COSMO-RS and experimental thermophysical properties of alkylammonium ionic liquids

Murilo L. Alcantara[1,2]; Gabriel L Bressan[1]; Paulo V. A. Santos [1]; Maria F. V. Nobre[1]; João A. P. Coutinho[2], Cláudio O. A. Nascimento[1], Luis A. F. Romero[1]*.

[1]*Chemical Engineering Department, Polytechnic School, University of São Paulo. São Paulo-Brazil.*

[2]*CICECO - Aveiro Institute of Materials, Chemistry Department, University of Aveiro, Aveiro, Portugal*

**follegatti@usp.br*

Supplementary material

S1 - Extra Figures and Tables

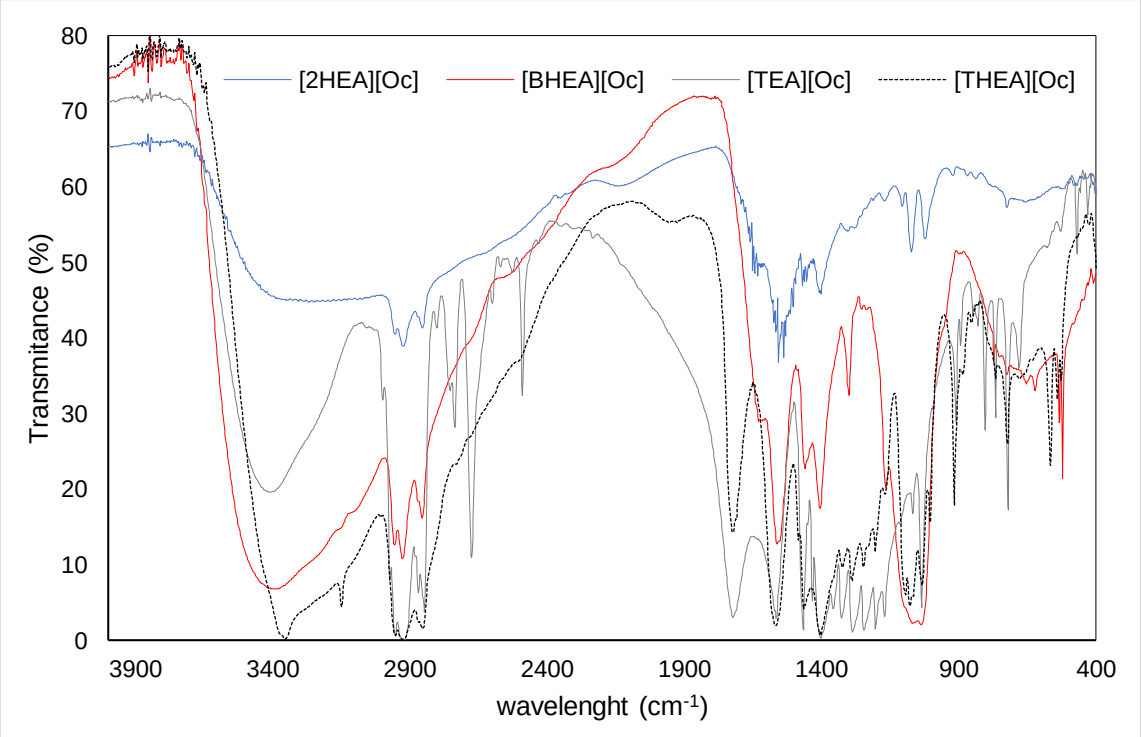

Figure S1. FT-IR spectra of the studied ILs. [2HEA][Oc] = [HEA][Oc] in the manuscript.

Figure S2 depicts the σ-profiles of the ILs' ions under study. These profiles provide a 2D representation of the charge distribution visualized in Figure 1, enabling quantitative analysis of the induced charge density concentration around each ion and their likely interactions.

The σ-profiles reveal a significant concentration of octanoate anions [Oc]-, characterized by one strong peak of neutral charges (-0.01 e/Å² to 0.01 e/Å²) and a secondary peak of concentrated induced positive charges (0.015 e/Å² to 0.03 e/Å²), a result of the negative site of the octanoate carboxyl group. All cations exhibited negative peaks (<-0.015 e/Å²), indicative of the positive charge sites. The order of negative induced charge concentration is $[HEA]^+$>$[BHEA]^+$>$[THEA]^+$>$[TEA]^+$, suggesting their relative polarities. Notably, the $[TEA]^+$ and $[THEA]^+$ cations showed minimal peaks of highly concentrated charges below -0.02 e/Å², indicating a more non-localized charge distribution. Additional analysis of sigma potentials can be found within Supplementary Material S1.

