Abstract Listing

Use your browser's Print button, or File-Print command sequence.

631605: Solute Dynamics in Room Temperature Ionic Liquids

IEC 0 [631605]: Solute Dynamics in Room Temperature Ionic Liquids

Frank V. Bright, Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, NY 14260-3000, Fax: 716-645-6963

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Room temperature ionic liquids (RTILs) have been the target of increased investigation. As an integral part of the Green Chemistry movement, RTILs have found application in catalysis, industrial cleaning, liquid/liquid extraction, polymerizations, separations, and synthesis. While much groundwork has been laid, the utilization of these solvents proceeds with an incomplete understanding of how these solvents solvate a solute. In this presentation we report on the steady-state and time-resolved spectroscopy of several small organic probe molecules when they are dissolved in 1-butyl-3-methylimidazolium hexafluorophosphate.

632167: Analytical Studies Using Ionic Liquids

IEC 0 [632167]: Analytical Studies Using Ionic Liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations*
Invited: *Y*
Preferred Presentation Format: *OralOnly*

Consider for Sci-Mix: *N*
Special Equipment Needs: *LCD Projector and Laser Pointer*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

We have recently employed polymeric surfactants (molecular micelles) in combination with capillary electrophoresis for enhanced separations of bioanalytical and environmental samples. We have also employed ionic liquids in combination with our polymeric surfactants to achieve some interesting separations. Our goal is to understand the factors which contribute to effective separations by use of polymeric surfactants in combination with ionic liquids. One of the methods that we have explored for probing molecular recognition is fluorescence anisotropy (FA)(JACS 2001, 123, 3173-3174). We have demonstrated that FA directly correlates with our chromatographic measurements and that it is possible to extract the difference in free energy of interaction between two analytes by use of FA measurements. This talk will highlight some of our recent studies in this area. Other analytical applications of ionic liquids in our laboratory will also be discussed.

635340: Green Chemistry: Halide Ionic Liquids in Action

IEC 0 [635340]: Green Chemistry: Halide Ionic Liquids in Action

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis*
Invited: *N*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Much interest has been shown in ionic liquids (ILs) for their unique physical and chemical properties. ILs are salts that melt at or near room temperature. In contrast to conventional organic solvents, ionic liquids exhibit negligible vapor pressure. Other important properties of ILs, include large liquid range, high thermal stability and ability to solvate compounds of widely varying polarity. Moreover, ILs that possess high ionic conductivity, high ion concentration, and good thermal and electrochemical stability should be beneficial in their utilities as heat transfer fluids, materials in solar cells and electrochemical capacitors. In our lab, halide ionic liquids have been used as both reaction media and reagents in organic synthesis. Halide ionic liquids have also been used as precursors for preparation of non-halide ionic liquids in a waste-free manner. These non-halide ionic liquids are being investigated as new materials.

636192: Issues affecting the use of ionic liquids in lithium-ion batteries

IEC 0 [636192]: Issues affecting the use of ionic liquids in lithium-ion batteries

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
Lithium-ion batteries have found a wide range of applications within consumer devices. These batteries are, for the most part, based on aprotic solvents with, in some instances, toxic lithium salts dissolved in them. For applications in aggressive and/or high temperature environments these solvents are inappropriate, and thus the use of ionic liquids has been explored, due to their numerous advantages. However, the amazing solubilizing properties of these materials introduces interesting electrochemical and engineering problems, such as the potential at which lithium-ions can be inserted into intercalation materials e.g. $LiMn_2O_4$ and graphite, the dissolution of elements within these materials and the solubility of the polymers used as binders in electrode foils. In this paper, experiments using various polymer binders and intercalation materials will be described, including results from lithium-ion cells using various combinations of electrode materials.

