

Supporting Information

Cation-Anion Interactions in 1-Ethyl-3-methylimidazolium-Based Ionic Liquids with Aprotic Heterocyclic Anions (AHAs)

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The Supporting Information file includes NMR data, density, and viscosity for each pure and deuterium exchanged IL.

1-ethyl-3-methylimidazolium 2-cyano-pyrrolide [emim][2-CNPyR].

- (1H NMR, DMSO-*d*6), δ=0.71(3H, t), 3.01(3H, s), 3.35(2H, q), 5.48(1H, m), 6.10(1H, m), 6.39(1H, s), 6.59(1H, d), 6.69(1H, d), 7.41(1H, s)

1-ethyl-3-methylimidazolium 4-triazolide [emim][4-Triaz].

- (1H NMR, DMSO-*d*6), δ=0.51(3H, t), 3.12(3H, s), 3.40(2H, q), 7.20(1H, s), 7.25(2H, s), 7.32(1H, s) 9.04(1H,s)

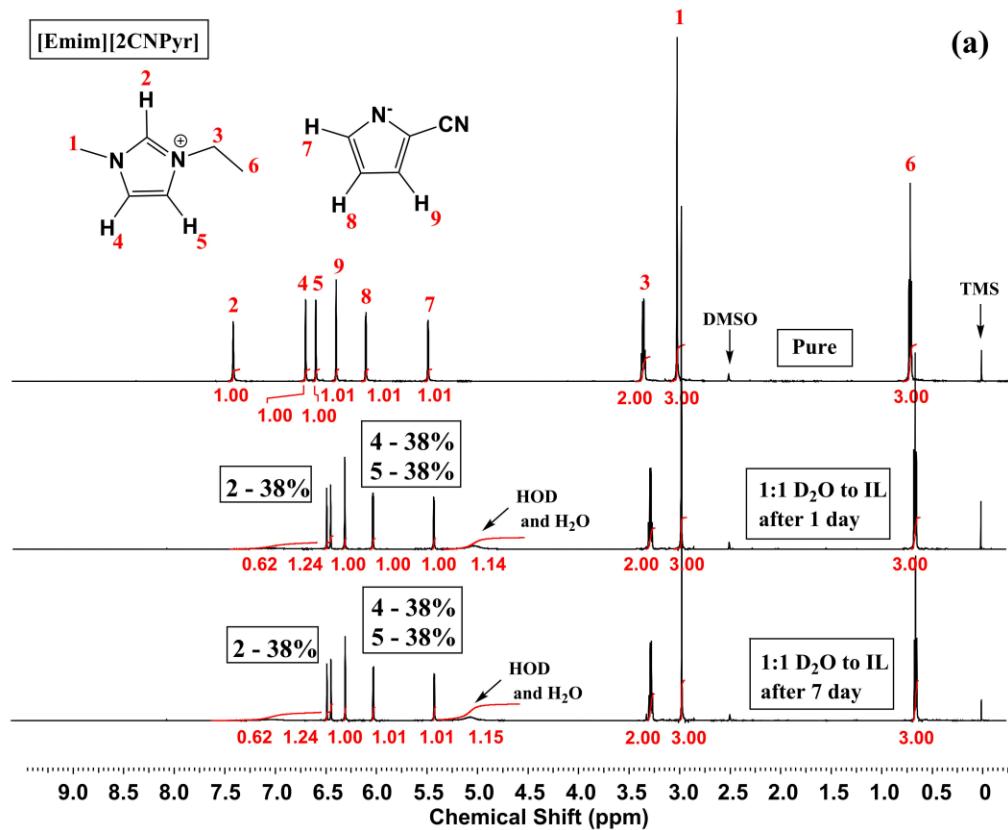
1-ethyl-3-methylimidazolium 3-triazolide [emim][3-Triaz].

