Electronic Supplementary Information (ESI) for

Effect of dielectric constant on estimation of properties of ionic liquids: An analysis of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide†

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Table S 1 Interaction energy (kJ.mol^{-1}) of C_1mimNTf$_2$ and C_4mimNTf$_2$, and cation-anion distance (Å) for these ILs as CA model for different dielectric constants

	$\mathbf{C_1mimNTf_2}$		$\mathbf{C_4mimNTf_2}$	
ε	ΔE_{int}	$\mathbf{d}_{H(C^+)-N(A^-)}$	ΔE_{int}	$\mathbf{d}_{H(C^+)-N(A^-)}$
1	-315.6	2.07	-308.5	2.10
2	-131.0	2.26	-131.2	2.17
10	-26.0	2.46	-25.1	2.50
33	-6.2	2.54	-6.7	2.61
78	-1.5	2.57	-0.8	2.69

Table S 2 Interaction energy (kJ.mol^{-1}) of C_{1-12}mimNTf$_2$ and cation-anion distance (Å) for these ILs as CA model

	ΔE_{int}		$\mathbf{d}_{H(C^+)-N(A^-)}$	
Ionic liquid	$\varepsilon = 1$	$\varepsilon = 78$	$\varepsilon = 1$	$\varepsilon = 78$
C_1mimNTf$_2$	-315.6	-1.5	2.07	2.57
C_2mimNTf$_2$	-314.6	-1.8	2.09	2.44
C_3mimNTf$_2$	-310.0	-1.0	2.10	2.59
C_4mimNTf$_2$	-308.5	-0.8	2.10	2.69
C_5mimNTf$_2$	-308.0	-1.0	2.10	2.58
C_6mimNTf$_2$	-307.1	-0.4	2.10	2.64
C_7mimNTf$_2$	-307.1	-0.6	2.10	2.78
C_8mimNTf$_2$	-306.6	-0.8	2.10	2.71
C_9mimNTf$_2$	-306.3	-0.5	2.10	2.73
C_{10}mimNTf$_2$	-306.3	-0.4	2.10	2.65
C_{11}mimNTf$_2$	-306.5	-0.9	2.11	2.58
C_{12}mimNTf$_2$	-306.6	-1.0	2.11	2.58

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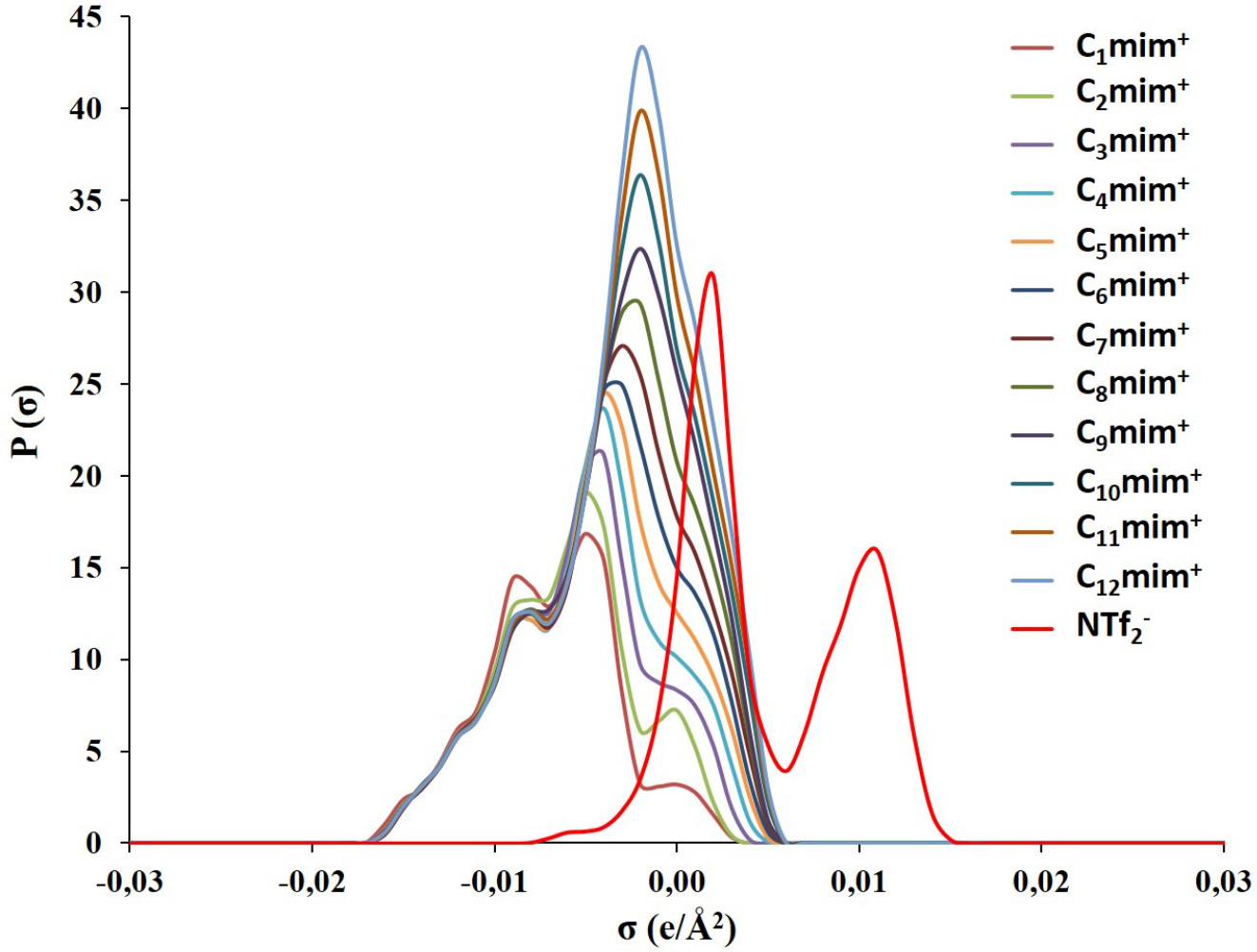