636967: Thermotropic-lyotropic, saturated, ionic liquid crystals

IEC 0 [636967]: Thermotropic-lyotropic, saturated, ionic liquid crystals

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Invited: *Y*

Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *Y*
Special Equipment Needs: *overhead projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

We report the properties of ionic liquid crystals, methyl-tri-*n*-decylphosphonium salts **(1P10A**, where the counter-ion **A** is Cl^-, $Cl^-\cdot H_2O$, NO_3^-, Br^-, or $Br^-\cdot H_2O$). Some are liquid crystalline at room temperature. The X-ray diffractograms of all of the salts are characteristic of smectic A phases. The **1P10A**, with **A**=NO_3^- or $Br^-\cdot H_2O$ exhibit dual thermotropic-lyotropic liquid-crystalline properties with high concentrations of small liquid molecules. Their low angle X-ray peaks are broadened but do not change position appreciably as the concentration of a solute, acetonitrile, is increased. The liquid-crystalline phases of both salts can be oriented in strong magnetic fields. By NMR spectroscopy, acetonitrile (≤ 10 wt %) exhibits one type of orientation in the nitrate salt. In the $Br^-\cdot H_2O$ salt, two types of orientations are detected at <1 wt % acetonitrile, but only one orientation is found at higher concentrations. Potential applications for these materials will be discussed.

637230: Ionic liquids as alternatives to organic solvents in liquid-liquid extraction of aromatics

IEC 0 [637230]: Ionic liquids as alternatives to organic solvents in liquid-liquid extraction of aromatics

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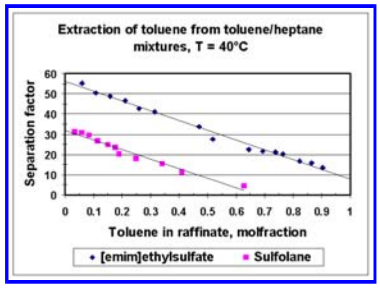
ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Fuels & Applications*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *Y*
Last Modified: *2003-05-10*

Abstract

Aromatic compounds present in cracker feeds (10-25%) are not converted into the desired olefin products. Removal of aromatic compounds would offer several advantages: higher capacity, higher thermal efficiency and less coke forming. Extraction of aromatics with ionic liquids would require less process steps and less energy consumption than extraction with conventional solvents due to the fact that ionic liquids have no or negligible vapour pressure. Liquid-liquid equilibrium data were collected for toluene/n-heptane mixtures at 40 and 75°C using [emim]

ethylsulfate and [mmim]methylsulfate. Equilibrium for extraction was reached within 5 minutes. The separation factor for the separation, at T=40°C, increases from 15 to 55 with decreasing toluene content in heptane, from 90 to 5 mol% (Figure 1). The distribution coefficient of toluene remained slightly above 0.2 over the entire concentration range. These separation factors are about 2-3 times higher compared to conventional solvents (Figure 1), while the capacity is lower.



638976: Solvation phenomena in ionic liquids

IEC 0 [638976]: Solvation phenomena in ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The principles of solvation are fundamental to the practice of chemistry, and the relationship between the chemical structure and solvation properties of molecular liquids are typically introduced within the first two years of undergraduate chemical training. Yet the novelty of ionic liquid solvents renders this "chemical intuition" moot, and demands the development of new principles for solvation in these systems. In this work, we present the results of molecular dynamics simulations aimed at understanding how the chemical structure of ionic liquids determines their behavior as solvents. We show that the highly structured nature of ionic liquid solvents makes solvent polarity a local property, and discuss how solvation processes such as cavity formation and solvent polarization differ in molecular and ionic liquids.

645110: Physical property measurements and a comprehensive data retrieval

system for ionic liquids

IEC 0 [645110]: Physical property measurements and a comprehensive data retrieval system for ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *standard equipment*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

By a judicious choice of its cation, anion, and substituent chemical groups, it is possible to tailor the physical properties of room-temperature ionic liquids (RTIL). Various research groups have reported physical properties for RTIL over ranges of temperature and pressure, including freezing points, densities, viscosities, solubilities, liquid-liquid phase equilibria, heat capacities, etc. To date, reports of some physical properties such as thermal conductivity are quite scarce. Benchmark physical properties of high accuracy are scarcer still. For these reasons, NIST has initiated a project to provide key physical properties of a subset of RTIL that represent a selection of cations, anions and substituent chemical groups.

As identified at the NATO Workshop in Heraklion, Greece, a verified, web-based, public-access database of RTIL properties data is an important need. NIST is addressing this need by evaluating published measurements and capturing the data into a comprehensive data retrieval system known as SOURCE. SOURCE is an archival system that presently captures more than 120 properties and contains 1.3 million data points on 17,000 different substances and 12,000 mixtures. The ionic liquids database will be built by using a record structure similar to Source and maintained by the Oracle relational database management system. Guided Data Capture (GDC) software will be used to speed collection of new experimental data directly from experimentalists. The RTIL database will archive important details including original publication details, method(s) used to make the measurements and the uncertainty of the measurements; it will be maintained by the Thermodynamics Research Center (TRC) on a public-access NIST file server with free, unlimited access to those who use it.

