Heat of Solution and Solvation of Water and Alcohols in ILs

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In this work the heat of solution at infinite dilution of water, 1-propanol, 1-butanol and 1-pentanol in ionic liquids was measured by Isothermal Titration Calorimetry (ITC). The alkyl chain length effect was explored in the 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquid series and the cation effect was evaluated by comparison of the solvation in the butyl cation derivatives, butilimidazolium butilpirrolidinium, butilpyridinium and butilpiperidinium Water and the alcohol series were used as molecular probes to elucidate the differentiation and magnitude of interaction of the –OH groups with the ILs. The trend of the heats of solvation along the alkyl chain length, as well as, the change of the molecular character will be presented and analysed to give insights into the structuration and nanostructuration of the ILs. Analyses of the results obtained by varying both the alcohol's and the IL's length allowed us to assess the trend shift in ΔHsol and in ΔHsolv values, and thus on solution interactions along this ILs series, reflecting the discrimination between the polar and non-polar regions of the ILs. It was thus possible to highlight and experimentally support the existence of a Critical Molecular Size (CMS) limit for the nanostructuration, starting at [C6C1im][NTf2], reflecting a change in the molecular structure of the liquid . A very small differentiation of the solvation was found by changing the cation, supporting the model that the solvation of the alcohols involves the interaction of the –OH group with the anion.

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