

## Supplementary material

# The Cation Effect on the Free Volume and the Solubility of H<sub>2</sub>S and CO<sub>2</sub> in Ionic Liquids Based on Bis(2-Ethylhexyl) Sulfosuccinate Anion

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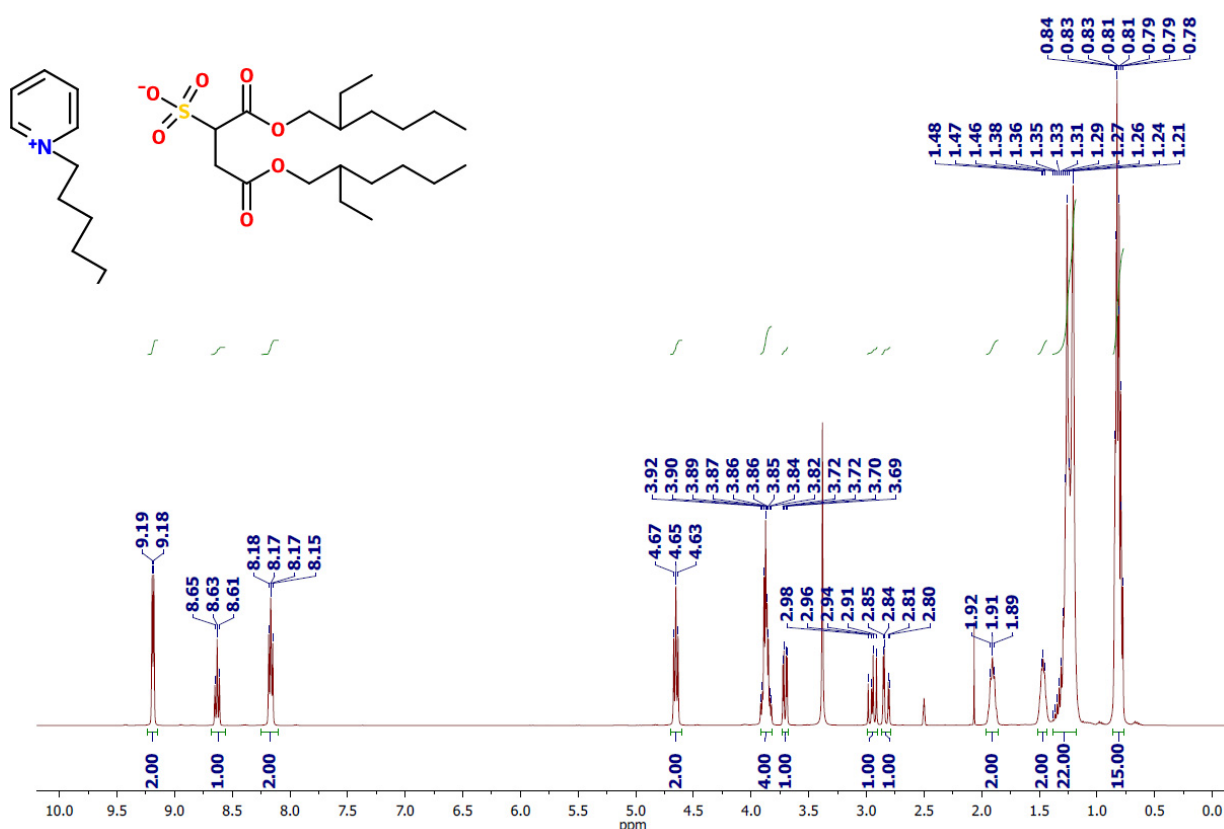
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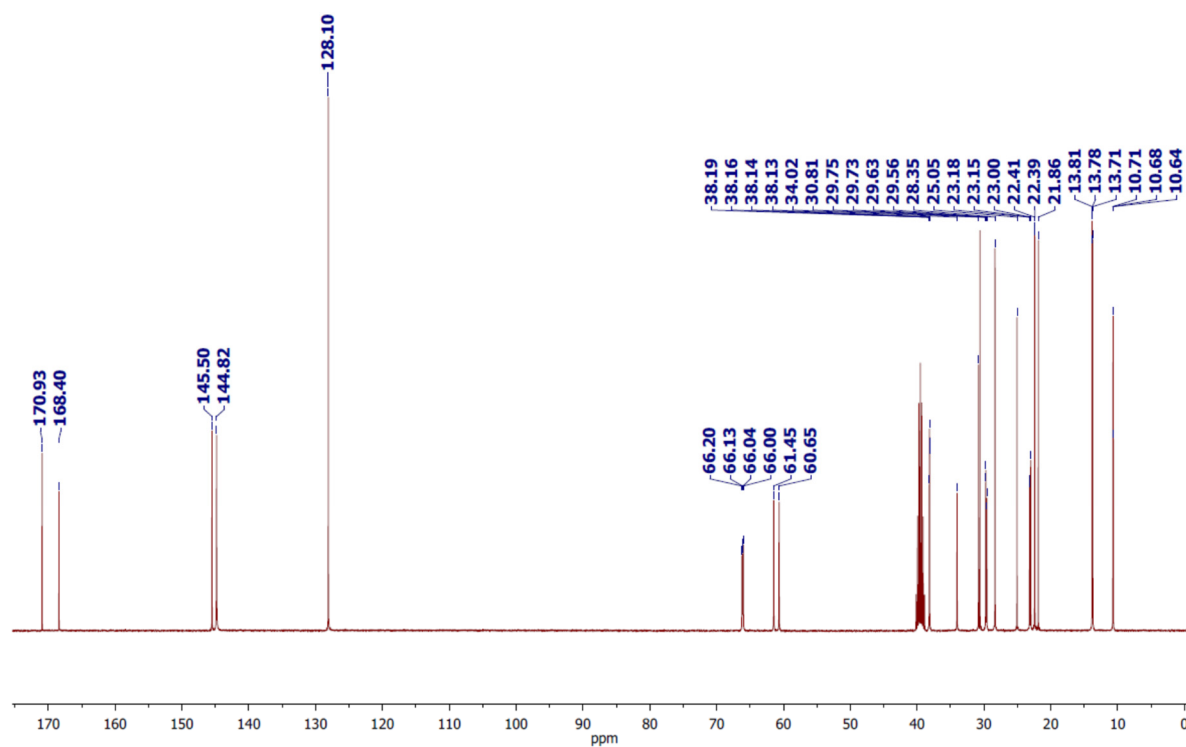
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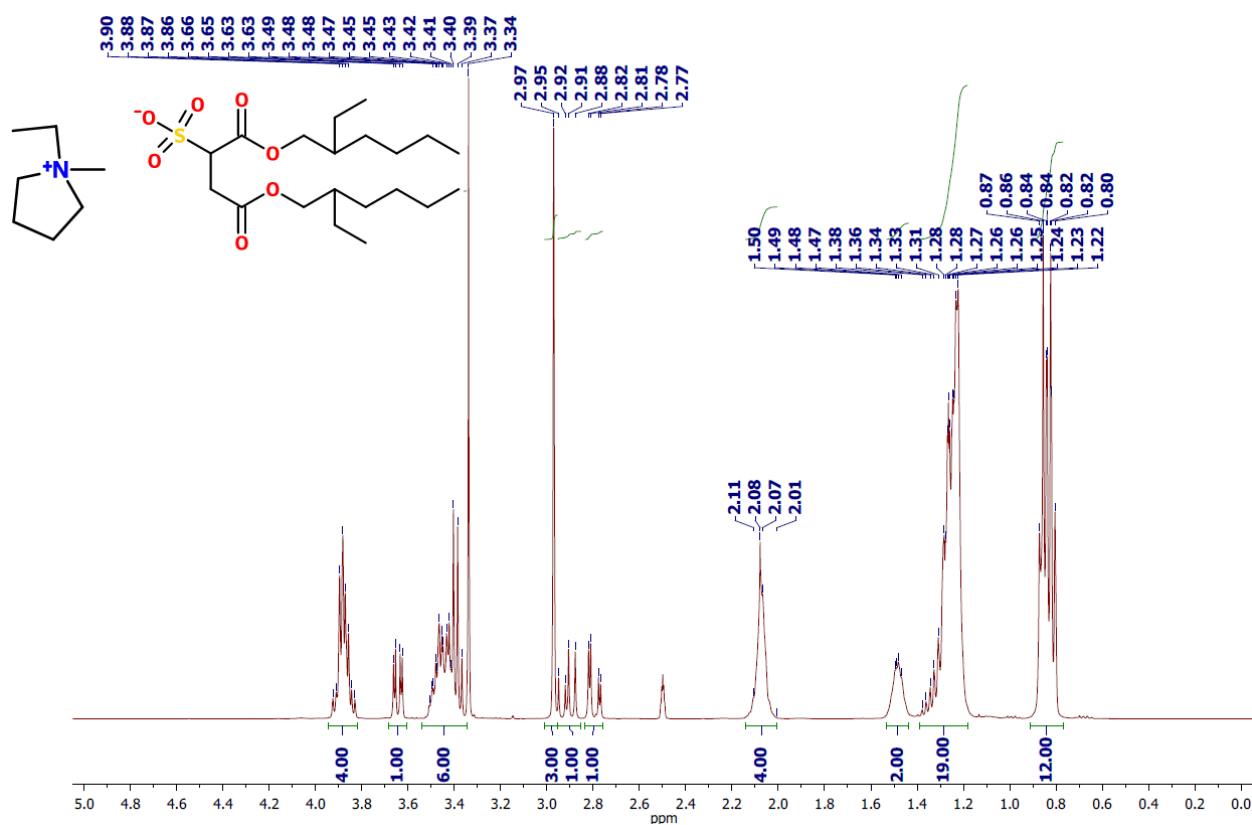