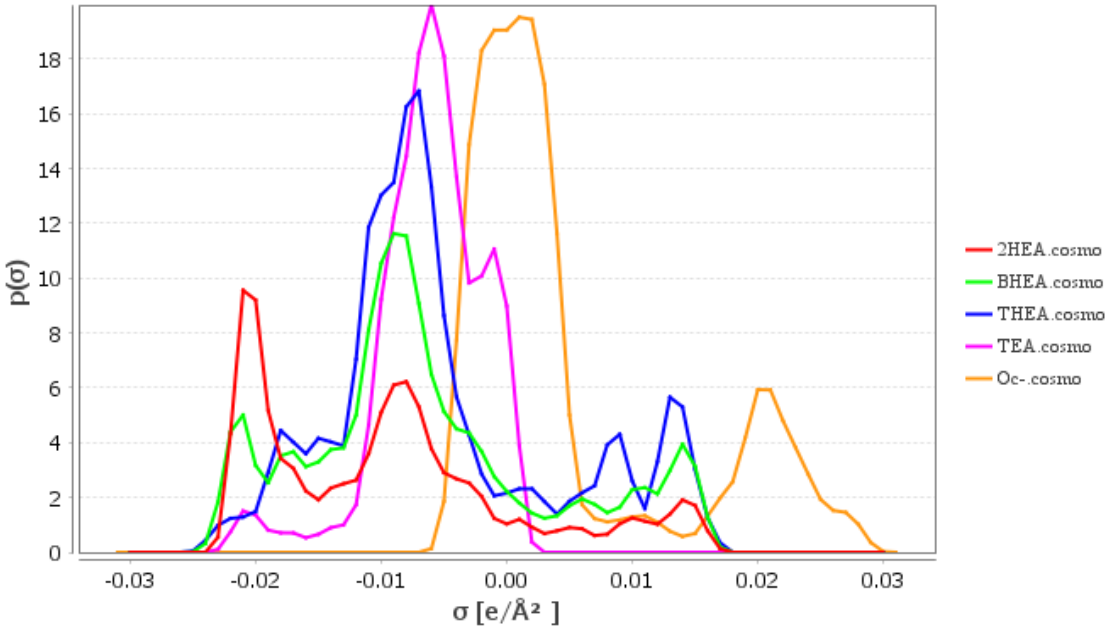

Figure S2. Sigma profile of all ions under study Octanoate [Oc], Tri-(2-Hydroxyethyl) Ammonium $[THEA]^+$, bis(2-Hydroxyethyl)Ammonium $[BHEA]^+$, N-Hydroxyethyl Ammonium $[HEA]^+$, triethylammonium $[TEA]^+$. [2HEA][Oc] = [HEA][Oc] in the manuscript.

