

Regional Electrophilic and Nucleophilic Fukui Functions Efficiently

Highlight the Lewis Acidic/Basic Regions in Ionic Liquids.

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Abstract.

The origin of catalysis and selectivity induced by room temperature ionic liquids (RTIL) in several organic reactions, have putatively been associated with the concept of *cation effect* (Hydrogen bond donor ability of the RTIL) or *anion effect* (Hydrogen bond accepting ability of the RTIL). In this work we show that there may be cases where this *a priori* classification may not be correctly assigned. Cations may concentrate both Lewis acidity/basicity functions in one fragment of the RTIL, an effect we tentatively call bi-functional distribution of the molecular Lewis acidity/basicity. The molecular distribution of the Lewis acidity/basicity may simply be assessed by evaluating the corresponding regional electrophilic/nucleophilic Fukui functions within a reference ion pair structure. The model is tested for a set of 81 RTIL currently used to run a variety of organic reactions. The usefulness of the model for the design of task specific RTIL is discussed.

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