

## *Supporting Information*

# Ionic liquids with anions based on fluorosulfonyl derivatives: from asymmetrical substitutions to a consistent force field model

*Andreia S. L. Gouveia,<sup>ab‡</sup> Carlos E. S. Bernardes,<sup>a‡</sup> Liliana C. Tomé,<sup>ab</sup>  
Elena I. Lozinskaya,<sup>c</sup> Yakov S. Vygodskii,<sup>c</sup> Alexander S. Shaplov,<sup>cd</sup>  
José N. Canongia Lopes<sup>a\*</sup> and Isabel M. Marrucho<sup>ab\*</sup>*

<sup>a</sup> Centro de Química Estrutural, Departamento de Engenharia Química, Instituto Superior Técnico,  
Universidade de Lisboa, Avenida Rovisco Pais, 1049-001 Lisboa, Portugal.

<sup>b</sup> Instituto de Tecnologia Química e Biológica António Xavier, Universidade Nova de Lisboa, Av. da  
República, 2780-157 Oeiras, Portugal.

<sup>c</sup> A.N. Nesmeyanov Institute of Organoelement Compounds Russian academy of sciences (INEOS RAS),  
Vavilov St., 28, 119991 Moscow, Russia

<sup>d</sup> Luxembourg Institute of Science and Technology (LIST), 5 avenue des Hauts-Fourneaux, L-4362,  
Esch-sur-Alzette, Luxembourg

\* Corresponding Authors:

Centro de Química Estrutural, Instituto Superior Técnico, 1049-001 Lisboa, Portugal.

E-mail: [jnlopes@tecnico.ulisboa.pt](mailto:jnlopes@tecnico.ulisboa.pt), [isabel.marrucho@tecnico.ulisboa.pt](mailto:isabel.marrucho@tecnico.ulisboa.pt)

<sup>‡</sup>Andreia S.L. Gouveia and Carlos E.S. Bernardes have equally contributed to this work.

**Table S1.** Experimental volumetric mass density,  $\rho$  ( $\text{g cm}^{-3}$ ), as a function of temperature for pure ILs ( $p = 0.1$  MPa).

$T$ (K)	$\rho$ ( $\text{g cm}^{-3}$ )					
	[C <sub>2</sub> mim] [FSI]	[C <sub>2</sub> mim] [TFSAM]	[C <sub>2</sub> mim] [TSAC]	[C <sub>2</sub> mim] [BETI]	[C <sub>2</sub> mim] [C <sub>4</sub> F <sub>9</sub> SO <sub>3</sub> ]	[C <sub>2</sub> mim] [NTf <sub>2</sub> ]*
293.15	1.448	1.352	1.459	1.599	-	1.524
298.15	1.443	1.347	1.454	1.593	-	1.519
303.15	1.438	1.343	1.449	1.588	1.542	1.514
308.15	1.434	1.339	1.444	1.582	1.536	1.509
313.15	1.429	1.335	1.439	1.577	1.531	1.504
318.15	1.425	1.330	1.434	1.572	1.526	1.499
323.15	1.420	1.326	1.429	1.566	1.521	1.494
328.15	1.416	1.322	1.424	1.561	1.516	1.489
333.15	1.411	1.318	1.419	1.555	1.510	1.485
338.15	1.407	1.314	1.414	1.550	1.505	1.480
343.15	1.402	1.310	1.409	1.544	1.500	1.475
348.15	1.398	-	1.404	1.539	1.495	-
353.15	1.394	-	1.399	1.534	1.490	-

\* Values taken from Tomé *et al.*<sup>1</sup>

**Table S2.** Experimental dynamic viscosity,  $\eta$  (mPa s), as a function of temperature for pure ILs ( $p = 0.1$  MPa).

$T$ (K)	$\eta$ (mPa s)					
	[C <sub>2</sub> mim] [FSI]	[C <sub>2</sub> mim] [TFSAM]	[C <sub>2</sub> mim] [TSAC]	[C <sub>2</sub> mim] [BETI]	[C <sub>2</sub> mim] [C <sub>4</sub> F <sub>9</sub> SO <sub>3</sub> ]	[C <sub>2</sub> mim] [NTf <sub>2</sub> ]*
293.15	22.4	23.7	30.4	85.5	-	39.1
298.15	19.3	20.2	25.3	68.3	-	32.4
303.15	16.8	17.4	21.3	55.2	109.7	27.2
308.15	14.8	15.1	18.1	45.3	86.1	23.1
313.15	13.1	13.1	15.6	37.6	68.7	19.9
318.15	11.6	11.6	13.6	31.6	55.7	17.3
323.15	10.4	10.3	11.9	26.9	45.7	15.2
328.15	9.4	9.2	10.5	23.0	38.0	13.4
333.15	8.5	8.2	9.4	20.0	32.0	11.9
338.15	7.8	7.5	8.4	17.4	27.2	10.7
343.15	7.1	6.8	7.6	15.3	23.3	9.7
348.15	6.5	-	6.9	13.5	20.2	-
353.15	6.0	-	6.3	12.1	17.6	-

\* Values taken from Tomé *et al.*<sup>1</sup>

## REFERENCES

1. L. C. Tomé, D. J. S. Patinha, C. S. R. Freire, L. P. N. Rebelo and I. M. Marrucho, *RSC Adv*, 2013, **3**, 12220-12229.