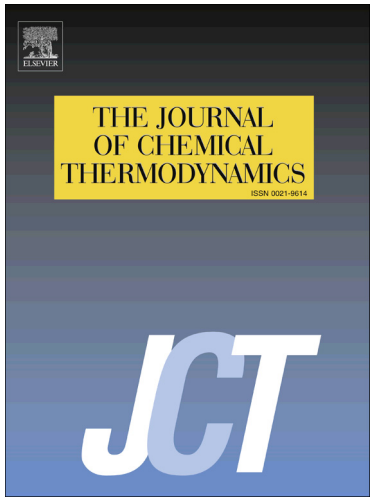

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Experimental and Theoretically study of interaction between organic compounds and tricyanomethanide based Ionic Liquids

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Abstract

Activity coefficients at infinite dilution ($\gamma_{1,2}^{\infty}$) for 35 solutes in two new tricyanomethanide containing Ionic Liquids were measured by inverse gas chromatography at temperatures from 318.15 to 368.15 K. Most organic compounds have stronger affinity with 1-butyl-4-methylpyridinium tricyanomethanide than 1-butyl-3-methylimidazolium tricyanomethanide. The retention data were further converted to gas-to-IL and analyzed using the Abraham solvation parameter model. The LSER treatment indicates that the most dominant interaction constants for this family of ILs are strong dipolarity, hydrogen bond basicity and acidity. Quantum chemical gas phase DFT calculations were performed on isolated ion pairs at the the 6-311 ++ G(d,p) level basis. It was found that the stacking structure of cation and anion is compact in the [BMIM][TCM] system and relatively loose in the [BMPY][TCM] system allowing a facile restructuring of the ionic liquid [BMPY][TCM] in the process of organic compounds dissolution.