Figure S 1 σ-profiles of C_{1-12}mimNTf_2 represented as C+A model with $\varepsilon = 1$

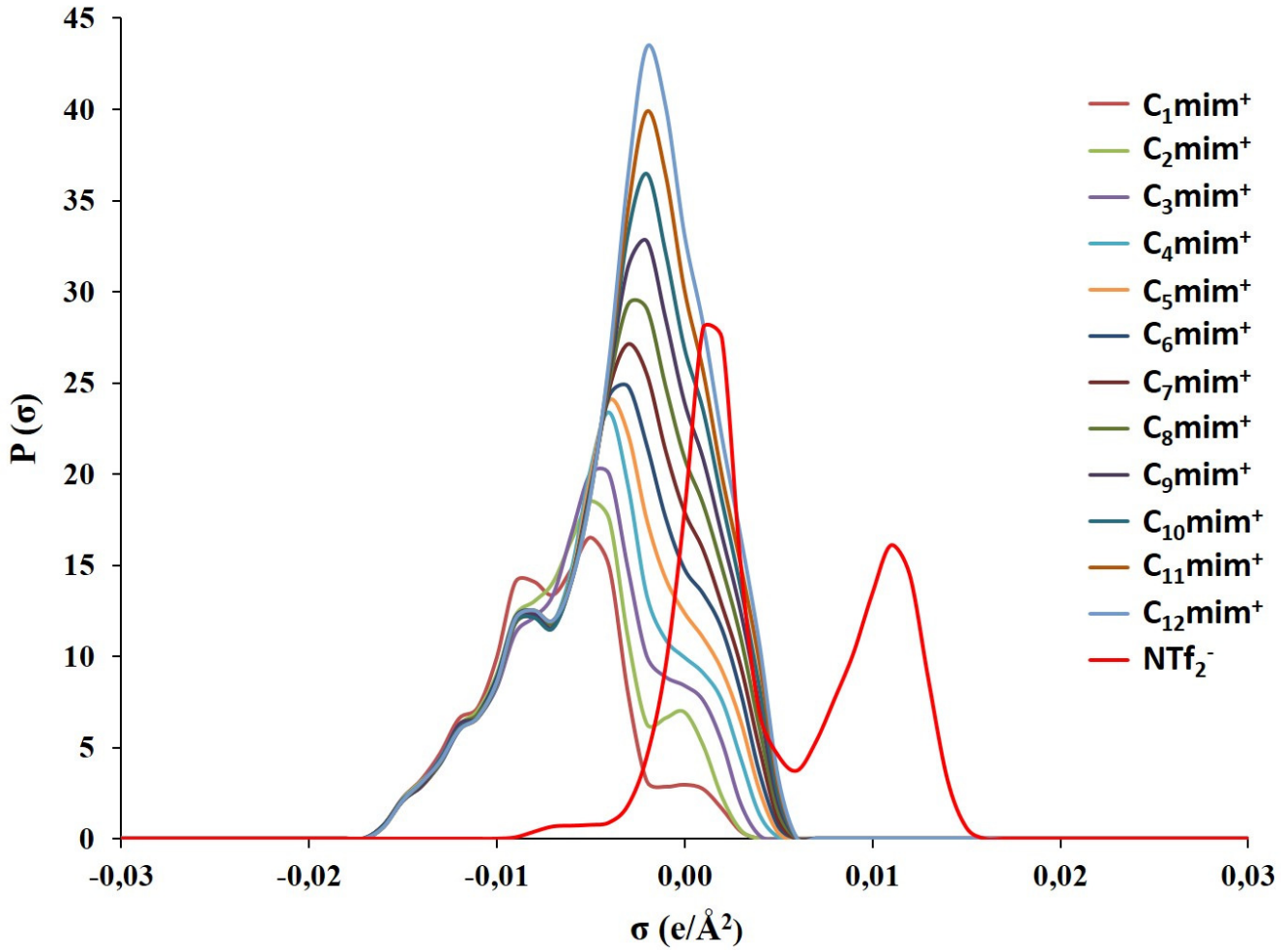

Figure S 2 σ-profiles of C_{1-12}mimNTf_2 represented as C+A model with $\varepsilon = 78$