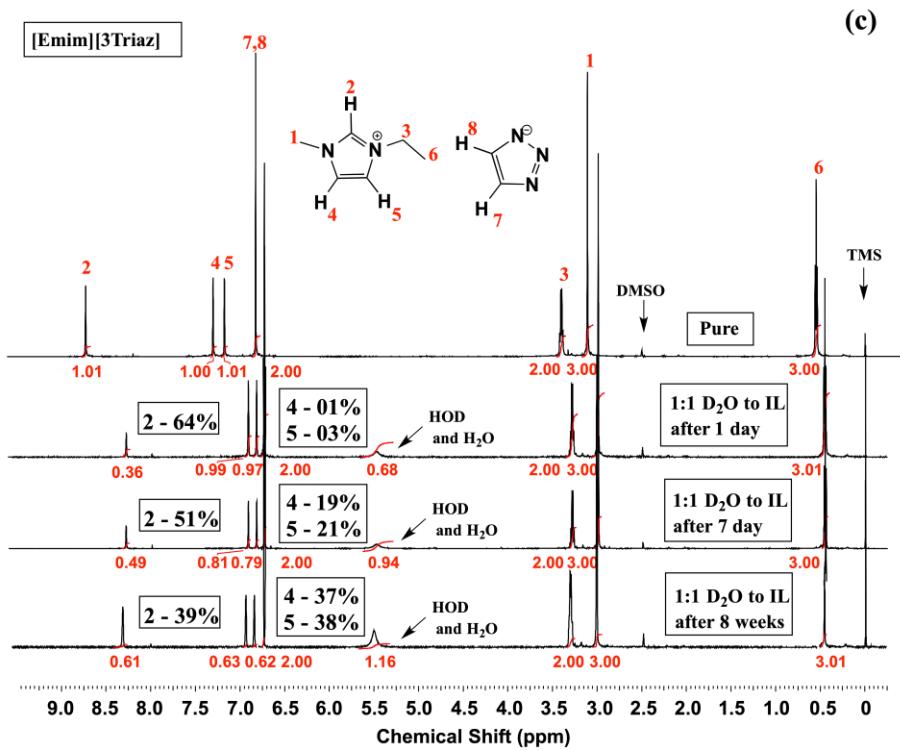
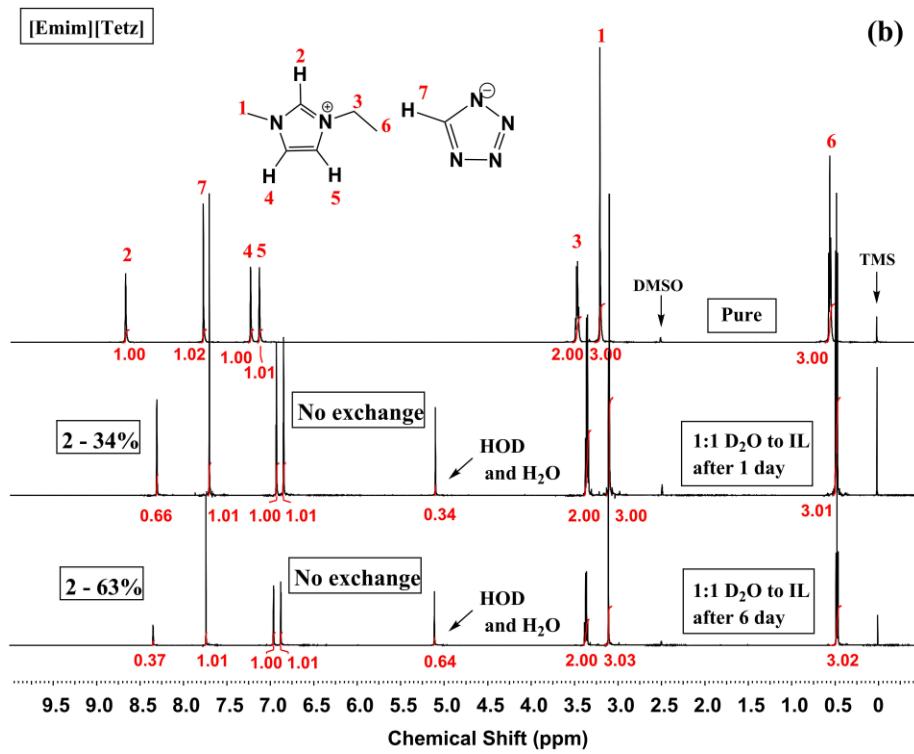
- (1H NMR, DMSO-*d*6), δ=0.55(3H, t), 3.11(3H, s), 3.41(2H, q), 6.83(2H, s), 7.18(1H, s), 7.31(1H, s) 8.73(1H,s)

1-ethyl-3-methylimidazolium tetrazolide [emim][Tetz].