645341: Preparation and properties of polymerized ionic liquids as film electrolytes

IEC 0 [645341]: Preparation and properties of polymerized ionic liquids as film electrolytes

Hiroyuki Ohno, and **Masahiro Yoshizawa**, Department of Biotechnology, Tokyo University of Agriculture & Technology, Koganei, Tokyo 184-8588, Japan, Fax: +81-42-388-7024, ohnoh@cc.tuat.ac.jp

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications: Polymers & Gels*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *LCD projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Ionic liquids are quite interesting materials for not only solvents but also electrolytes. In spite of non-volatility, liquid state restricts some applications especially industrial use. Polymerized ionic liquids should broaden the application area of this interesting material. Introduction of vinyl group on some imidazolium cations induced no effect on the ionic liquid formation with proper anions. Similarly, anions containing vinyl groups made liquid salts with vinyl imidazolium cations. Copolymerizations of these vinyl monomeric ions as well as homopolymerization of either polymerizable cations or anions containing non-polymerizable counter ions have been examined. Introduction of spacer groups in between charged site and vinyl group was revealed to be effective to lower the glass transition temperature and accordingly to improve ionic conductivity. Their electrochemical characteristics and physico-chemical properties will further be discussed with their structure.

645571: Catalysis in Environmentally Friendly Solvents

IEC 0 [645571]: Catalysis in Environmentally Friendly Solvents

REJECTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*
Comments to Organizer: *Poster, oral.*
Preferred Presentation Format: *Poster*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Abstract text not available.

646342: Zwitterionic liquids as non-volatile and non-migrate solvents under potential gradient

IEC 0 [646342]: Zwitterionic liquids as non-volatile and non-migrate solvents under potential gradient

Masahiro Yoshizawa, Asako Narita, and Hiroyuki Ohno, Department of Biotechnology, Tokyo University of Agriculture & Technology, 2-24-16 Nakacho, Koganei 184-8588, Japan, Fax: +81-42-388-7024, yopy@cc.tuat.ac.jp

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications: Polymers & Gels*
Invited: *N*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *LCD projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Ionic liquids have attractive properties such as non-volatility, non-flammability, low viscosity, and quite high ionic conductivity. It is however impossible to realize a selective ion conduction in the ionic liquids. To overcome this drawback, new ionic liquids have been designed. One is the zwitterionic liquid in which both cation and anion are tethered. We have prepared more than 30 kinds of zwitterionic liquids. Most are solids at room temperature, but a few samples are obtained as liquid. The other is the mixture of zwitterionic liquid and LiTFSI. This is obtained as liquid and shows relatively high ionic conductivity of about 10-5 S cm-1 at ambient temperature. The effect of cation, anion, and spacer structure on their melting points will be discussed.

646354: Zwitterionic-liquid-in-polymer electrolytes

IEC 0 [646354]: Zwitterionic-liquid-in-polymer electrolytes

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*

Preferred Presentation Format: *PosterOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

We have designed several zwitterionic liquids, in which both cation and anion are tethered, as a new family of electrolyte material to realize target ion transport in ionic liquids. Although these zwitterionic liquids contain no carrier ions, they showed relatively high ionic conductivity of about 10-5 S cm-1 at ambient temperature when LiTFSI was added to them. In addition, the lithium transference number of zwitterionic liquid containing equimolar amount of LiTFSI is 0.56 which is better than that in typical organic solvents (below 0.4). These zwitterionic liquids are expected as new non-volatile solvents for ionics technology. We prepared polymer gel electrolytes containing zwitterionic liquids as a polar solvent. These polymer gel electrolytes are extremely stable ion conductive polymer in a wide temperature range.

