



Developing a new correlation for the aliphatic and aromatic hydrocarbon diffusion coefficients at infinite dilution in ionic liquids

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ABSTRACT

In this work the Taylor dispersion technique has been used to measure the diffusion coefficients of *n*-heptane and toluene at infinite dilution in four ionic liquids, namely 1-ethyl-3-methylimidazolium thiocyanate ([emim][SCN]), 1-ethyl-3-methylimidazolium tricyanomethanide ([emim][TCM]), 1-butyl-3-methylimidazolium tricyanomethanide ([bmim][TCM]), and 1-butyl-4-methylpyridinium tricyanomethanide ([4bmpy][TCM]), at the range temperatures from (298.2–333.2) K. The hydrocarbon diffusion is faster at higher temperatures because of the lower ionic liquid viscosity, and toluene diffuses faster than *n*-heptane due to its smaller molecular volume. In addition, it is seen that the values of the *n*-heptane diffusion coefficients decrease with an increase in the molecular weight and molar volume of the ionic liquid. The same is observed for the diffusion coefficients of toluene in the most viscous ionic liquids ([bmim][TCM], [4bmpy][TCM] and [4empy][Tf₂N]), but, conversely, they increase for the least viscous ionic liquids ([emim][SCN], [emim][DCA], and [emim][TCM]). This behavior suggests that the strength of the toluene-ionic liquid chemical interactions have a significant effect on diffusion. A new empirical correlation has been proposed as a variation of the Wilke–Chang equation. Two additional variables have been introduced in this correlation; the molar fraction of the maximum hydrocarbon solubility, to take into account the toluene-ionic liquid interactions, as well as the molar volume of the ionic liquid, because of the huge difference between them and the solute. This new correlation satisfactorily fits the experimental data with an average deviation of 9.6%.

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