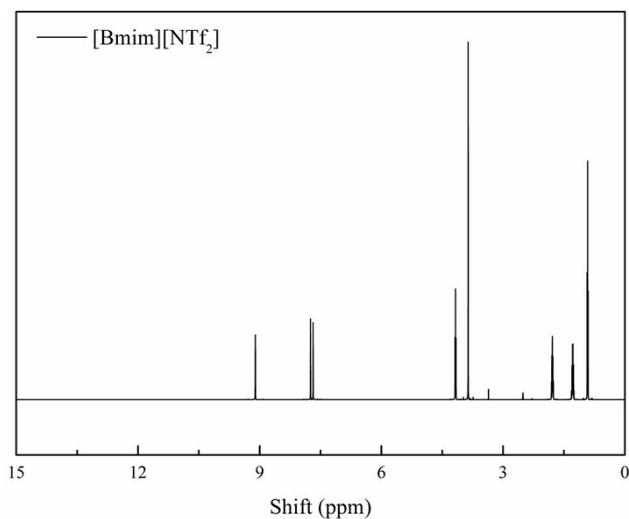


Figure S5. ¹H-NMR spectrum of [Bmim][NTf₂] in DMSO

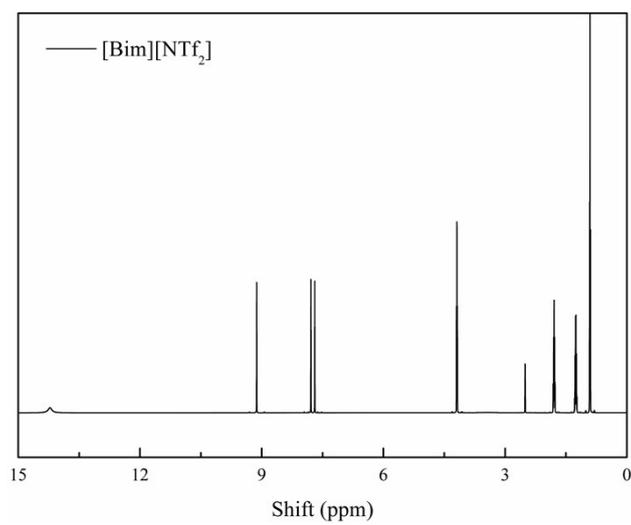


Figure S6. ¹H-NMR spectrum of [Bim][NTf₂] in DMSO

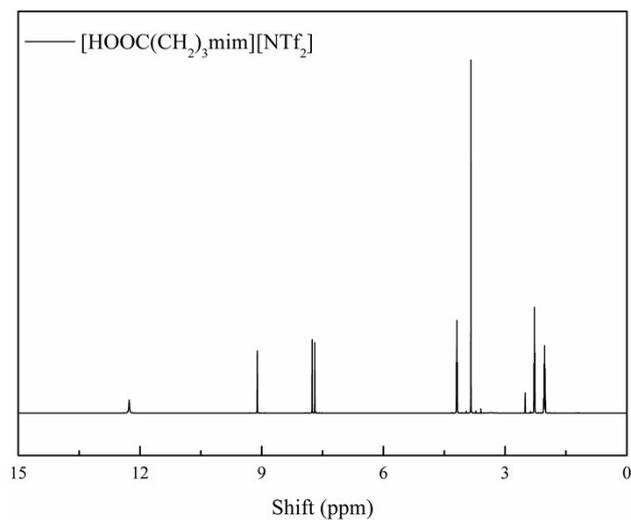


Figure S7. ¹H-NMR spectrum of [HOOC(CH₂)₃mim][NTf₂] in DMSO

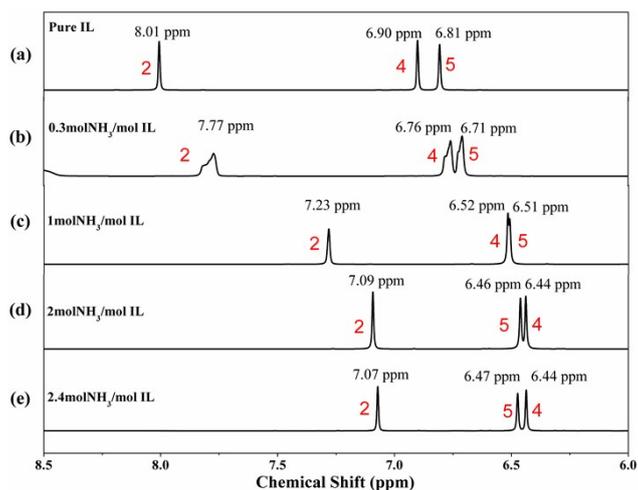


Figure S8. ^1H -NMR spectra of $[\text{Bim}][\text{NTf}_2]$ with different concentrations of NH_3 in drive pipe in DMSO