646550: Ionic liquids at Degussa: Catalyst heterogenization in an industrial process

IEC 0 [646550]: Ionic liquids at Degussa: Catalyst heterogenization in an industrial process

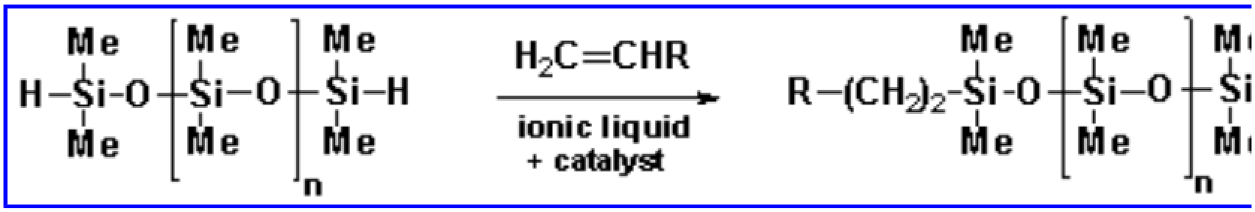
Bernd Weyershausen, Kerstin Hell, and Ute Hesse, R&D Department, Oligomers/Silicones, Degussa AG, Goldschmidtstrasse 1, 45127 Essen, Germany, Fax: ++49-201-1731839, bernd.weyershausen@degussa.com

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis*
Invited: *Y*
Comments to Organizer: *I would appreciate to have the opportunity to present this paper either on Monday 11/8/2003 or Tuesday 11/9/2003 (I won't be able to give the presentation on Thursday 11/11/2003 as I'll have to leave the conference on Wednesday).*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *LCD projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

One of the most fundamental and elegant methods of laboratory and industrial synthesis of organomodified polydimethylsiloxanes is the transition metal catalyzed hydrosilylation of CC-double bond containing compounds with SiH-functionalized polydimethylsiloxanes. Usually, the reaction is homogeneously catalyzed which means that after completion of the reaction the catalyst either remains within the product or has to be costly removed. From an economic and ecological point of view it is desirable to not only separate the expensive catalyst from the

product, but also to recycle and reuse it. We addressed this problem and developed a hydrosilylation process for the synthesis of organosilicon compounds using ionic liquids for the immobilization, respectively, heterogenization of the catalyst. The use of an ionic liquid in this process enables conventional hydrosilylation catalysts to be easily recycled, respectively, to be immediately reused without any further treatment after separation from the product at the end of the reaction. Employing this method different kinds of organomodified polydimethylsiloxanes can be synthesized.



646698: Ionic liquid 'polarity' effects on chemical reactions

IEC 0 [646698]: Ionic liquid 'polarity' effects on chemical reactions

Thomas Welton, N. Llewellyn Lancaster, L. Crowhurst, and J. M. Perez-Arlandis, Department of Chemistry, Imperial College, Exhibition Road, South Kensington, London SW7 2AY, United Kingdom, Fax: 44 (0)20 7594 5804, t.welton@ic.ac.uk

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Fuels & Applications*
Invited: *N*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *No special needs*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
Ionic liquids have become a subject of great activity in recent years. One of the most active areas is that of the synthesis of organic compounds. However, little is known of how to predict which reactions are likely to benefit from the use of ionic liquids and, just as importantly, which will not. There is also little understanding of which ionic liquid will be the ideal one for any given reaction. The work presented in this study seeks to address this problem. We analyse how the ionic liquids interact with solute species an see how this effects the rates of a number of fundamental reactions.

647288: Near-Infrared spectroscopic investigations of water absorption by room-temperature ionic liquids

IEC 0 [647288]: Near-Infrared spectroscopic investigations of water absorption by room-temperature ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Near-infrared (NIR) spectrometry has been successfully used to characterize and to determine kinetics of water absorption by different room-temperature ionic liquids (RTILs) including 1-butyl-3-methylimidazolium tetrafluoroborate ([BuMIm+][BF4-]), [BuMIm+] [PF6-] and [BuMIm+] [Tf2N-]. Interactions between water and ionic liquids were found to be strongly dependent on anions of the ionic liquids, and that the stronger the interactions, the higher is concentration of absorbed water.

