Thermodynamic Modeling of Ionic Liquid Density with Heterosegmented Statistical Associating Fluid Theory

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Heterosegmented statistical associating fluid theory is used to represent the density of an ionic liquid. An ionic liquid molecule is divided into several groups representing the alkyls, cation head, and anion. The cation of the ionic liquid is modeled as a chain molecule that consists of one spherical segment representing the cation head, and groups of segments of different types representing different substituents (alkyls). The anion of the ionic liquid is modeled as a spherical segment of different type. To account for the electrostatic/polar interaction between the cation and anion, the spherical segments representing the cation head and anion each have one association site, which can only cross associate to each other. The parameters for alkyls are obtained from those of the corresponding n-alkanes and the parameters of groups representing the cation head and anion, including the two association parameters, are fitted to a group of experimental ionic liquid data. The performance of the model is examined by describing the densities of three important series of imidazolium-based ionic liquids, i.e., $[C_n\text{mim}][Tf_2N]$, $[C_n\text{mim}][BF_4]$, and $[C_n\text{mim}][PF_6]$. The model is found to well represent the densities of these ionic liquids from 293.15 to 415 K and up to 650 bar, and capture well the effects of temperature, pressure, and alkyl types on density.