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Molecular Modeling and Prediction of the Physicochemical Properties of Carbohydrates and Polyols

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ROQUETTE is a producer of plant-based ingredients. Modeling, simulation, and predictive thermodynamic models are the tools to characterize the physicochemical properties of the matter flows in order to optimize and control their industrial processes. This relates to aqueous mixtures of carbohydrates and polyols with a high dry matter content. The polyols mannitol and sorbitol are diastereoisomers that have a nearly identical chemical structure, but very different physicochemical properties – for example, the solubility of sorbitol in water is 2.5 kg/kg of water, while mannitol has a solubility of 250 g/kg of water at 25°C. Therefore, predicting liquid-solid equilibrium properties in this case requires sophisticated solution models that cannot be based solely on chemical groups. In this context, previous works carried out by Institut Pascal's GePEB axis have shown that robust consideration of the solvation phenomena of polyols is essential for accurately predicting water activity in such systems. Focusing its efforts on modeling the residual terms of activity coefficients using COSMO-type models, the team has developed the COSMO-UCA model, which has the structural advantage of using quantum mechanics tools to predict formation and phase equilibrium properties. In this work, we present a methodology to predict physicochemical properties of complex solutions, taking as sole input the three-dimensional structure of the molecules in the medium. Computational chemistry tools are used to generate the input data for the model. Finally, we model certain physicochemical properties (activities and solubilities) of aqueous solutions of mannitol and sorbitol.

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[2] Vincent Dumouilla (2022): **Modélisation thermodynamique et spectroscopique des solutions aqueuses d'hydrates de carbone et de polyols**, *Institut Pascal, Axe Génie des Procédés, Energétique et Biosystèmes (GePEB).*

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