

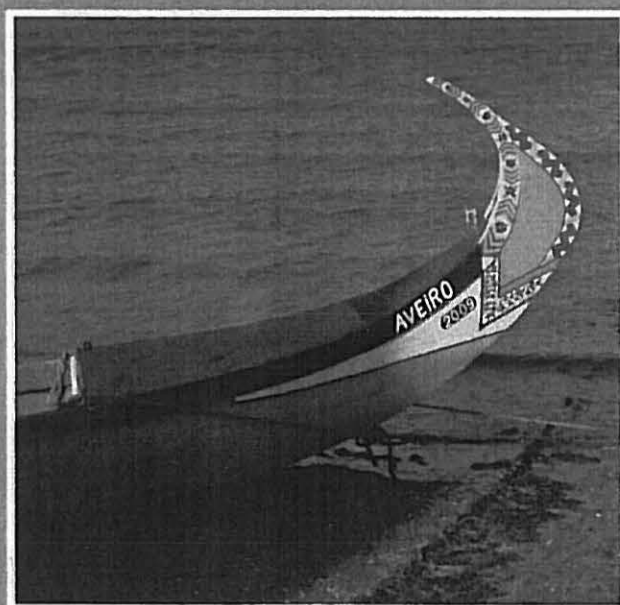
 **SOCIEDADE PORTUGUESA DE QUÍMICA**

## Book of abstracts

**9<sup>o</sup> Encontro Nacional de Química Física  
1<sup>st</sup> Iberian Meeting on Ionic Liquids**



**June 15-16<sup>th</sup>, 2009  
University of Aveiro**



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## Phase Equilibria of Phenolic Compounds in Aqueous, Organic and Supercritical Solvents

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Phenolic compounds are relevant chemicals in industrial and biological processes. Their production, either by synthesis or extraction from biological media, requires the knowledge of phase equilibrium data that is lacking considerably in the open literature. For this reason, we have been performing at our laboratory a series of experimental measurements of solubility in water<sup>[1,2]</sup> and organic solvents, focused on two important families of phenolics: hydroxybenzoic and phenylpropenoic acids.

The analytical shake flask method was employed for generating the saturated solutions, followed by quantitative analysis by Uv-vis spectrophotometry and/or gravimetry<sup>[1,2]</sup>. Alternatively, a synthetic method using DSC is being implemented, as this is faster and requires smaller amounts of solid.

For a better understanding of the solubilization process, the corresponding melting properties were determined by DSC, with the exception of those phenolics that decompose upon melting, such as *o*-coumaric, gallic and caffeic acids. For these, the Marrero and Gani group-contribution procedure<sup>[3]</sup> was used to generate estimates of the melting properties<sup>[1]</sup>.

Since the studied molecules are organic acids, dissociation constants were also determined by potentiometric titration.

As these compounds represent a class of associating molecules containing different associating groups such as hydroxyl and carboxyl (in many cases with multiple substitutions), a new methodology for modeling these multifunctional compounds with the cubic-plus-association (CPA) equation of state was developed. In this, the three cubic term parameters ( $a_c$ ,  $c_1$  and  $b$ ) are obtained from correlations involving the critical temperature and pressure, and van der Waals volumes, while the association term parameters depend on the nature and position of each associating group<sup>[1,2]</sup>.

Results showed that this methodology for the pure component parameters can lead to a good description of the aqueous solubility of phenolics using a single, small and temperature independent binary interaction parameter in the physical contribution of CPA.

Further results for organic and supercritical solvents using the same methodology will be presented during the meeting.

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