648073: Phase equilibria (SLE, LLE) of N,N-Dialkylimidazolium Hexafluorofosphate or Chloride

IEC 0 [648073]: Phase equilibria (SLE, LLE) of N,N-Dialkylimidazolium Hexafluorofosphate or Chloride

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *PC with Office windows XP(1998-2000) version of Powerpoint*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The solubility of 1-ethyl-3-methylimidazolium hexafluorophosphate, [emim][PF6] in aromatic hydrocarbons and in alcohols as well as of 1-butyl-3-methyl-imidazolium hexafluorophosphate, [bmim][PF6] in the same aromatic hydrocarbons, in n-alkanes and in cyclohydrocarbons has

been measured by a dynamic method from 290 K to the melting point of ionic liquid or to the boiling point of the solvent. The solubility of [emim][PF6] and [bmim][PF6] in aromatic hydrocarbons and in an alcohols decreases with an increase of the molecular weight of the solvent. The differences on the solubility in o-, m- p-xylene are not significant. In every case, with the exception of methanol, the mutual liquid-liquid equilibrium was observed. Also the solubilities of 1-butyl-,or decyl-, or dodecyl-3-methylimidazolium chloride [C4, or C10, or C12mim][Cl] in alcohols has been measured by the same method. The melting point, enthalpy of fusion, and enthalpies of different solid-solid phase transitions were determined by differential scanning calorimetry (DSC) for every ILs. The data were correlated by means of the Wilson, UNIQUAC ASM and modified NRTL equations utilizing parameters derived from the solid-liquid equilibrium (SLE). The root-mean-square deviations of the solubility temperatures for all calculated data depend on the particular system and the equation used. The solubilities of 1-alkyl-3-methylimidazolium chloride, [Cnmim][Cl], where n=4, 8, 10, 12 in octan-1-ol and water have been measured and used to calculate the octan-1-ol/water partition coefficients as a function of temperature and alkyl substituent. Experimental partition coefficients (log P) are negative in three temperatures, what is the evidence of the possibility of using these ionic liquids as a green solvents.

648364: Electrochemical synthesis in 1-butyl-2, 3-dimethylimidazolium hexafluorophosphate

IEC 0 [648364]: Electrochemical synthesis in 1-butyl-2, 3-dimethylimidazolium hexafluorophosphate

Michael A. Matthews, John W. Weidner, and Inas M AlNashef, Department of Chemical Engineering, University of South Carolina, Swearingen Engineering Center, S. Main Street, Columbia, SC 29208, matthews@engr.sc.edu

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry*
Invited: *N*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

We previously demonstrated the electrochemical generation of a stable superoxide ion in room temperature ionic liquids (RTIL) solvents. We also showed that superoxide ion could be utilized to synthesize carboxylic acids and ketones from the corresponding primary and secondary alcohols, respectively. In most of the synthesis processes that we carried out in 1-butyl-3-methylimidazolium hexafluorophosphate, [bmim] [HFP], the presence of 1-butyl-3-methylimidazolidone in the ether extract was observed using GC/MS. This compound was not found before the electrolysis process; hence we suspect that superoxide ion is reacting with the RTIL. But when we used 1-butyl-2,3-dimethylimidazolium hexafluorophosphate, [bdmim]

[HFP], to see the effect of blocking the C2 position no apparent oxidation of the ionic liquid was detected. The conversion of benzhydrol to benzophenone increased from 40% in [bmim] [HFP] to 95% in [bdmim] [HFP]. The vast majority of our results to date have been generated in conventional electrolytic two-compartment cell with fritted glass separating the cathode and anode compartments. We here discuss the design of a novel membrane reactor that will increase current efficiencies and production in the electro-organic syntheses utilizing superoxide ion. The new membrane reactor design will increase current efficiency and reaction rates in the electrolysis of oxygen. The novel reactor will employs a thin polymer membrane, infiltrated with the RTIL, to separate the anode and cathode compartments. This membrane reactor will serve as a model system for simulating large-scale production aimed at reducing the energy needed for electrolysis.

648768: ionic liquids: solvents for electrochemical nanotechnology

IEC 0 [648768]: ionic liquids: solvents for electrochemical nanotechnology

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

In the recent years ionic liquids have gained rising interest in electrochemistry. These are liquids that are based on organic cations (e.g. 1-Butyl-3-methylimidazolium [BMIm]) and organic and / or inorganic anions (e.g. Bis(trifluoromethyl-sulfonyl)imide [BTA] or e.g. hexafluorophosphate PF6), and besides a high chemical stability and low vapour pressures even at elevated temperatures they can have electrochemical windows of more than 6 Volt. Most of the studies hitherto were performed in liquids based on highly hygroscopic AlCl3, which can have electrochemical windows of up to 4 V, depending on the composition. These liquids are well established and many less noble metals like e.g. Al and its alloys can be electrodeposited, even in nanocrystalline form (e.g. Al and Al-Mn). This can be achieved by pulsed electrodeposition and organic additives, resulting in shining and nanocrystalline bulk materials. For example, the hardness of nanocrystalline Al can be 100 – 200 % higher compared to microcrystalline Al, as will be shown in this talk. The rather new air and water stable ionic liquids like [BMIm]PF6 or [BMIm]BTA are of high interest for the electrodeposition of semiconductors, especially as thin layers. It could be shown with the in situ Scanning Tunneling Microscope that epitaxial 20 nm thin Ge(111) layers as well as narrowly distributed semiconducting Ge nanocrystallites can be obtained. It will also be shortly demonstrated that nanocrystalline Si can be obtained by electrodeposition from ionic liquids.

