

Prediction of Thermophysical Properties of Deep Eutectic Solvents Using the SAFT- γ Mie Group-Contribution Equation of State

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Deep eutectic solvents are increasingly recognized as appropriate materials for use as active pharmaceutical ingredients or formulation additives. Among different deep eutectic solvents choline and geranate (CAGE) have been demonstrated to offer promising properties such as powerful antibacterial activity against several drug-resistant bacteria, fungi, and viruses [1] and enhancement of the transdermal delivery of proteins and antibacterial drugs [1,2]. However, little is known on the thermophysical properties of CAGE. Molecular theory enables us to predict thermodynamic properties of solutions. We have developed an accurate coarse-grained intermolecular potential of CAGE by using the SAFT- γ Mie group contribution approach. This method is based on the formulation of the statistical associating fluid theory for Mie potentials [3]. Indeed, it allows an estimation of the parameters of the Mie force-field, which can be directly used for coarse-grained simulations of aggregation and transport phenomena. Modelling CAGE using SAFT- γ Mie requires the determination of group interaction parameters. The functional groups are developed in a successive manner, namely the determination of new group interaction parameters is based on those of previous groups. The group interaction parameters to model CAGE are estimated using experimental data for phase equilibria of pure components (i.e. n-alkanes, n-alkenes, branched alkenes) and mixtures (i.e. branched alkenes and carboxylic acids/water), such as vapor pressure, saturated liquid density, vapor-liquid equilibrium, or solubility. The models developed for CAGE extend the set of functional groups developed using SAFT- γ Mie presented previously [4]. It further provides an accurate intermolecular potential of CAGE which allows the prediction of a broad range of thermophysical properties at different thermodynamics state of mixtures containing CAGE.

References:

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