

Supplementary Information

Efficient Absorption of Ammonia with Hydroxyl-functionalized Ionic Liquids

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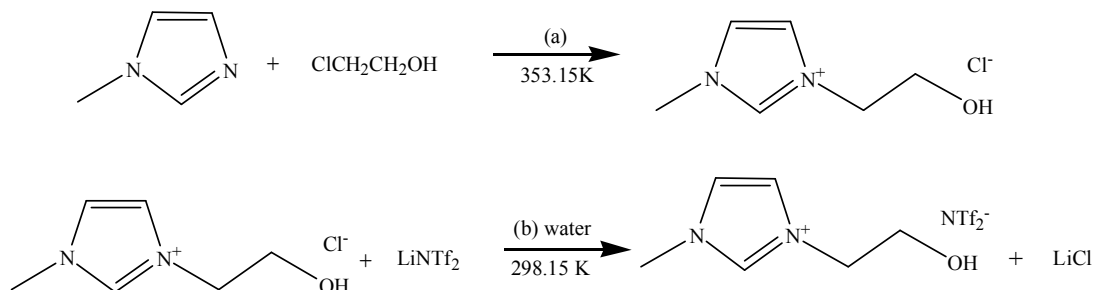
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1. Synthetic route of [EtOHmim][NTf₂].



Scheme S1. Synthetic route of [EtOHmim][NTf₂].

2. NMR data of ILs.

[EtOHmim][Cl]: ¹H NMR (*d*₆-DMSO): 9.21(s, 1H), 7.76(t, 1H), 7.72(t, 1H), 5.38(s, 1H), 4.23(t, 2H), 3.88(s, 3H), 3.72(t, 2H); ¹³C NMR (*d*₆-DMSO): 136.84, 123.26, 122.64, 59.25, 51.53, 35.62.

[EtOHmim][NTf₂]: ¹H NMR (*d*₆-DMSO): 9.07(s, 1H), 7.70(t, 1H), 7.66(t, 1H), 5.16(s, 1H), 4.22(t, 2H), 3.87(s, 3H), 3.74(t, 2H); ¹³C NMR (*d*₆-DMSO): 136.78, 123.23, 122.56, 120.51, 118.38, 59.25, 51.59, 35.54.

[EtOHmim][PF₆]: ¹H NMR (*d*₆-DMSO): 9.04(s, 1H), 7.67(t, 1H), 7.63(t, 1H), 5.18(s, 1H), 4.21(t, 2H), 3.86(s, 3H), 3.74(t, 2H); ¹³C NMR (*d*₆-DMSO): 136.72, 123.20, 122.55, 59.27, 51.59, 35.49.

[EtOHmim][BF₄]: ¹H NMR (*d*₆-DMSO): 9.01(s, 1H), 7.68(t, 1H), 7.64(t, 1H), 5.15(s, 1H), 4.21(t, 2H), 3.87(s, 3H), 3.74(t, 2H); ¹³C NMR (*d*₆-DMSO): 136.68, 123.20, 122.51, 59.29, 51.57, 35.54.

[EtOHmim][SCN]: ¹H NMR (*d*₆-DMSO): 9.04(s, 1H), 7.67(t, 1H), 7.63(t, 1H), 5.18(s, 1H), 4.21(t, 2H), 3.86(s, 3H), 3.74(t, 2H); ¹³C NMR (*d*₆-DMSO): 136.76, 123.31,

122.62, 59.29, 51.63, 35.68.

[EtOHmim][DCA]: ^1H NMR (d_6 -DMSO): 9.07(s, 1H), 7.71(t, 1H), 7.68(t, 1H), 5.15(s, 1H), 4.21(t, 2H), 3.87(s, 3H), 3.73(t, 2H); ^{13}C NMR (d_6 -DMSO):136.77, 123.31, 122.62, 119.04, 59.28, 51.61, 35.65.

