

Properties of *N*-Functionalized Imidazoles and Comparisons to Imidazolium-based Ionic Liquids

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N-functionalized imidazoles are a class of heterocyclic organic molecules, and are well-known as components of pharmaceuticals and also serve as building blocks for imidazolium-based ionic liquids (ILs). While IL-based solvents have been the focus of many research efforts in areas such as CO₂ capture, imidazoles have not been considered for these same applications. Imidazoles possess many of the same desirable characteristics as ILs such as tunable chemical structures, low vapor pressure and good chemical/thermal stability. Despite these promising features, it has only been very recently that reports on the the relationships between imidazole structure and physical properties were reported, and the study of imidazoles as tailored solvents is still dwarfed by the body of knowledge available for ILs. Our research in this area has focused on developing structure-property relationships *N*-functionalized imidazoles, with emphasis on density, viscosity, heat capacity. solubility of CO₂, CH₄ and other gases, as well as the underlying thermodynamics. Furthermore, we have utilized COSMOtherm as a means to computationally predict properties as well as parametrically study the influences of various functional groups (e.g. alkyl, ethers, nitriles, etc.) on physical properties. While imidazoles have some similar properties to ILs, other properties such as viscosity can be an order of magnitude (or more) different. Furthermore, some unique chemistries are available due to the basicity/nucleophilicity of imidazoles that are unavailable in ILs. This presentation will detail our synthetic methods, property characterizations, COSMO modeling and provide comparisons to these properties in ILs.