

Solvent effects in ionic liquids: Empirical linear energy-density relationships

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Multiparameter linear energy-density relationships to model solvent effects in room temperature ionic liquids (RTILs) are introduced and tested. The model incorporates two solvent dependent and two specific solute-solvent parameters represented by a set of electronic indexes derived from the conceptual density functional theory. The specific solute-solvent interactions are described in terms of the electronic chemical potential for proton migration between the anion or cation and the transition state structure of a specific reaction. These indexes provide a quantitative estimation of the hydrogen bond (HB) acceptor basicity and the hydrogen bond donor acidity of the ionic solvent, respectively. A sound quantitative scale of HB strength is thereby obtained. The solvent dependent contributions are described by the global electrophilicity of the cation and nucleophilicity of the anion forming the ionic liquid. The model is illustrated for the kinetics of cycloaddition of cyclopentadiene t