- (1H NMR, DMSO-*d*6), δ=0.54(3H, t), 3.2(3H, s), 3.47 (2H, q), 7.14(1H, t), 7.24 (1H, t), 7.79 (1H, s), 8.69 (1H,s)

Figure S1. Full NMR spectra of pure ILs and D₂O-IL mixtures with quantification of the amount of deuterium exchanged measured at various times, with the reactions eventually reaching equilibrium. (a)-[Emim][2CNPyr] (b) [Emim][Tetz] (c) [Emim][3Triaz] (d) [Emim][4Triaz]





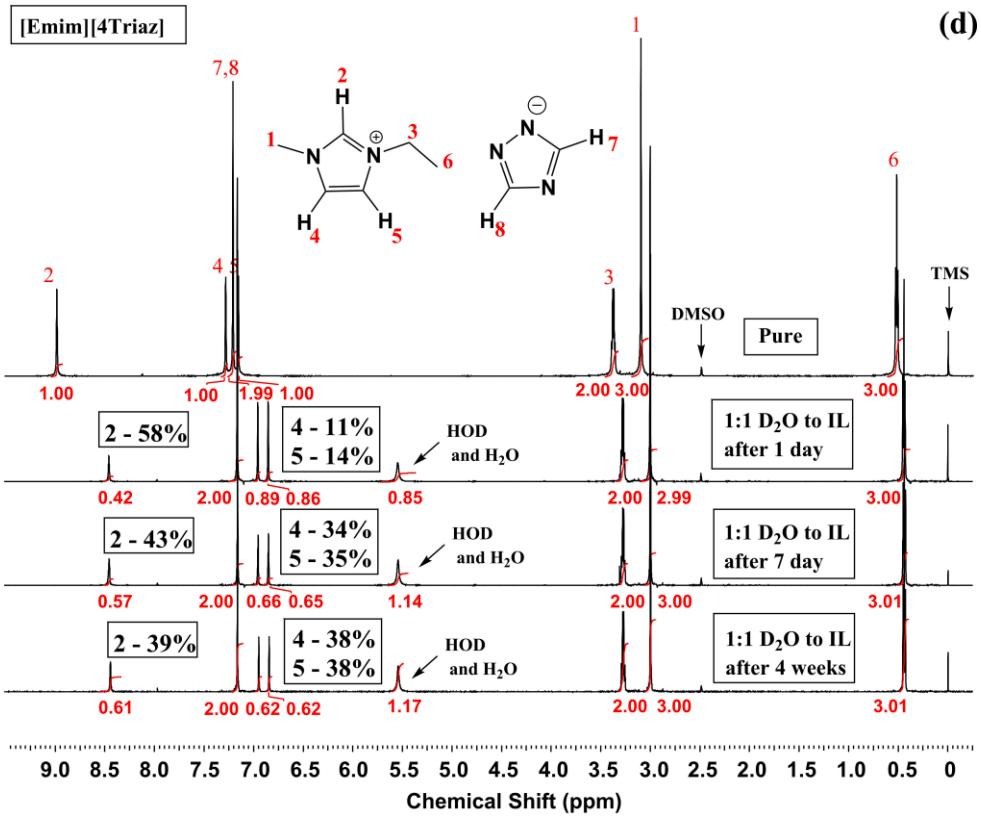
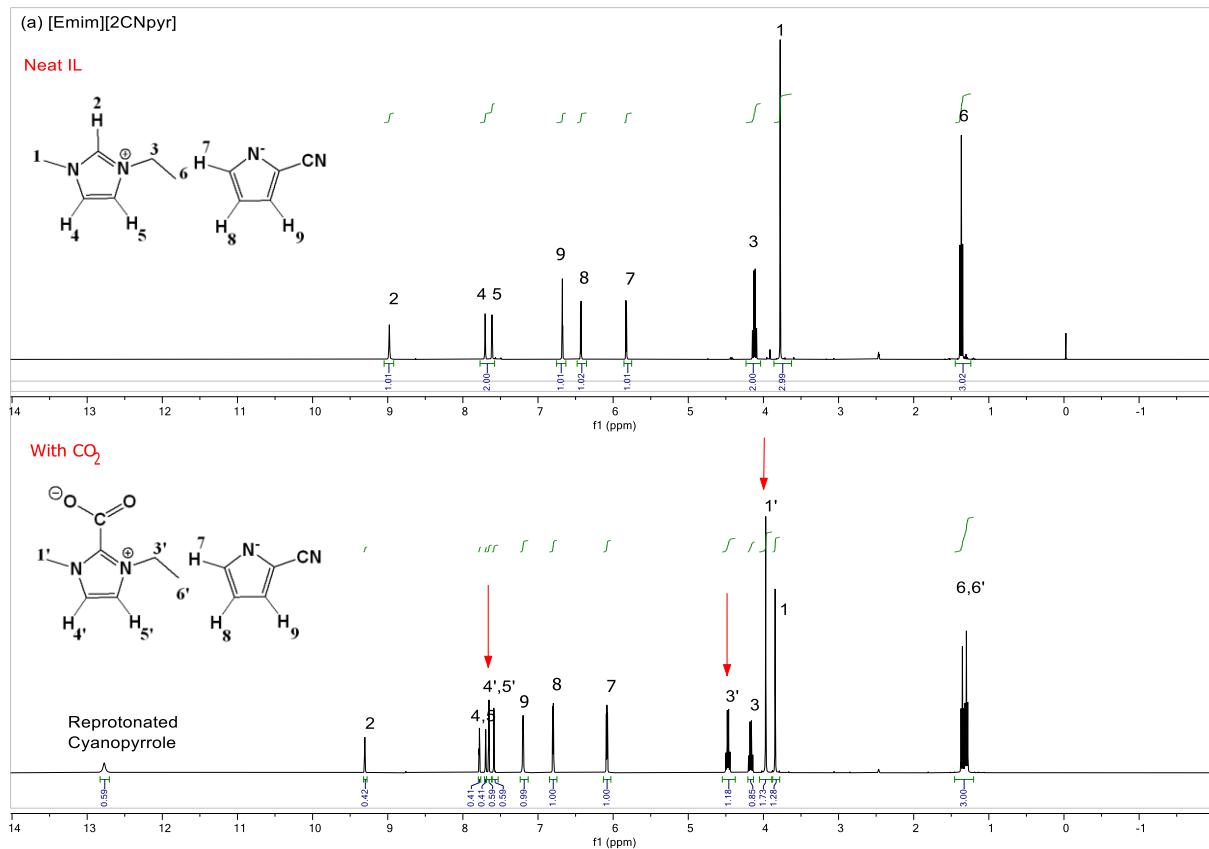


