Abstract Listing

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419056: Solution thermodynamics of imidazolium-based ionic liquids and water

IEC 0 [419056]: Solution thermodynamics of imidazolium-based ionic liquids and water

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ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Properties of Ionic Liquids*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2000-11-24*

Abstract

This work presents the vapor-liquid equilibrium and the liquid-liquid equilibrium phase behavior and associated thermodynamic properties of water with three ionic liquids: 1-*n*-butyl-3-methylimidazolium hexafluorophosphate ([bmim][PF_6]), 1-*n*-octyl-3-methylimidazolium hexafluorophosphate ([C8mim][PF_6]), and 1-*n*-octyl-3-methylimidazolium tetrafluoroborate ([C8mim][BF_4]). Due to the negligible volatility of ionic liquids, we were able to measure vapor-liquid equilibrium using a gravimetric analyzer, which was designed to measure adsorption on solids. These results provide insight on how the natures of the cation and the anion affect the thermodynamic properties, such as Henry's constants and enthalpies and entropies of absorption. In addition, we show that ionic liquids can be removed from aqueous solutions with granular activated carbon.

419153: Gas solubility in ionic liquids

IEC 0 [419153]: Gas solubility in ionic liquids

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ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and*

Supercritical Fluids: Properties of Ionic Liquids
Invited: *Y*
Preferred Presentation Format: *Poster*
Consider for Sci-Mix: *N*
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Abstract

Previously we have shown that CO2 is a viable solvent to extract solutes from ionic liquids. Significant amounts of CO2 dissolve in the ionic liquids but no measurable ionic liquid dissolves in the CO2. Thus, separations without cross-contamination of the extract with the ionic liquid are possible. Here we explore the solubility of a variety of gases, ranging from simple nonpolar compounds to more complex polar gases capable of hydrogen bonding, in a variety of ionic liquids, including [bmim][PF6], [C8-mim][PF6], and [C8-mim][BF4]. Thus, these studies seek to elucidate the factors that control gas solubility in ionic liquids.

419291: Intellectual property rights with special reference to ionic liquids

IEC 0 [419291]: Intellectual property rights with special reference to ionic liquids

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ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Properties of Ionic Liquids*
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Abstract

In the early 90s Covalent began to work on what were then known as "room temperature molten salts," a class of materials now identified as ionic liquids. We were particularly interested in those non-haloaluminate containing ionic liquids that would be stable to air and moisture, and also immiscible with water. We believed that such hydrophobic ionic liquids would open the door to a broad spectrum of industrial applications such as thermally stable solvents, advanced electrolytes for power sources, "ionic plasticizers," and biphase catalysis. In this regard, it has been gratifying for us to observe how the need for environmentally benign chemical processes has brought ionic liquids to the forefront of Green Chemistry.

Covalent's business strategy is to invent and characterize new materials for many applications, particularly in the field of power sources. The ionic liquids fit into this strategy which involves the licensing of our technology for specific applications and/or the manufacture and sale of ionic liquids to supply the needs of the industry for all applications. Over the past few years, we have generated significant intellectual property in the form patents, patent applications and know-how. In this paper, we will consider those families of ionic liquids that fall under the scope of Covalent's patents as well as

a number of commercial applications enabled by our ionic liquid technology.

419331: Research opportunities derived from the Molten Salt Database project

IEC 0 [419331]: Research opportunities derived from the Molten Salt Database project

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ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Properties of Ionic Liquids*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *computer Powerpoint presentation*
Conforms to Bylaw 6: *Y*
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Abstract

The Molten Salt Database project was designed to provide the research community with the physical property data necessary for designing new experimental systems as well as modeling/prediction of new salt systems. The database currently focuses on high temperature salt systems because there are significant industrial interests to drive the collection and critical evaluation of data. In keeping with the goals of this symposium, the opportunities and challenges of including data from the room-temperature salt systems will be discussed in this presentation. Specifically: • What data are necessary to provide a critical assessment of current knowledge? • What are the current and future industrial data requirements for the room-temperature molten salt systems? • Is it possible to identify data needs to meet industrial technological challenges?

442196: The Influence of Chloride, Water and Organic Solvents on the Physical Properties of Ionic Liquids

IEC 0 [442196]: The Influence of Chloride, Water and Organic Solvents on the Physical Properties of Ionic Liquids

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ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Properties of Ionic Liquids*
Invited: *N*
Preferred Presentation Format: *Oral*

Consider for Sci-Mix: *Y*
Special Equipment Needs: *power point presentation preferred*
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Abstract

We present here the first systematic study of the effect of impurities and additives (e.g., water, chloride and co-solvents) on the physical properties of room temperature ionic liquids. Remarkably, it was discovered that the viscosity of mixtures was dependent mainly upon the mole fraction of added molecular solvents and only to a lesser extent upon their identity, allowing viscosity changes during the course of a reaction to be entirely predictable. While the addition of such molecular solvents decreases the viscosity and density, chloride impurities, arising from the preparation of the ionic liquids, increase viscosity dramatically. The commonly used methods of preparation were validated with respect to chloride impurity.

442209: Viscosity and Density of 1-alkyl-3-methylimidazolium Ionic Liquids

IEC 0 [442209]: Viscosity and Density of 1-alkyl-3-methylimidazolium Ionic Liquids

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Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Properties of Ionic Liquids*
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Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *Y*
Special Equipment Needs: *power point presentation preferred*
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Abstract

We report here the viscosity and density of 1-alkyl-3-methylimidazolium salts of tetrafluoroborate, hexafluorophosphate, chloride, trifluoromethanesulfonate and nitrate. Viscosity decreases as a function of temperature and increases with increasing alkyl chain length, while density decreases with increasing temperature and longer alkyl chain length. Viscosity data were fitted to the VFT equation. The ionic liquids were found to exhibit Newtonian behaviour when isotropic, whereas they act as non-Newtonian shear thinning materials at the liquid crystalline mesophase temperatures.

442601: Free Energy Relationships and Solvatochromic Properties of Room Temperature Ionic Liquids based on Methylimmidazolium cations

IEC 0 [442601]: Free Energy Relationships and Solvatochromic Properties of Room Temperature Ionic Liquids based on Methylimmidazolium cations

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Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Properties of Ionic Liquids*
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Abstract

Linear Free Energy Relationships and Solvatochromic parameters have provided a convenient means of characterizing the properties of molecular solvents because of their ability to encapsulate such important practical properties as solubilities, partition constants and reaction rates. We have attempted to characterize the solute distribution and solvatochromic properties of a series of room temperature ionic liquids (RTIL) based on methylimmidazolium cations in combination with a variety of different anions using these two approaches. The first is based on the solvatochromic shift in the wavelength of absorption of various dyes, including 4-nitroanisole, Reichardt's betaine and 4-nitrophenol when dissolved in the ionic liquid. The second involves determination and correlation of the distribution of selected solutes between the water/ionic liquid phases of water immiscible ionic liquids. The results of these studies will be reported and the solvent properties of this class of ionic liquids discussed.

445123: Intermission

0 [445123]: Intermission

ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Properties of Ionic Liquids* ***Preferred Presentation Format:*** *Break*
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Abstract: Abstract text not available.

445124: Discussion

0 [445124]: Discussion

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Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Properties of Ionic Liquids* ***Preferred Presentation Format:*** *Break*

Consider for Sci-Mix:
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