A

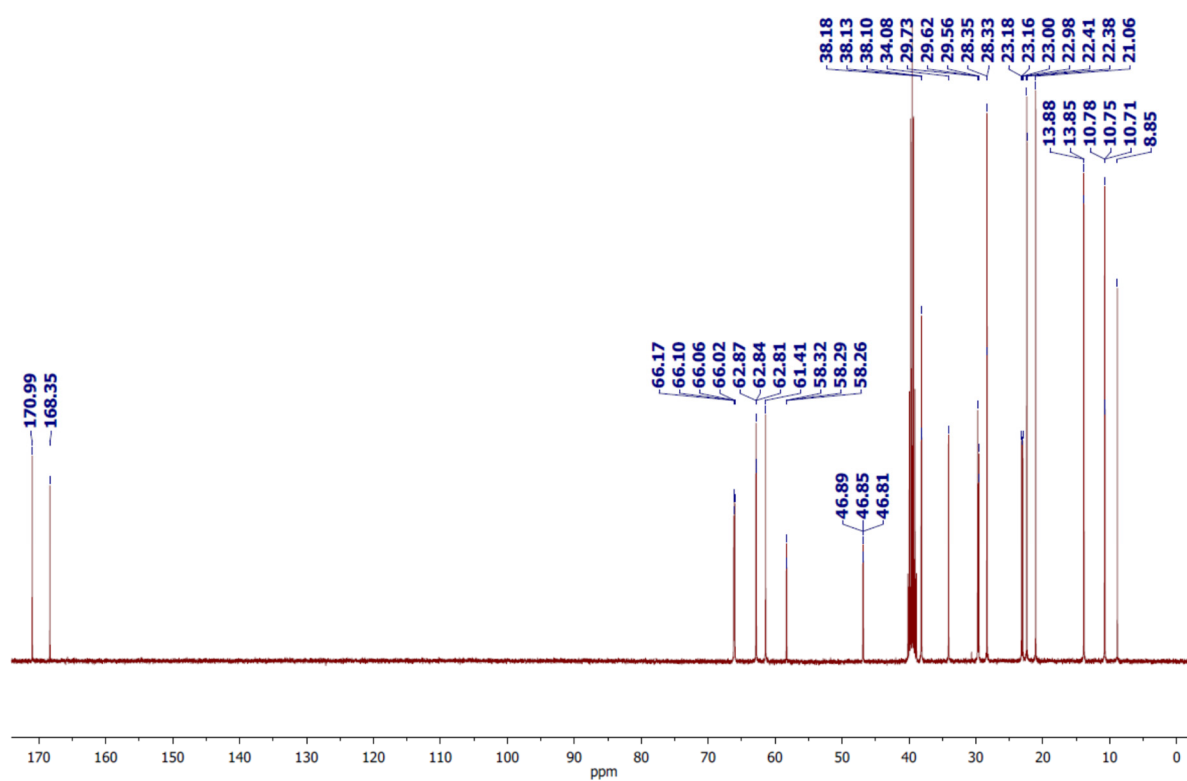


B

**Figure S1.** The <sup>1</sup>H (a) and <sup>13</sup>C NMR (b) of 1-hexylpyridinium bis(2-ethylhexyl) sulfosuccinate.

