

Linear Free Energy Relationships to Describe Solute Partitioning in Room Temperature Ionic Liquids

R.D. Rogers,^{1,2} J.G. Huddleston,² A.E. Visser,¹ and R.P. Swatloski¹

¹Department of Chemistry and ²Center for Green Manufacturing

The University of Alabama

Tuscaloosa, AL 35487 U.S.A.

Room temperature ionic liquids are emerging as novel replacements for volatile organic compounds traditionally used as industrial solvents, however, the lack of fundamental data which describes and predicts the basic science and engineering needs for practical application may be artificially holding back utilization of these green solvents. Detailed assessment of the solvent properties can be obtained by studying the partition of an extensive solute set whose properties have already been parameterized by partition in a series of solvents of known properties. The partitioning behavior is governed by a linear solvent free energy relationship (LFER). By generating a corresponding LFER to describe the partition, we expect to be able to arrive at a detailed, objective, and comparative description of the important forces governing solubility in ionic liquids and to show how these vary when the synthesized molecular structure is changed.