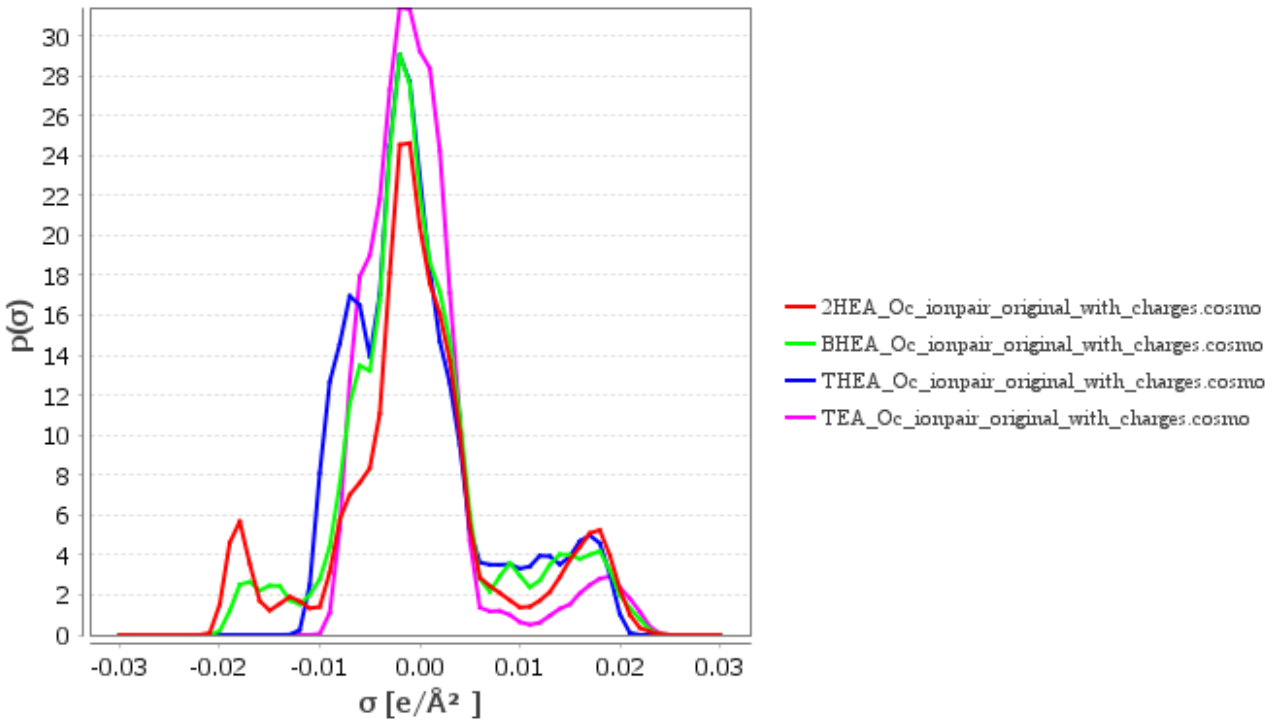

Figure S3. Sigma profile of ion-pairs under study: 2-Hydroxyethylammonium Octanoate [HEA][Oc], bis(2-Hydroxyethyl)ammonium Octanoate [BHEA][Oc], Tri-(2-Hydroxyethyl)ammonium Octanoate [THEA][Oc], Triethylammonium Octanoate [TEA][Oc]. [2HEA][Oc] = [HEA][Oc] in the manuscript.

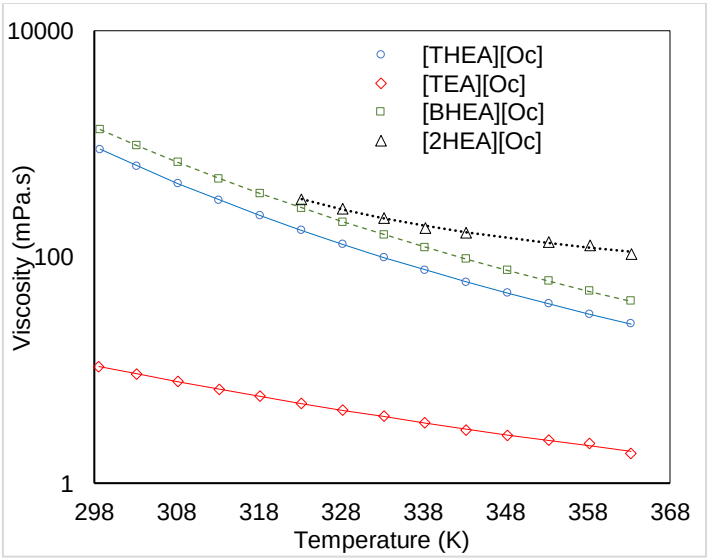

Figure S4. Experimental (dots) and fitted viscosities by Vogel-Tammann-Fulcher of the studied ILs: 2-Hydroxyethylammonium Octanoate [HEA][Oc], bis(2-Hydroxyethyl)ammonium Octanoate [BHEA][Oc], Tri-(2-Hydroxyethyl)ammonium Octanoate [THEA][Oc], Triethylammonium Octanoate [TEA][Oc]. [2HEA][Oc] = [HEA][Oc] in the manuscript.

Table S1. Parameters of Vogel-Tammann-Fulcher for viscosity of: 2-Hydroxyethylammonium Octanoate [HEA][Oc], bis(2-Hydroxyethyl)ammonium Octanoate [BHEA][Oc], Tri-(2-Hydroxyethyl)ammonium Octanoate [THEA][Oc], Triethylammonium Octanoate [TEA][Oc].

Parameters	**[HEA][Oc]**	**[BHEA][Oc]**	**[THEA][OC]**	**[TEA][OC]**
a	2.60E+01	3.36E-03	4.83E-03	2.06E-03
b	1.37E+02	2.24E+03	1.88E+03	2.19E+03
t0	2.69E+02	1.25E+02	1.43E+02	4.23E+01
r^2	0.99601	0.99999	0.99999	0.99969