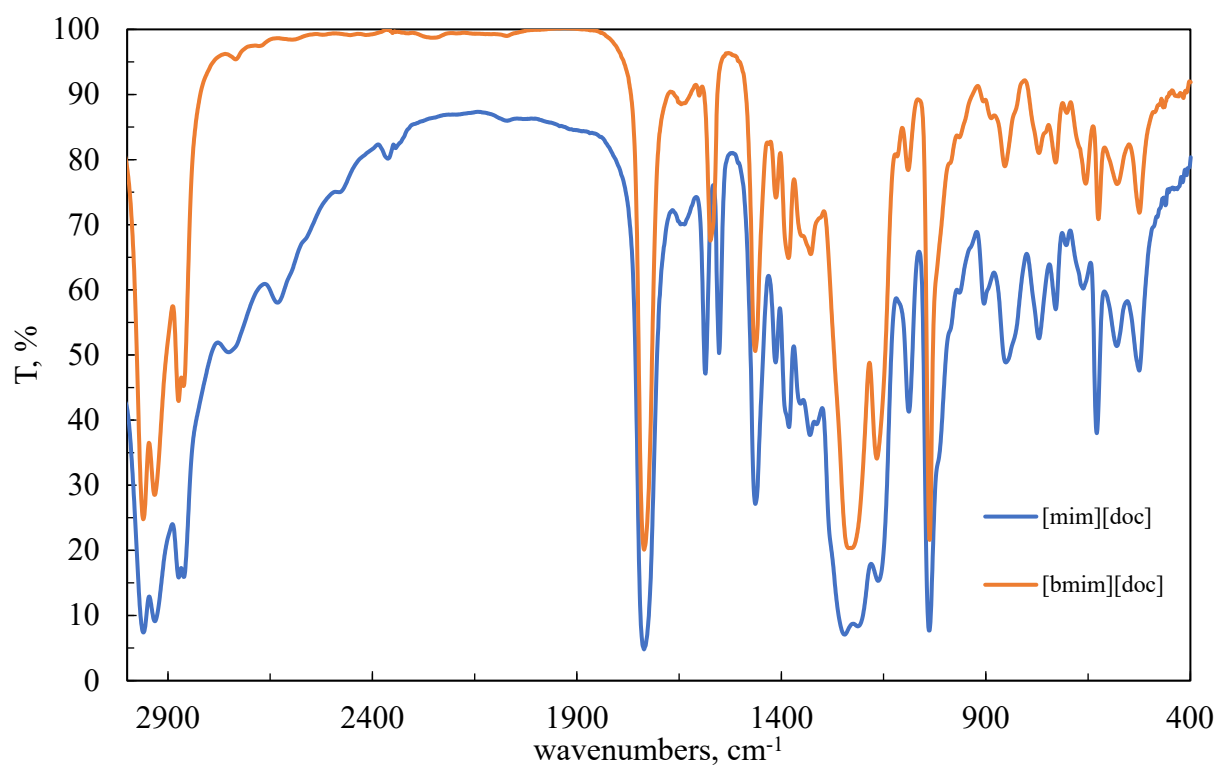


A



B

**Figure S2.** The  $^1\text{H}$  (a) and  $^{13}\text{C}$  NMR (b) of 1-ethyl-1-methylpyrrolidinium bis(2-ethylhexyl) sulfosuccinate.