649462: Novel Separation Processes Based on Unique Solvation Properties of Ionic Liquids

IEC 0 [649462]: Novel Separation Processes Based on Unique Solvation Properties of Ionic Liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *LCD projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
The uses of ionic liquids in designing new separation processes have been recently explored. For example, large distribution coefficients for the extraction of metal ions based on the ionic liquids containing complexing ligands have been observed. The enhanced distribution coefficients are fundamentally correlated to the unique interactions of ionic liquids with solutes. The wide variation in the strength of the interaction forces allows us to rationally design a "smart" ionic solvent for a specific separation process. We will discuss our recent results on fundamental studies concerning the solvation properties of ionic liquids, the effects of second coordination shells in ionic liquids, and their applications in designing new separation processes.

649581: Recyclable catalysts and reagents using ionic liquids based on biorenewable materials

IEC 0 [649581]: Recyclable catalysts and reagents using ionic liquids based on biorenewable materials

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis*
Invited: *Y*

Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The interest in and application of room temperature ionic liquids (RTILs) continues to grow. The beneficial properties with respect to volatility, flammability, and toxicity have resulted in RTILs being considered a promising class of "green" solvents. To date, the most common use of RTILs is as inert, recyclable solvents for transition-metal-catalyzed reactions. At the same time, there are a considerable number of important volatile and toxic organic solvents that would be worthwhile candidates for safer replacements but do not fall into the category of "inert." A prime example of this is pyridine, which is a widely used acylation catalyst and reaction buffer and is also highly carcinogenic. Our research has focused on developing new, functionalized RTILs based on natural products as the starting material. Two main areas will be discussed. First is Lewis basic RTILs based on nicotine that can serve as acylation catalysts and as mild acid catalysts for a variety of reactions. Second is protic RTILs based on fructose that can be used as supports for soluble, supported reagents.

649723: Imidazolium-2-carboxylates: Versatile intermediates for the synthesis of ionic liquids and ligands

IEC 0 [649723]: Imidazolium-2-carboxylates: Versatile intermediates for the synthesis of ionic liquids and ligands

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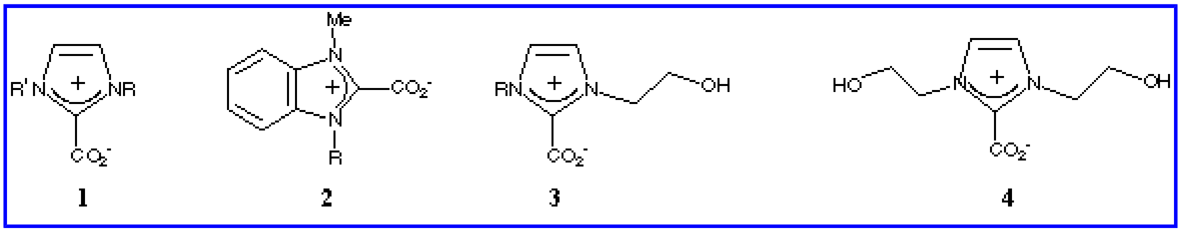
ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *OH or LCD projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The recently discovered alkylation of methylimidazole by dimethyl carbonate to dimethylimidazolium–2–carboylate,[1,2] has been extended to other imidazole derivatives, including benzimidazoles, and to other dialkyl carbonates like cyclic carbonates. Generic structures 1–4 are obtained in good yields and selectivities.[3] The corresponding ionic liquids are obtained by controlled protonation of the C–2 carboxylates, followed either by thermal

treatment or base-catalyzed decarboxylation. Details on these different reactions will be presented and the reaction mechanisms discussed. Additional examples of the use of imidazolium-2-carboxylates will be introduced, demonstrating the flexibility of these readily accessible intermediates.