[EtOHmim][NO₃]: ^1H NMR (d_6 -DMSO): 9.17(s, 1H), 7.76(t, 1H), 7.73(t, 1H), 5.26(s, 1H), 4.24(t, 2H), 3.89(s, 3H), 3.74(t, 2H); ^{13}C NMR (d_6 -DMSO):136.86, 123.30, 122.61, 59.33, 51.57, 35.52.

[Emim][NTf₂]: ^1H NMR (d_6 -DMSO): 9.04(s, H) 7.74 (t, 1H), 7.66 (t, 1H), 4.19 (t, 2H), 3.85 (s, 3H), 1.42 (t, 3H).

3. The viscosity activation energy (E_a) of ILs.

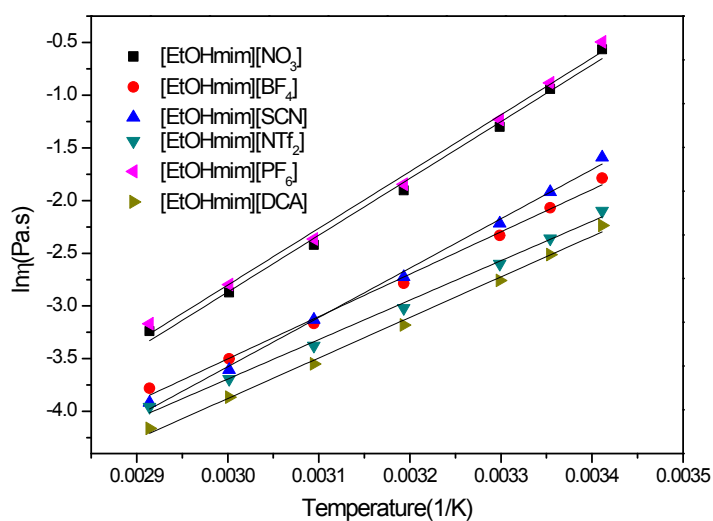


Figure S1. Semi-logarithmic Arrhenius-like plots.

Table S1. Fitted Arrhenius parameters of ILs with the [EtOHmim] cation.

[EtOHmim]X	E_a (kJ/mol)
[PF ₆]	-44.81
[NO ₃]	-44.79
[SCN]	-38.89

[BF ₄]	-33.39
[NTf ₂]	-31.11
[DCA]	-31.10

4. TGA results of hydroxyl-functionalized ILs.

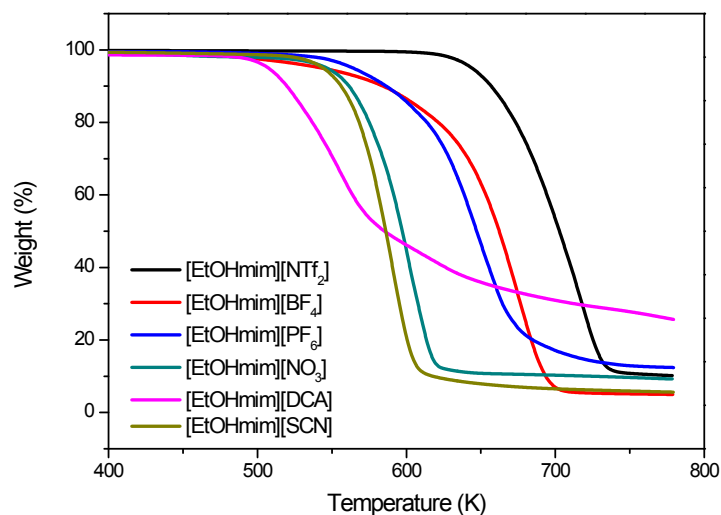


Figure S2. TGA traces of task-specific ILs.

5. Solubility of NH₃ in hydroxyl-functionalized ILs.

Table S2. The solubilities of NH₃ in task-specific ILs.