Figure S2. ^1H NMR spectra of neat ILs and CO_2 saturated ILs in deuterated DMSO with peak area integrations. (a)-[Emim][2CNPyr] (b) [Emim][4Triaz] (c) [Emim][3Triaz]



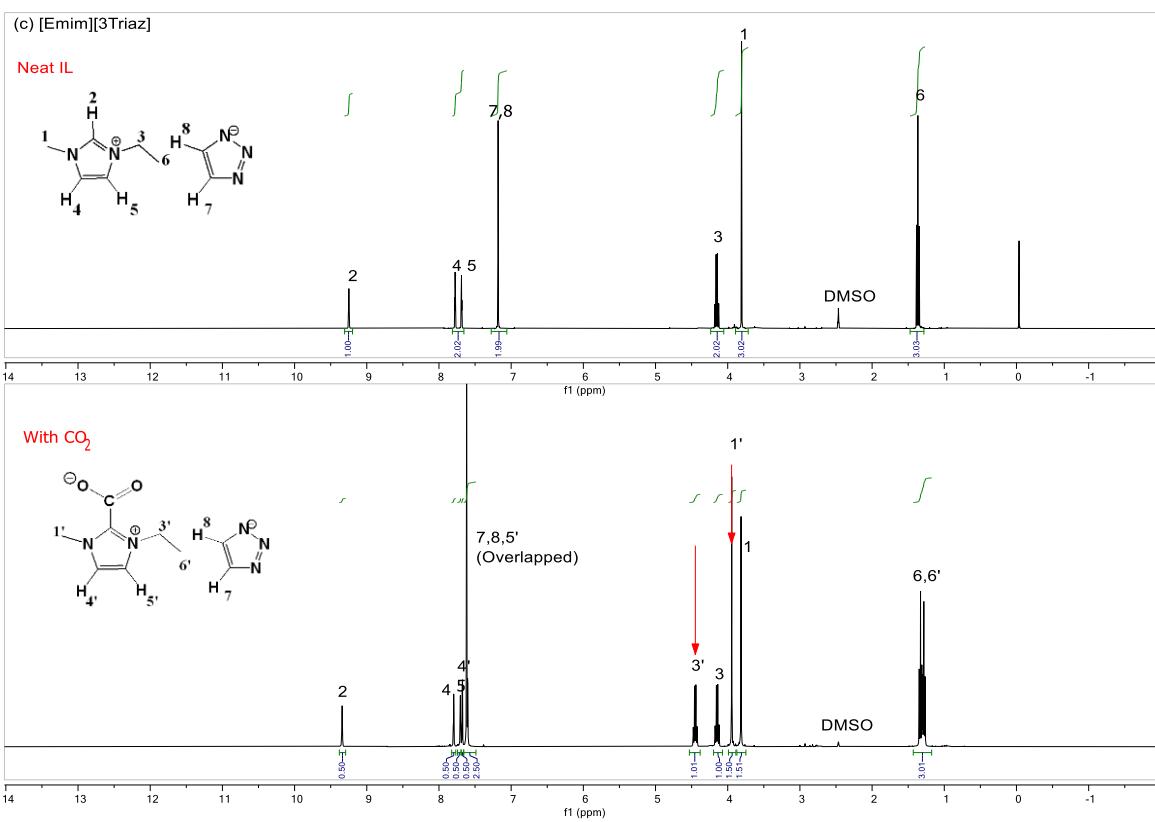
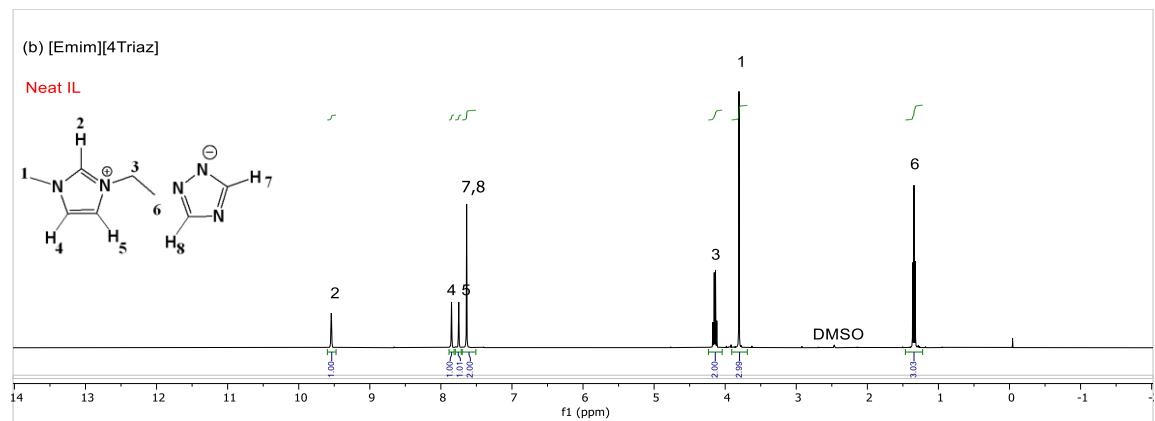


