

Application of Virial-Based Mixing Rules for Correlation to Excess Molar Volumes of (trioctylmethylammonium bis(trifluoromethylsulfonyl)imide + Acetates) at Different Temperatures

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As part of a systematic study of ionic liquid systems, binary excess molar volumes for the ionic liquid trioctylmethylammonium bis(trifluoromethylsulfonyl)imide and methyl acetate (or ethyl acetate) were determined experimentally from density data (at 25, 30 and 40 °C) obtained with a densitometer. The results were correlated with Virial-Based Mixing Rules. The correlation model draws upon the exact mathematics of mixing rules established for virial coefficients of gases. Perturbations from ideal mixing are modeled akin to successive terms in the virial expansion, resulting in the name “Virial-Based Mixing Rules” (VBMR). Each perturbation reduces to zero for pure components, and adopts the composition order of the corresponding virial coefficient it represents. For example, the first perturbation represents the second virial coefficient and implements a quadratic mixing rule, while allowing one adjustable binary interaction parameter. The next term employs cubic mixing and allows multiple interaction parameters, including a ternary interaction parameter which may be fine-tuned for ternary and higher mixtures. The VBMR correlated the densities of the binary liquid mixtures for the low boiling ionic liquid and the acetates within experimental uncertainty. The interaction parameters obtained from the correlation are presented as a function of temperature.