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BOOK OF ABSTRACTS

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Solubility of Phenolic Compounds in Water, Organic and Supercritical Solvents

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Phenolic compounds represent a class of important chemicals with both biological and industrial importance. Their production, either by chemical synthesis or extraction from different biological media requires the adequate knowledge of phase equilibria. Particularly, the solubility in aqueous systems, organic and supercritical solvents are fundamental for a better design of separation and purification processes.

Although their importance, there is still a considerable lack of data on phase equilibria of phenolic compounds. Due to this reason, we have implemented a series of experimental measurements of solubility in water [1,2] and organic solvents. Our experimental studies have been focused on two of the most important families of phenolics: hydroxybenzoic (gallic, salicylic, protocatechuic, and syringic acids) and phenylpropenoic acids (trans-cinnamic, ferulic, caffeic and o-coumaric).

Measurements have been performed using the analytical shake flask method with quantitative analysis by Uv-vis spectrophotometry and/or gravimetry [1,2]. Alternatively, the synthetic method for determining the solubility of phenolics in organic solvents by DSC is being implemented as this is a faster method, requiring considerably smaller sample amounts, when compared with the classical analytical shake flask method.

For a better understanding of the solubilization process of these solid compounds, melting temperatures and enthalpies of fusion were also determined by DSC, with the exception of o-coumaric, gallic and caffeic acids, that decompose upon melting. For these, the Marrero and Gani group contribution procedure [3] was used to generate estimates of the melting properties. This group contribution method was previously evaluated for the estimation of the melting temperatures and enthalpies of fusion of the other phenolics [1].

As the studied molecules are organic acids, in order to understand the extent of acid dissociation in water, dissociation constants were determined by potentiometric titration, as well as the pH of the corresponding saturated aqueous solutions.

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_0 , 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 [1,2].

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.

References.

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