References [1] Poinsot D., Tkatchenko I., Tommasi I., French Demande 02 12 692 (University of Burgundy, 10/10/02). [2] Holbrey J., Reichert D. W. M., Tkatchenko I., Bouajila E., Walter O., Tommasi I., Rogers R. D., Chem. Commun. 2003, 28-29. [3] Poinsot D., Tkatchenko I., Tommasi I., submitted.



650869: Applications of vibrational spectroscopy to ionic liquids

IEC 0 [650869]: Applications of vibrational spectroscopy to ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
The possibility of combining chemical reactions in Ionic Liquids (IL) with separations using supercritical CO2 is potentially valuable. However, detailed information of the phase behaviour of high-pressure CO2/IL systems and a molecular-level insight into the state of CO2 dissolved in IL is needed. The presence of water in IL may affect solubility of CO2 in IL and other solvent properties of IL. Therefore, molecular state of water dissolved in IL also needs to be elucidated. Vibrational spectroscopy (IR and Raman) plays an important role in probing molecular structure of IL and interactions between solutes and IL. Spectroscopy also allows one to monitor in situ chemical processes in IL. In this paper, we report applications of ATR-IR, transmission IR and Raman spectroscopy to study ionic liquids subjected to CO2 at different pressures, and to water in the range of different humidity. Applications of spectroscopic imaging to IL will also be discussed.

651798: Catalysis in environmentally friendly solvents

IEC 0 [651798]: Catalysis in environmentally friendly solvents

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*
Preferred Presentation Format: *Poster*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

In recent years, one of the prime concerns of chemists is the search for replacements to conventional organic solvents. In this context, room temperature ionic liquids (RTILs) are attracting increasing interest as environmentally benign reaction media for chemical synthesis and catalysis. We have investigated a number of reactions in RTILs. These include the use of Lewis acidic ionic liquids, e.g. [BMIM]Cl-(x)$ZnCl_2$ (BMIM=1-butyl-3-methylimidazolium, x=1.0 – 2.5), as catalyst and reaction medium for Diels-Alder reactions and Fisher-Indole synthesis. The effect of the composition of the IL on yield and selectivity will be described.

Copper triflate complexed with a bisoxazoline will catalyse a number of reactions e.g. Diels-Alder, cyclopropanation, allylic oxidation with good e.e. and in some cases asymmetric induction is dependent on anion. Therefore, we have investigated some of these reactions in [BMIM][OTf], [BMIM][PF_6], [BMIM][NTf_2], [BMIM][BF_4] and examined the affect of anion on yield and enantioselectivity. The possibility of recovery and reuse of the catalyst ionic liquid solution will also be discussed in selected cases.

651920: Molecularly organized assemblies within room-temperature ionic liquid-based solutions?

IEC 0 [651920]: Molecularly organized assemblies within room-temperature ionic liquid-based solutions?

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry &*

Engineering and Separation Science & Technology subdivisions): Spectroscopy
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

A room-temperature ionic liquid (RTIL) is a novel solvent which holds great promise for enabling new environmentally-responsible technologies. However, research carried out recently has exposed obstacles to their wider use due to solubility limitations. One effective way to tune such solubility is via the formation of a suitable molecularly organized assembly, a feature of which is often high local concentration within the organized heterogeneous assembly. Applications of such assemblies include, increased rate, product distribution, or turnover number of a chemical reaction, lower analyte detection limits, higher chromatographic efficiency, and improved time release in drug delivery vehicles. We present our research efforts to explore the formation of organized assemblies within RTIL solutions using optical spectroscopic techniques. Our strategy entails not only an exploration of the influence of the nature of the amphiphile and cosolvents leading to self-assembly in RTIL systems but also the development of a much needed fundamental, molecular-level view of the underlying system heterogeneity.