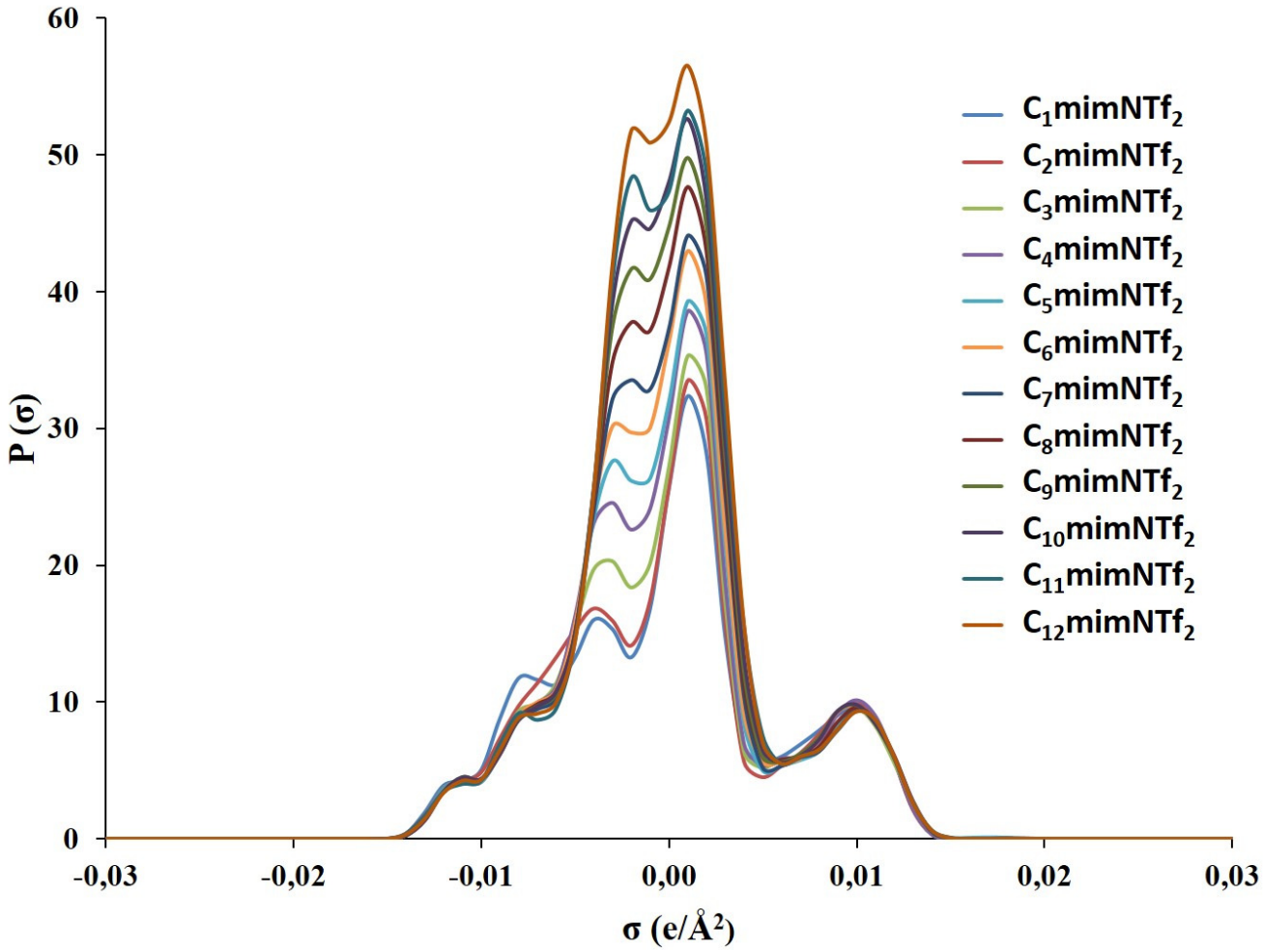

Figure S 3 σ-profiles of C_{1-12}mimNTf$_2$ represented as CA model with $\varepsilon = 1$