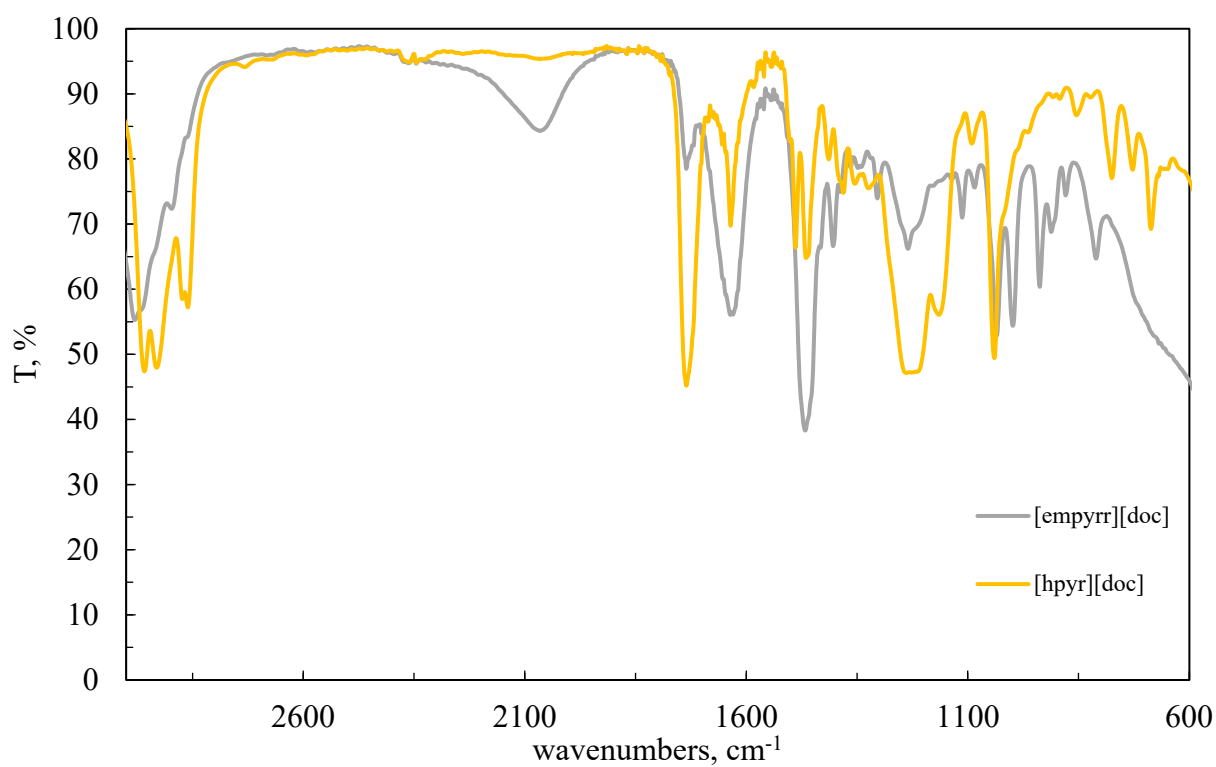


Figure S3. The FTIR spectra of the [doc] – based ILs.

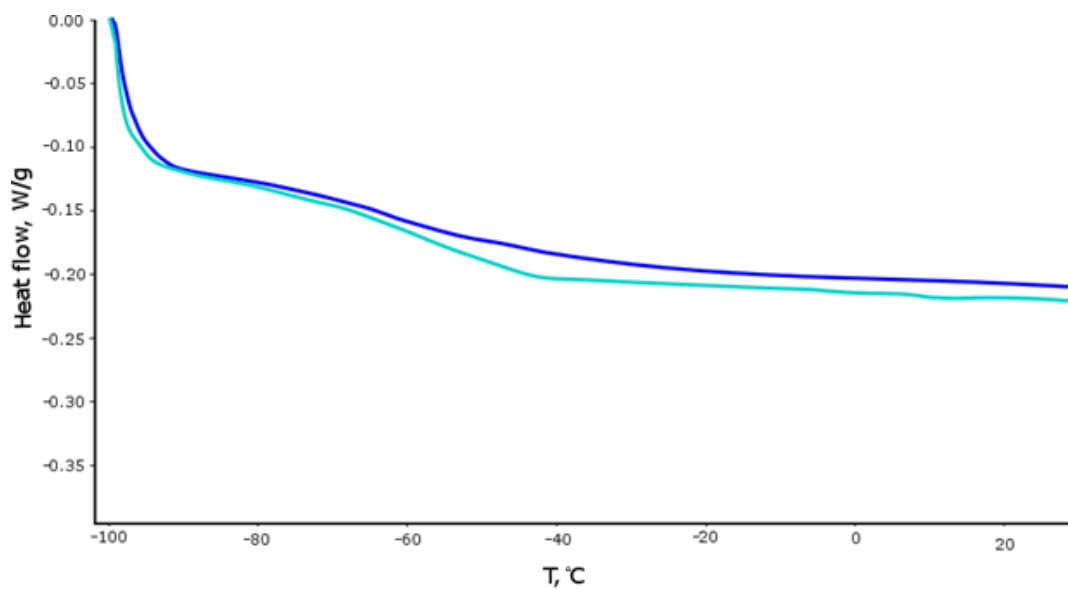


Figure S4. DSC thermograms of and 1-ethyl-1-methylpyrrolidinium bis(2-ethylhexyl) sulfosuccinate (a) 1- hexylpyridinium bis(2-ethylhexyl) sulfosuccinate (b).

