

J. Phys. Chem. B, 2015, 119 (41), pp 13160–13166
DOI: 10.1021/acs.jpcc.5b05305

Lewis Acidity/Basicity Changes in Imidazolium Based Ionic Liquids Brought About by Impurities

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Abstract

We herein report on the effect that water molecules, present as impurities, in the vicinity of an ionic liquid model structure, may induce on the Lewis acidity/basicity patterns normally observed in these materials. Depending on the position and orientation of water, the Lewis acidity/basicity pattern changes from “normal distribution” (i.e., the basicity located at the anion moiety and the acidity located at the cation fragment) to “bifunctional distribution” (i.e., the acidity and basicity located at the cation moiety). In some specific cases, there appears a third Lewis acidity/basicity distribution, where water may bind both the cation and the anion of the ion pair; a response we tentatively call “amphoteric”. These effects are clearly traced to the hydrogen bond formation ability of water to coordinate different regions of pure ionic liquids taken as references.