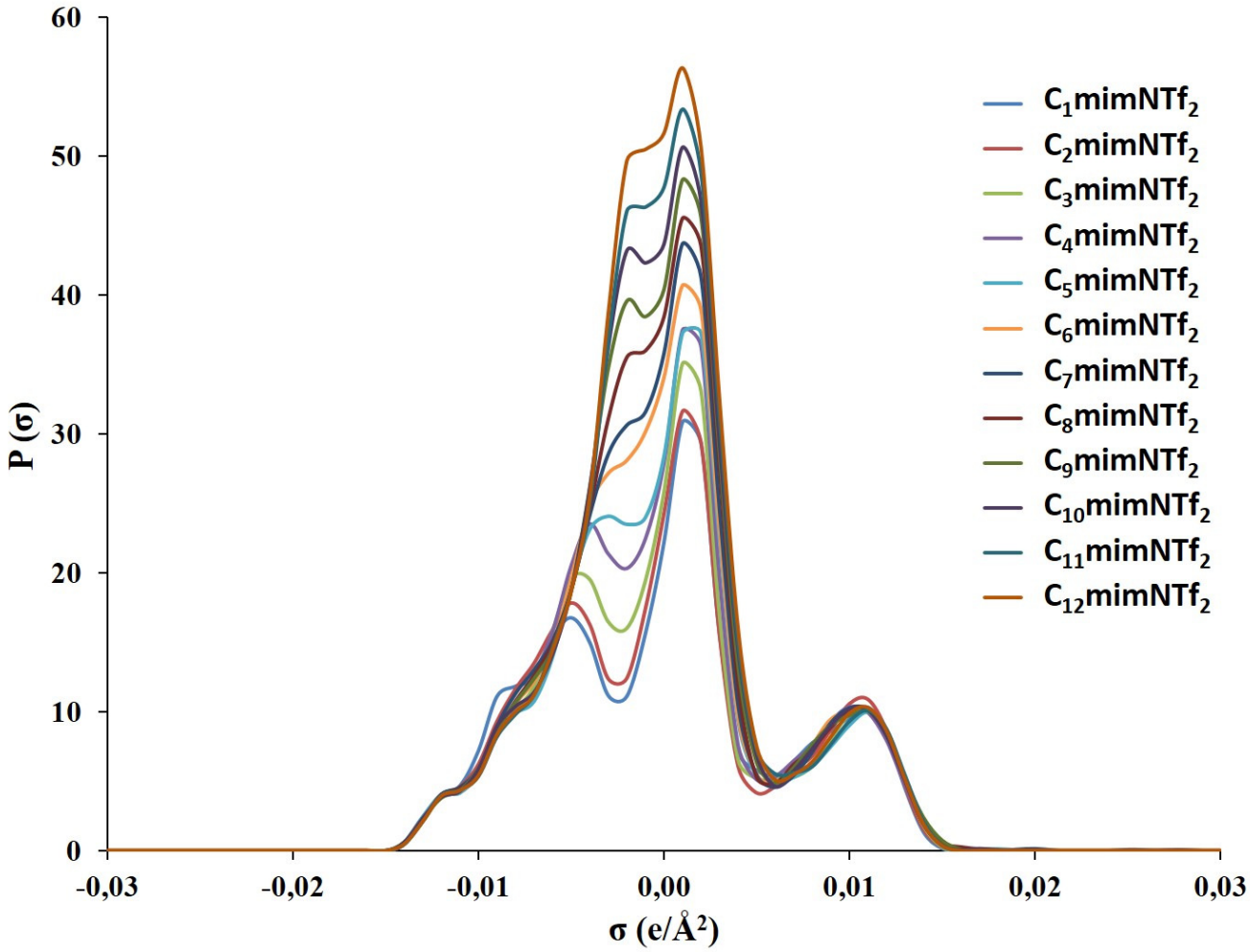

Figure S 4 σ-profiles of C_{1-12}mimNTf$_2$ represented as CA model with $\varepsilon = 78$