T=298.15 K		T=313.15 K		T=323.1 K		T=333.15 K		T=343.15 K	
P / kPa	X _{NH3}	P / kPa	X _{NH3}	P / kPa	X _{NH3}	P / kPa	X _{NH3}	P / kPa	X _{NH3}
[EtOHmim][NTf ₂]									
105.50	0.4944	127.79	0.4536	163.45	0.4689	116.83	0.3544	114.41	0.3299
209.51	0.6046	206.36	0.5298	325.05	0.5853	216.76	0.4628	239.24	0.4554
307.40	0.6733	305.74	0.5956	440.77	0.6392	387.66	0.5693	397.31	0.5485
406.95	0.7287	400.10	0.6438	498.83	0.6613	473.28	0.6067	539.22	0.6066
517.48	0.7805	599.77	0.7241	580.56	0.6903	620.21	0.6617	649.52	0.6428
[EtOHmim][PF ₆]									
106.80	0.4954	107.91	0.4026	128.36	0.4170	99.00	0.3316	44.76	0.1870
169.58	0.5579	212.12	0.5070	236.46	0.5040	214.35	0.4427	118.23	0.3147
250.38	0.6184	311.68	0.5709	339.36	0.5596	290.24	0.4894	218.99	0.4089

322.08	0.6628	432.22	0.6316	456.57	0.6093	390.81	0.5368	367.49	0.4910
474.91	0.7424	519.34	0.6686	575.44	0.6514	538.29	0.5912	460.58	0.5293
[EtOHmim][BF ₄]									
98.94	0.4515	115.56	0.3974	98.82	0.3231	102.72	0.2736	185.60	0.3237
208.96	0.5659	196.55	0.4801	208.22	0.4418	170.32	0.3551	269.70	0.3856
293.29	0.6247	336.04	0.5714	318.45	0.5159	286.04	0.4434	364.25	0.4457
344.47	0.6549	408.83	0.6062	415.32	0.5645	407.15	0.5069	468.45	0.4917
426.89	0.6983	500.62	0.6451	566.52	0.6240	547.02	0.5629	604.42	0.5425
[EtOHmim][SCN]									
95.29	0.3522	94.73	0.2370	67.98	0.1653	106.65	0.1867	68.91	0.1095
134.67	0.4205	186.49	0.3719	127.05	0.2645	171.22	0.2598	134.29	0.1803
191.13	0.4932	307.78	0.4855	219.92	0.3684	314.50	0.3784	204.68	0.2450
307.60	0.5979	409.85	0.5538	317.62	0.4463	406.22	0.4351	333.04	0.3357
421.64	0.6720	487.59	0.5971	562.04	0.5793	592.38	0.5255	562.25	0.4545
[EtOHmim][DCA]									
75.04	0.2985	139.81	0.2646	39.96	0.1051	42.10	0.0354	53.68	0.0828
108.48	0.3754	241.15	0.4068	98.45	0.2159	96.79	0.1076	159.36	0.2050
206.36	0.5231	295.52	0.4629	213.61	0.3634	199.05	0.2420	244.81	0.2790
309.45	0.6222	368.11	0.5241	320.60	0.4552	298.62	0.3370	328.21	0.3393
397.68	0.6856	457.18	0.5854	446.72	0.5363	542.50	0.4956	572.65	0.4714
[EtOHmim][NO ₃]									
61.85	0.2455	61.84	0.1169	70.58	0.1511	71.88	0.1176	75.23	0.0994
106.62	0.3427	103.46	0.2020	143.76	0.2546	116.27	0.1723	230.89	0.2384
201.72	0.4754	206.33	0.3470	205.99	0.3201	224.75	0.2777	302.74	0.2880
314.28	0.5766	301.46	0.4389	326.35	0.4191	312.98	0.3432	413.78	0.3516
454.15	0.6665	532.16	0.5862	559.65	0.5494	517.06	0.4589	516.03	0.4033

