

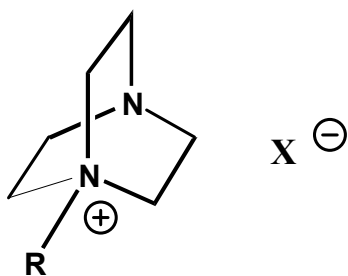


DABCO-BASED IONIC LIQUIDS: PROPERTIES AND APPLICATIONS

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New basic ionic liquids, composed of monosubstituted dabco (diazabicyclo[2.2.2]octane) cations and polyatomic anions, were synthesized and characterized. The key properties of these salts - phase transitions, thermal stability, density, viscosity and conductivity- were measured and compared to those of other common ILs. Moreover, ESI-MS measurements were performed at different concentrations to evaluate the degree of ion association in the liquid state, whereas solvatochromic dyes were used to assess the solvation properties. The structural effect on all above properties was intensively investigated in terms of the identity of the anion and of the variation of the side chain in the cation (i.e. alkyl chain length and introduction on the alkyl chain of specific functional groups).



These ionic liquids have been used as solvents in metal catalyzed reactions that generally are performed in the presence of a base (Heck reaction, Cu(I) catalyzed azide-alkyne coupling). Comparative studies were finalized to identify the most efficient ILs and at the same time to address some crucial issues such as the solubility of reagents, the extraction of the products, the recovery and reuse IL and catalyst. In the case of Cu(I) catalyzed Huisgen cycloaddition reaction, depending on the reaction conditions dabco-based ILs gave a different product distribution and different yields. The ability of these ionic liquids to affect the kinetic and/or regiochemical behavior of this reaction has been attributed to the different aptitude of the ionic liquid components to interact with the catalyst; effects ranging from catalyst stabilization to sequestration have been assumed depending on cation/anion structure. *Ab initio* calculations have been performed to support this hypothesis. Finally, the possibility to perform some of these reactions under MW dielectric heating was evaluated.