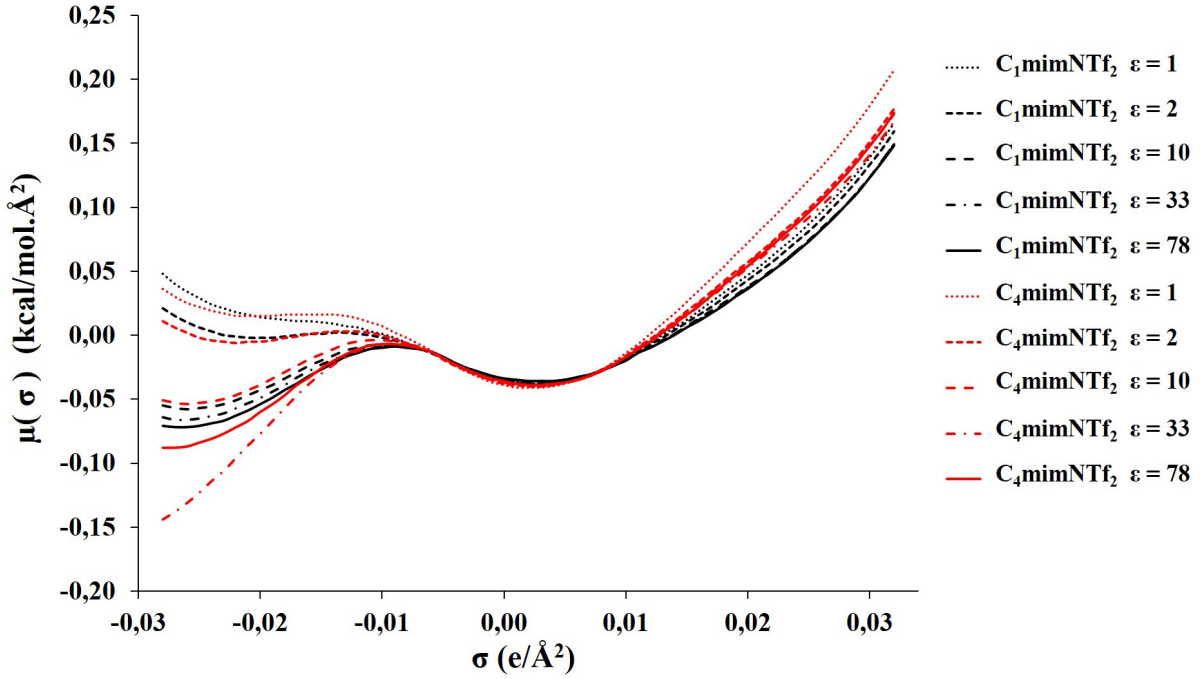

Figure S 5 σ-potentials of C_1mimNTf$_2$ (black lines) and C_4mimNTf$_2$ (red lines) represented as CA model with different values of ε

Table S 3 Vaporization enthalpy (kJ.mol^{-1}) of C_{1-12}mimNTf$_2$ for $\varepsilon = 1$ and $\varepsilon = 78$ with both models, including experimental data

	ΔH_{vap} CA model		ΔH_{vap} C+A model		
Ionic liquid	$\varepsilon = 1$	$\varepsilon = 78$	$\varepsilon = 1$	$\varepsilon = 78$	$\Delta H^{a)}_{vapExp}$
C_1mimNTf$_2$	108.4	123.8	168.8	173.2	-
C_2mimNTf$_2$	107.2	122.9	167.1	171.6	133.2
C_3mimNTf$_2$	111.3	125.9	167.4	172.0	133.8
C_4mimNTf$_2$	116.0	131.8	168.5	173.1	139.2
C_5mimNTf$_2$	118.4	131.8	169.9	174.3	145.4
C_6mimNTf$_2$	122.9	139.2	171.3	175.8	150.1
C_7mimNTf$_2$	125.5	144.2	172.9	177.4	153.7
C_8mimNTf$_2$	130.4	145.2	174.6	179.1	155.2
C_9mimNTf$_2$	134.3	150.2	176.3	180.8	-
C_{10}mimNTf$_2$	138.2	153.3	178.1	182.6	165.2
C_{11}mimNTf$_2$	140.9	154.4	179.8	180.2	-
C_{12}mimNTf$_2$	144.9	158.5	185.8	186.1	171.5