**Table S1.** Mole Fraction Solubility of Carbon Dioxide Gas.

T/K	[bmim][doc]		[mim][doc]	
	P (bar)	$m_{CO_2}/(mol_{CO_2}/kg_{IL})$	P (bar)	$m_{CO_2}/(mol_{CO_2}/kg_{IL})$
303.2	2.210	0.207	2.073	0.067
	3.618	0.322	3.477	0.111
	5.152	0.433	4.878	0.153
	6.590	0.527	6.275	0.193
313.2	2.362	0.193	2.312	0.071
	3.928	0.301	3.654	0.110
	5.515	0.403	5.130	0.152
	6.877	0.490	6.411	0.187
323.2	2.516	0.186	2.652	0.077
	3.999	0.279	3.995	0.114
	5.589	0.377	5.487	0.155
	6.985	0.460	6.813	0.189
333.2	2.658	0.1818	2.925	0.080
	4.351	0.2773	4.283	0.115
	5.876	0.3626	5.750	0.153
	7.279	0.438	7.066	0.186
	[hpyr][doc]		[empyrr][doc]	
	P (bar)	$m_{CO_2}/(mol_{CO_2}/kg_{IL})$	P (bar)	$m_{CO_2}/(mol_{CO_2}/kg_{IL})$
303.2	2.191	0.095	2.088	0.103
	3.577	0.140	3.505	0.154
	4.662	0.169	5.016	0.197
	6.286	0.205	6.187	0.224
313.2	2.213	0.088	2.225	0.096
	3.672	0.132	3.671	0.142
	4.776	0.160	5.184	0.183
	6.392	0.195	6.383	0.210
323.2	2.230	0.078	2.239	0.084
	3.784	0.121	3.687	0.128
	4.934	0.148	5.258	0.168
	6.655	0.183	6.410	0.194
333.2	2.478	0.074	2.375	0.078
	3.994	0.110	3.797	0.117
	5.180	0.135	5.419	0.156
	6.904	0.167	6.588	0.181

**Table S2.** Mole Fraction Solubility of Hydrogen Sulfide Gas.

T/K	[bmim][doc]		[mim][doc]	
	P (bar)	$m_{CO_2}/(mol_{CO_2}/kg_{IL})$	P (bar)	$m_{CO_2}/(mol_{CO_2}/kg_{IL})$
303.2	2.010	0.722	1.995	0.247
	3.183	1.187	3.365	0.426
	4.277	1.657	4.280	0.550
	6.110	2.457	5.428	0.711
313.2	2.122	0.626	2.179	0.252
	3.343	1.038	3.529	0.414
	4.439	1.394	4.402	0.527
	6.301	2.055	5.606	0.674
323.2	2.355	0.591	2.293	0.249
	3.620	0.940	3.651	0.340
	4.690	1.252	4.527	0.505

333.2	[hpyr][doc]		[empyrr][doc]	
	P (bar)	$m_{H_2S}/(mol_{H_2S}/kg_{IL})$	P (bar)	$m_{H_2S}/(mol_{H_2S}/kg_{IL})$
	2.311	0.247	2.209	0.303
	3.545	0.410	3.451	0.512
	4.700	0.590	4.507	0.718
303.2	5.789	0.789	6.848	1.312
	2.449	0.241	2.291	0.267
	3.643	0.388	3.520	0.443
	4.776	0.550	4.645	0.631
313.2	5.902	0.740	6.990	1.143
	2.451	0.216	2.420	0.269
	3.714	0.355	3.621	0.436
	4.953	0.517	4.779	0.626
323.2	6.201	0.713	7.216	1.166
	2.580	0.201	2.491	0.250
	3.785	0.317	3.763	0.412
	5.008	0.455	4.962	0.595
333.2	6.315	0.630	7.279	1.075

**Table S3.** Density and viscosity of the ILs as a function of temperature.

T / K	$\rho$ (g·cm <sup>-3</sup> )		$\eta$ (mPa·s)	
	[mim][doc]	[bmim][doc]	[mim][doc]	[bmim][doc]
293.15	1.0874	1.0875	3381.1	3441.7
303.15	1.0801	1.0802	1439.9	1454
313.15	1.0728	1.0729	683.91	692.32
323.15	1.0654	1.0655	359.48	363.28
333.15	1.0584	1.0583	204.86	206.52
T / K	$\rho$ (g·cm <sup>-3</sup> )		$\eta$ (mPa·s)	
	[empyrr][doc]	[hpyr][doc]	[empyrr][doc]	[hpyr][doc]
303.15	-	1.0859	-	4342.2
313.15	1.0879	1.0788	2670	1895.2
323.15	1.0795	1.0717	1242.3	893.16
333.15	1.07227	1.0647	628.36	468.13
343.15	1.0652	1.0578	346.75	267.58
353.15	1.05826	-	207.47	-