Extension of COSMO-RS-ES for the calculation of phase equilibria in highly concentrated electrolytes

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Electrolytes are present in a wide range of industrial processes and their description has gained even more attention in recent years, not only because of their challenging nature, but also because of the introduction of ionic liquids and salt-based deep eutectic solvents, which contain large polyatomic ions. These components and mixtures can be promising sustainable alternatives to traditional solvents in various specific processes.

Describing the thermodynamic behavior of systems containing these substances is of paramount importance for process and product design. However, when experimental data is scarce or difficult to produce, predictive models like COSMO-RS become a valuable tool. COSMO-RS is a model that relies on quantum chemistry and statistical thermodynamics to describe the intermolecular interactions that take place in a liquid phase. The model can accurately describe the trends observed in experimentally determined phase equilibria of neutral species and has proven capable of describing some liquid phases with highly concentrated ionic liquids and deep eutectic solvents.

![Figure 1: Calculation of the mean ionic activity coefficient of choline chloride in water](image)

The electrolyte model COSMO-RS-ES is a modified COSMO-RS combined with Debye-Hückel theory that accurately predicts aqueous mean ionic activity coefficients, salting out effects and solubilities of alkali and alkali-earth inorganic salts in mixed and pure organic solvents. The aim of this work is to extend COSMO-RS-ES in order to include a general treatment for more complex polyatomic ions and describe their behavior in a wide concentration range.