[a)] M. A. A. Rocha, C. F. R. A. C. Lima, L. R. Gomes, B. Schröder, J. A. P. Coutinho, I. M. Marrucho, J. M. S. S. Esperança, L. P. N. Rebelo, K. Shimizu, J. N. Canongia Lopes and L. M. N. B. F. Santos, *J. Phys. Chem B*, 2011, **115**, 10919–10926.

Table S 4 Density (g.mL^{-1}) of C_{1-12}mimNTf$_2$ for $\varepsilon = 1$ and $\varepsilon = 78$ with both models, including experimental data

	ρ CA model		ρ C+A model		
Ionic liquid	$\varepsilon = 1$	$\varepsilon = 78$	$\varepsilon = 1$	$\varepsilon = 78$	ρ_{Exp}
C_1mimNTf$_2$	1.539	1.520	1.565	1.572	1.570[a)]
C_2mimNTf$_2$	1.495	1.472	1.517	1.519	1.515[a)]
C_3mimNTf$_2$	1.460	1.437	1.473	1.476	1.476[b)]
C_4mimNTf$_2$	1.419	1.399	1.438	1.439	1.436[a)]
C_5mimNTf$_2$	1.391	1.370	1.406	1.407	1.404[b)]
C_6mimNTf$_2$	1.360	1.340	1.375	1.376	1.371[a)]
C_7mimNTf$_2$	1.336	1.315	1.351	1.351	-
C_8mimNTf$_2$	1.311	1.297	1.326	1.327	1.319[a)]
C_9mimNTf$_2$	1.288	1.277	1.300	1.304	-
C_{10}mimNTf$_2$	1.270	1.260	1.285	1.285	1.278[a)]
C_{11}mimNTf$_2$	1.250	1.236	1.268	1.267	-
C_{12}mimNTf$_2$	1.231	1.220	1.249	1.250	1.245[a)]

[a)] M. Tariq, P. A. S. Forte, M. F. Costa Gomes, J. N. Canongia Lopes and L. P. N. Rebelo, *J. Chem. Thermodyn.*, 2009, **41**, 790–798.

[b)] J. M. S. S. Esperança, Z. P. Visak, N. V. Plechkova, K. R. Seddon, H. J. R. Guedes and L. P. N. Rebelo, *J. Chem. Eng. Data*, 2006, **51**, 2009–2015.

Table S 5 Viscosity (cP) of C_{1-12}mimNTf$_2$ for $\varepsilon = 1$ and $\varepsilon = 78$ with both models, including experimental data

	η CA model		η C+A model		
Ionic liquid	$\varepsilon = 1$	$\varepsilon = 78$	$\varepsilon = 1$	$\varepsilon = 78$	$\eta^{a)}_{Exp}$
C_1mimNTf$_2$	28.81	66.22	33.96	42.29	33.00
C_2mimNTf$_2$	26.33	64.87	38.87	49.79	45.75
C_3mimNTf$_2$	29.76	75.86	47.73	61.26	50.62
C_4mimNTf$_2$	43.58	120.30	59.07	76.49	57.81
C_5mimNTf$_2$	50.77	117.19	72.70	93.82	70.61
C_6mimNTf$_2$	72.46	208.59	88.33	114.41	81.11
C_7mimNTf$_2$	82.61	313.29	105.48	136.98	93.05
C_8mimNTf$_2$	121.35	326.30	125.63	162.54	106.41
C_9mimNTf$_2$	157.80	464.09	147.39	192.12	120.18
C_{10}mimNTf$_2$	207.49	589.22	172.89	222.85	-
C_{11}mimNTf$_2$	236.29	588.21	199.42	203.99	154.33
C_{12}mimNTf$_2$	310.15	783.61	229.97	297.61	-

[a)] M. Tariq, P. J. Carvalho, J. A. P. Coutinho, I. M. Marrucho, J. N. Canongia Lopes and L. P. N. Rebelo, *Fluid Phase Equilibr.*, 2011, **301**, 22–32.