6. The equilibrium time of [EtOHmim][NTf₂] and [Emim][NTf₂] at 313.15 K.

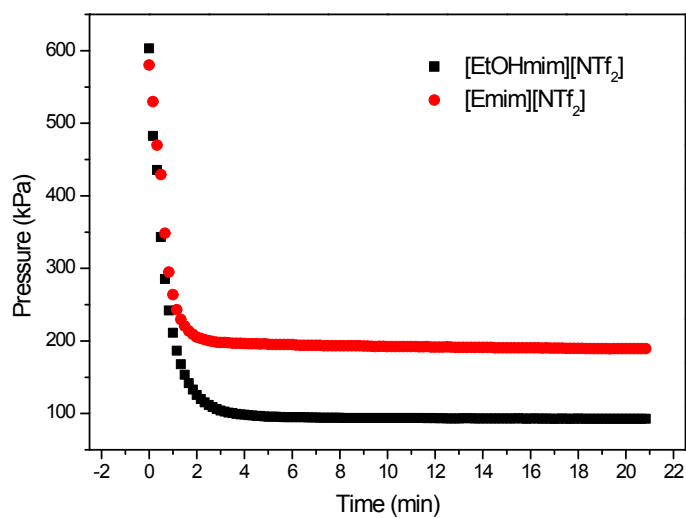


Figure S3. The variation of pressure with time for ammonia absorption in [EtOHmim][NTf₂] and [Emim][NTf₂] at 313.15 K.

7. FT-IR and ¹H NMR spectra of ILs.

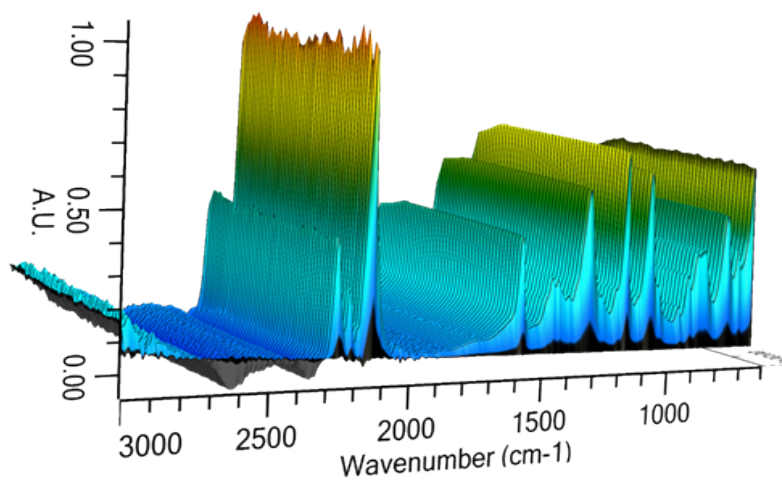


Figure S4. The variation of in-situ IR spectra of [EtOHmim][DCA] in NH₃ absorption process.

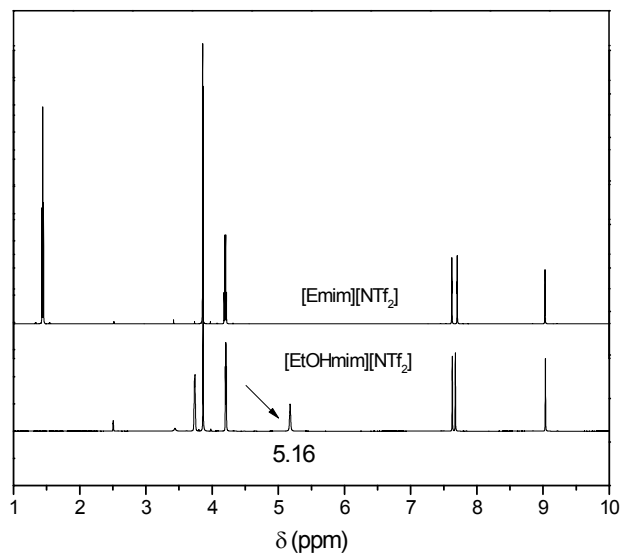


Figure S5. ^1H NMR spectra of $[\text{EtOHmim}][\text{NTf}_2]$ and $[\text{Emim}][\text{NTf}_2]$.