

Supplementary Materials

Chronopotentiometric Evaluation of Ionization Degree and Dissociation Constant of Imidazolium-Based Ionic Liquid [C₆Meim][NTf₂] in Polymeric Plasticized Membranes

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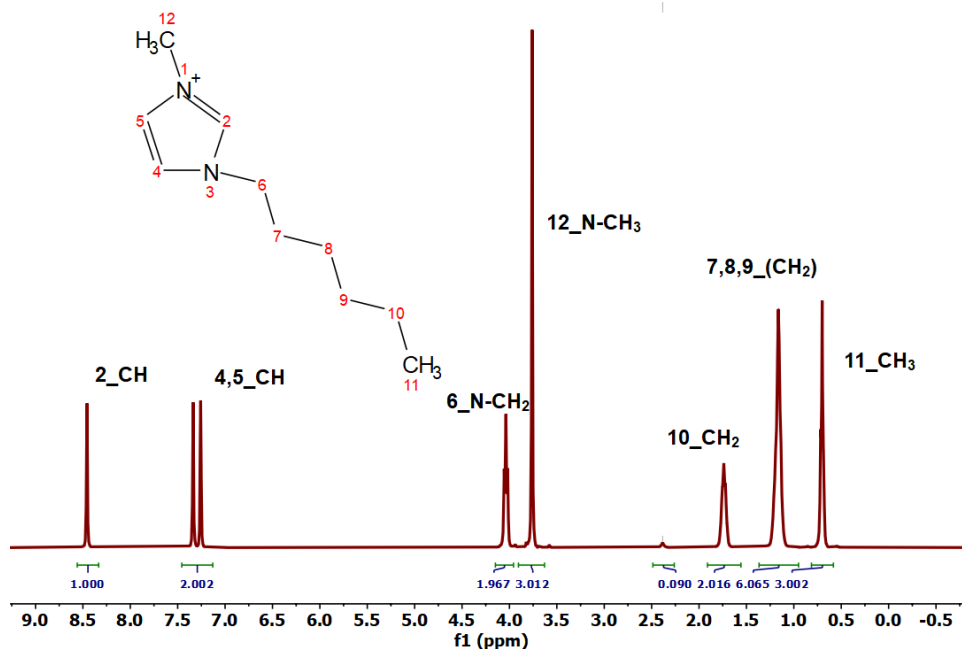


Figure S1. ^1H NMR spectrum of pure IL $[\text{C}_6\text{Meim}][\text{NTf}_2]$.

Table S1. Composition of the prepared PVC- $[\text{C}_6\text{Meim}][\text{NTf}_2]$ -DOS membranes.

Target IL Content															
(ω_{IL} , % in plasticizing mixture)		0	12.4	20.8	29.2	37.3	40.9	50	53.5	54.1	59.1	70.8	79.2	87.6	100
Target IL Content															
(C_{IL} , mol/L of the membrane volume)		0	0.211	0.351	0.494	0.634	0.691	0.840	0.907	0.916	0.999	1.195	1.332	1.487	1.687
Mem-brane Composition	IL, (mg)	0	23.5	38	54.1	71	76.1	91.1	100.4	101.4	110	131	144.3	165.8	184.4
	DOS, (mg)	184.4	165.8	144.3	131	119.3	110	91.4	87.1	86	76.1	54.1	38	23.5	0
	PVC, (mg)	60													

