

***Invited Contribution from AIChE Area 1a***

**Is the Difference in Hydrogen Bond Ability of Anions an Exclusive Descriptor of Nonideality in Binary Ionic Liquid Mixtures?**

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Ionic liquids (ILs) are molten salts composed entirely of ions that exist as liquids under ambient conditions. The traditional approach for tuning the property behavior of ionic liquid has taken advantage of a proper ion selection. Recently, the use of ionic liquid mixtures has been proposed as a strategy to obtain task-specific properties of ionic liquid solvent systems. As a result of which, a thorough understanding of the structure-property relationships is only now beginning to be probed for binary ionic liquid mixtures. One of the outstanding questions in the binary ionic liquid mixture research is whether there are molecular descriptors that can be used to predict the non-ideal behavior of such mixture systems. In an effort to answer this question, atomistic molecular dynamics (MD) simulations were carried for a total of 15 ionic liquid-ionic liquid mixtures sharing the common cation 1-n-butyl-3-methylimidazolium [C<sub>4</sub>mim]<sup>+</sup> and the anions with a range of hydrogen bonding ability. The non-ideality in these mixtures was assessed in terms of the local organization of the anions around the cation and the extent to which such organizations differ from those for the ionic liquids being mixed. Our calculations revealed that the generation of non-native structures requires a significant difference in the anion hydrogen bonding basicity as well as a substantial difference in the ionic liquid molar volumes. The effect of non-native structures on the solubility of gases such as CO<sub>2</sub> will be discussed.