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Elena Lukoshko, Fabrice Mutelet, Urszula Domanska

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

Elena LUKOSHKO^a, Fabrice MUTELET^b, Urszula DOMANSKA^{a,c}

a- Warsaw University of Technology, Faculty of Chemistry, Department of Physical Chemistry, Noakowskiego 3, 00-664 Warsaw, Poland.

b- Université de Lorraine, Ecole Nationale Supérieure des Industries Chimiques, Laboratoire Réactions et Génie des Procédés (UMR CNRS 7274), 1 rue Grandville, 54000 NANCY, France.

c- University of KwaZulu-Natal, Howard College Campus, School of Chemical Engineering, Thermodynamic Research Unit, King George V Avenue, Durban 4001, South Africa.

(* author to whom the correspondence should be addressed: e-mail: fabrice.mutelet@univ-lorraine.fr - Telephone number: +33 3 83 17 51 31 - Fax number: +33 3 83 17 53 95

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.

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