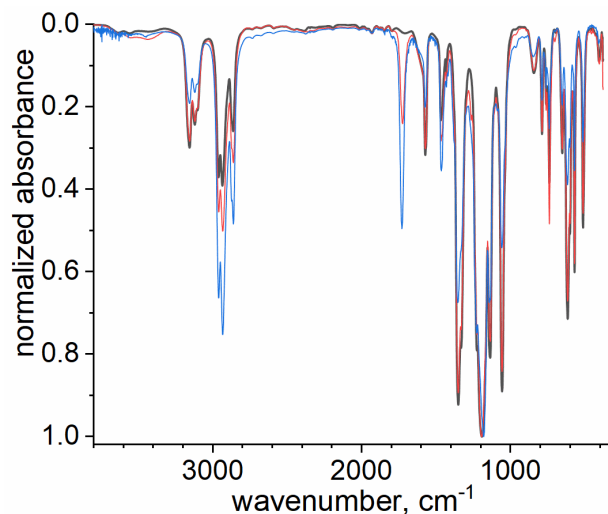


Figure S2. IR absorption spectra of pure $[\text{C}_6\text{Meim}][\text{NTf}_2]$ (black), membrane exudate (red), and $[\text{C}_6\text{Meim}][\text{NTf}_2]$ -DOS mixture ($\omega_{\text{DOS}} = 5\%$, blue).

Table S2. Recalculated IL content in the membranes cast from THF- and CH-based liquid compositions.

Target IL Content (ω_{IL} , % in plasticizing mixture)		0	12.4	20.8	29.2	37.3	40.9	49.9	53.5	54.1	59.1	70.8	79.2	87.6	100
Found IL Content (ω_{IL} , % in plasticizing mixture)	THF	0	4.8	10.1	14.4	26.9	28.9	42.2	41.9	45.4	51.6	67.4	64.2	78.5	-
	CH	0	outlier	10.6	3.8	-	outlier	38.6	-	-	38.3	54	67.3	74.8	-

Table S3. The data obtained from fitting chronopotentiometric curves registered with PVC membranes doped with various amount of [C₆Meim][NTf₂], with Equation 4.

Target IL Content (ω_{IL} , % in plasticizing mixture)	Found IL Content (ω_{IL} , % in plasticizing mixture)	mean $\chi^2 \times 10^9$	mean τ , (s)	log C_i	log D_i
0	0	-	-	-4.1 ± 0.2	-
12.4	4.8	0.98	1.6	-2.3 ± 0.3	-8.35 ± 0.29
20.8	10.1	1.9	3.7	-2.0 ± 0.1	-8.32 ± 0.14
29.2	14.4	3.1	3.4	-1.5 ± 0.2	-7.94 ± 0.23
40.9	28.9	3.9	3.7	-1.2 ± 0.2	-6.63 ± 0.15
49.9	42.2	7.3	4.7	-2.3 ± 0.3	-6.92 ± 0.17
59.1	51.6	4.9	2.8	-2.5 ± 0.3	-7.17 ± 0.11
70.8	64.2	4.2	4.9	-2.6 ± 0.2	-7.31 ± 0.16
79.2	67.4	3.4	6.6	-2.5 ± 0.2	-7.62 ± 0.21
87.6	78.5	2.9	4.7	-2.6 ± 0.1	-8.03 ± 0.24
100	100	2.2	5.9	-2.8 ± 0.1	-7.15 ± 0.15