5. Optimized structures and interaction energies for $[\text{Bim}]^+-3\text{NH}_3$

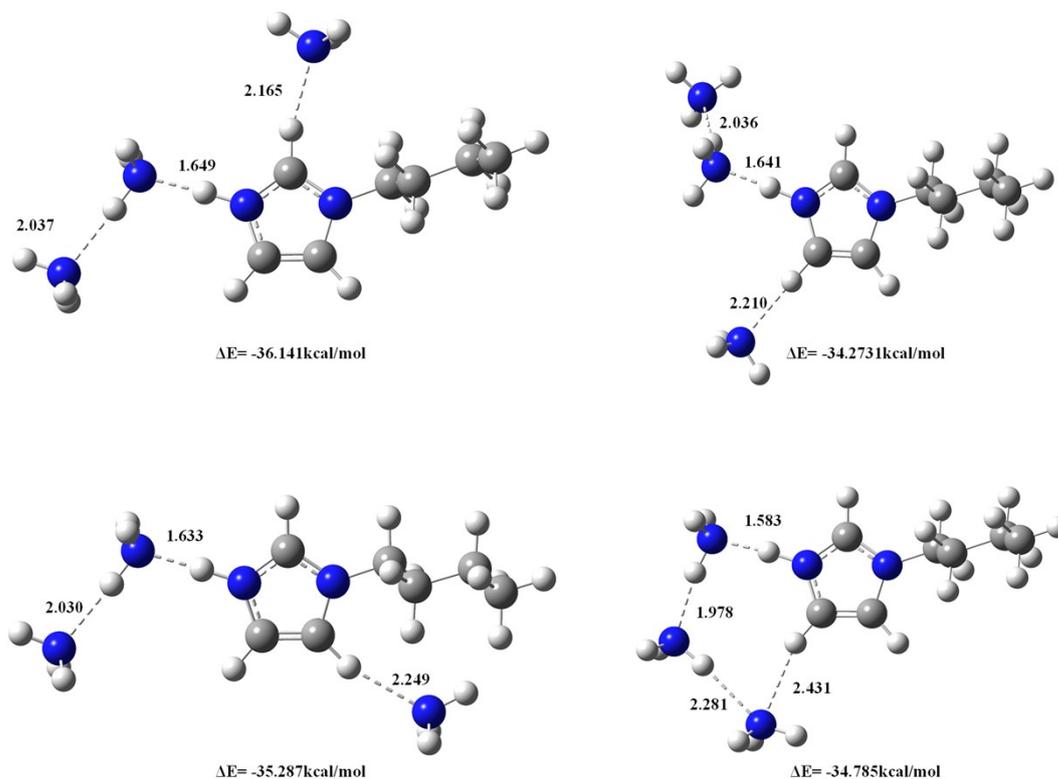


Figure S9. Optimized structures and interaction energies for $[\text{Bim}]^+-3\text{NH}_3$ (N, blue; H, white; C, gray)

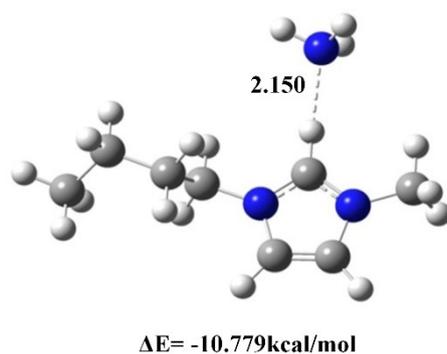


Figure S10. Optimized structures and interaction energies for [Bmim]⁺- NH₃ (N, blue; H, white; C, gray)