Table S1. Density data of [Emim][2CNPyr], [Emim][Tetz], [Emim][3Triaz], and
 [Emim][4Triaz]

Temp (°C)	Density data (g/cm ³)							
	[Emim][2CNPyr]		[Emim][4Triaz]		[Emim][3Triaz]		[Emim][Tetz]	
	Pure	+D ₂ O*	Pure	+D ₂ O*	Pure	+D ₂ O*	Pure	+D ₂ O*
15	1.091	1.098	1.145	1.152	1.138	1.143	1.174	1.175
20	1.088	1.095	1.141	1.149	1.135	1.140	1.171	1.172
23	1.086	1.093	1.140	1.147	1.133	1.138	1.169	1.170
25	1.085	1.092	1.138	1.146	1.132	1.137	1.168	1.169
30	1.082	1.089	1.135	1.143	1.289	1.133	1.165	1.166
40	1.076	1.082	1.129	1.136	1.123	1.127	1.158	1.159
50			1.123		1.117	1.121	1.152	
60			1.117		1.111	1.115	1.146	

* Amounts of exchanged acidic protons are specified in TABLE 5 of the main article.

Table S2. Viscosity data of [Emim][2CNPyr], [Emim][Tetz], [Emim][3Triaz], and
 [Emim][4Triaz]

Temp (°C)	Viscosity data (cP)							
	[Emim][2CNPyr]		[Emim][4Triaz]		[Emim][3Triaz]		[Emim][Tetz]	
	Pure	+D ₂ O*	Pure	+D ₂ O*	Pure	+D ₂ O*	Pure	+D ₂ O*
15	121.6	123.2	152.1	155.8	134.6	140.2	65.5	66.9
20	85.7	87.4	110.0	112.7	100.3	105.2	52.0	54.0
23	70.6	72.4	92.0	94.0	84.7	85.8	45.4	45.9
25	62.7	66.1	83.0	84.4	76.0	80.2	42.3	43.8
30	48.2	50.0	63.8	67.1	60.1	61.7	35.1	35.2
40	30.5	30.1	39.5	40.5	37.8	38.6	24.8	24.1
50			27.2		26.2	26.8		
60			19.3		18.9	19.2		

* Amounts of exchanged acidic protons are specified in TABLE 5 of the main article.