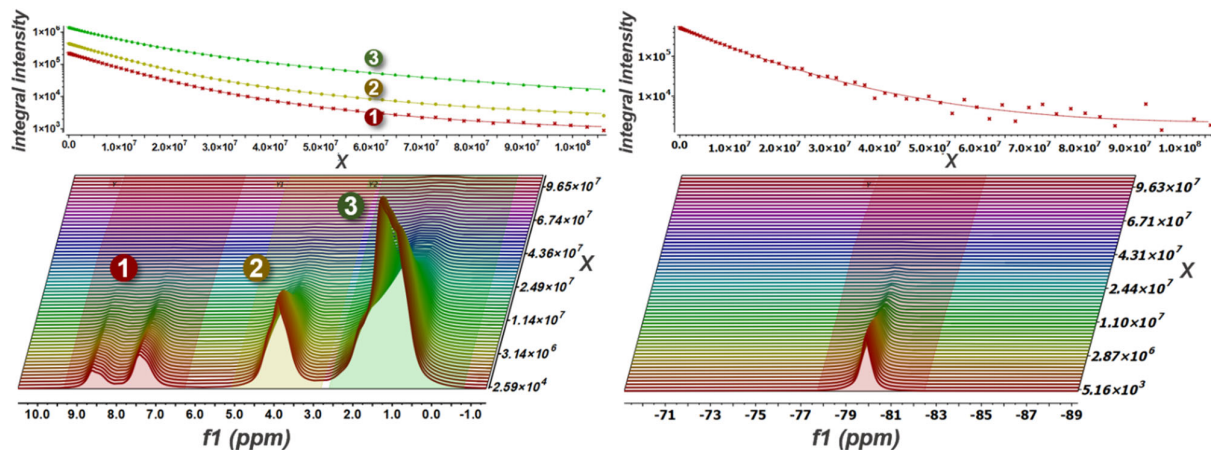
**Figure S3.** A stack of ^1H (left panel) and ^{19}F (right panel) spectra of the membrane with 45.4 wt.% of IL in the plasticizing mixture at different values of the gradient amplitude. Insets: the respective experimental (symbols) and fitted with Equation 117 (lines) dependences of the integral intensity on the square of gradient amplitude (x) for ^1H and ^{19}F spectra.

Table S4. Diffusion coefficients obtained from fitting integral intensities in ^1H and ^{19}F NMR spectra registered with PVC membranes doped with various amount of $[\text{C}_6\text{Meim}][\text{NTf}_2]$, versus square of the gradient amplitude (x); D_1 —“fast” component, D_2 —“slow” component in Equation 17.

Found IL Content (ω_{IL} , % in plasticizing mixture)	obtained from cation peaks in ^1H spectra, $\times 10^7 \text{ cm}^2/\text{s}$		obtained from anion (fluorine) peaks in ^{19}F spectra, $\times 10^7 \text{ cm}^2/\text{s}$		mean D_1 , log units	mean D_2 , log units
	D_1	D_2	D_1	D_2		
26.9	1.108 ± 0.011	0.574 ± 0.009	1.285 ± 0.018	0.498 ± 0.081	-6.928 ± 0.006	-7.272 ± 0.044
41.9	1.731 ± 0.008	0.558 ± 0.009	1.295 ± 0.012	0.531 ± 0.024	-6.825 ± 0.004	-7.264 ± 0.016
45.4	1.192 ± 0.008	0.446 ± 0.021	1.303 ± 0.074	0.592 ± 0.142	-6.905 ± 0.025	-7.290 ± 0.087
pure $[\text{C}_6\text{Meim}][\text{NTf}_2]$	2.055 ± 0.006	-	2.002 ± 0.013	-	-	-

Table S5. The target and found IL concentrations in the studied membranes, and the respective values of $[\text{C}_6\text{Meim}][\text{NTf}_2]$ ionization degree.

Target IL Content	Found IL Content		ionization degree, $\alpha_{[\text{C}_6\text{Meim}][\text{NTf}_2]}$
ω_{IL} , % in plasticiz- ing mixture	$\omega_{\text{IL}}^{\text{corr}}$, % in plasti- cizing mixture	C_{IL} , mol/l of the membrane volume	
12.4	4.8	0.080	0.13 ± 0.09
20.8	10.1	0.164	0.13 ± 0.03
29.2	14.4	0.231	0.25 ± 0.12
40.9	28.9	0.466	0.32 ± 0.15
49.9	42.2	0.685	$(16 \pm 12) \times 10^{-3}$
59.1	51.6	0.836	$(6 \pm 5) \times 10^{-3}$
70.8	67.4	1.107	$(4.0 \pm 1.9) \times 10^{-3}$
79.2	64.2	0.917	$(6 \pm 3) \times 10^{-3}$
87.6	78.5	1.133	$(4.0 \pm 1.9) \times 10^{-3}$
100	100	1.518	$(1.2 \pm 0.5) \times 10^{-3}$