652613: Multiphase equilibrium in mixtures of [C4mim][PF6] with supercritical carbon dioxide, water and ethanol: applications in catalysis

IEC 0 [652613]: Multiphase equilibrium in mixtures of [C4mim][PF6] with supercritical carbon dioxide, water and ethanol: applications in catalysis

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *LCD projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The ionic liquid [C4mim][PF6] and supercritical carbon dioxide produce multiphase systems when mixed with ethanol and water. Mixtures of these four "green" solvents can be made to go through a succession of phase changes. By small changes in composition or carbon dioxide

pressure, the system exhibits the following pattern: one phase (IL) - two phases (IL+water)- one phase (IL/water/ethanol) - two phases (IL/water/ethanol + CO2) - three phases (IL-rich + water/ethanol-rich + CO2-rich) + two phases. (IL-rich + water/ethanol/CO2). Increasing carbon dioxide pressure induces first the appearance of an intermediate liquid phase and later the merging of this phase with the gas, leaving all the ionic liquid in a separate, denser liquid. This succession is suitable to carry out reaction cycles in ionic liquid-based solvents. An epoxidation reaction, catalysed by sodium hydroxide, was rapidly carried out in these conditions, with complete recovery of the reaction product by CO2 decompression.

653058: Dialkyl imidazolium benzoates – room temperature ionic liquids useful in the peracetylation and perbenzoylation of simple and sulfated saccharides

IEC 0 [653058]: Dialkyl imidazolium benzoates – room temperature ionic liquids useful in the peracetylation and perbenzoylation of simple and sulfated saccharides

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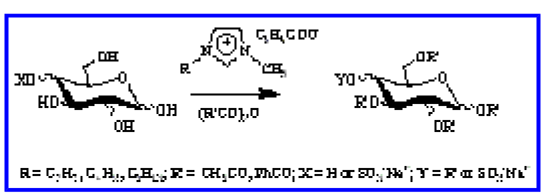
ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
Dialkyl imidazolium benzoates, room temperature ionic liquids including 1-ethyl-3-methyl imidazolium benzoate, 1-butyl-3-methyl imidazolium benzoate and 1-hexyl-3-methyl imidazolium benzoate were used in the peracetylation and perbenzoylation of several simple and sulfated carbohydrates. Organic solvents and catalysts were not required in the syntheses and these ionic liquids gave excellent yields in short reaction times.



653470: Phase behavior and thermodynamic properties of ionic liquids, ionic

liquid mixtures, and ionic liquid solutions

IEC 0 [653470]: Phase behavior and thermodynamic properties of ionic liquids, ionic liquid mixtures, and ionic liquid solutions

Luis P.N. Rebelo, Vesna Najdanovic-Visak, Ricardo Gomes de Azevedo, José M. Esperança, Manuel Nunes da Ponte, Henrique J. Guedes, Zoran P. Visak, Herminio C. de Sousa, Jerzy Szydlowski, and José N. Canongia Lopes, Instituto de Tecnologia Quimica e Biologica, Universidade Nova de Lisboa, Portugal, Av Republica, Apartado 127, 2781-901 Oeiras, Portugal, Fax: 351-21-4411277, luis.rebelo@itqb.unl.pt

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *overhead and LCD*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

This contribution reports on (i) experimental and theoretical studies of critical liquid-liquid demixing of some ionic liquid solutions and on their relationship with solutions' non-ideality; and (ii) on speed of propagation of ultrasound waves in pure ILs from which several other thermodynamic properties such as compressibilities, expansivities and heat capacities, can be derived. Research has been carried out at a broad range of pressures, typically up to 1600 bar, sometimes inside the metastable liquid region. The current study focuses on [Cnmim][PF6], [Cnmim][NTf2], and [Cnmim][BF4] where n is usually 4, but generally $2 < n < 10$. The first experimental evidence of a Lower-CST for critical demixing has just been found. A phenomenological approach based on an extended Flory-Huggins-type gE-model coupled with the statistical-mechanical theory of isotope effects is used. Combination of the model's parameters with the T-p slope of the critical lines enables us to discuss the magnitude and sign of the enthalpic and volumetric excess properties of these solutions as well as mode frequency shifts upon dilution.

653537: Thermodynamic Properties of Mixtures Containing Ionic Liquids

IEC 0 [653537]: Thermodynamic Properties of Mixtures Containing Ionic Liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry &*

Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *overhead projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The unique properties of ionic liquids open up a wide range for various applications. Ionic liquids have proven to be viable reaction media for numerous types of reactions. Separation of the reaction products from the ionic liquid requires the knowledge of the thermodynamic properties of such mixtures, as well as of properties of the pure individual compounds. Vapor-liquid equilibrium of the mixtures of high boiling solvents: ethyl benzoate, dimethyladipate, benzylamine, and octylamine with the ionic liquid 1-methyl-3-ethyl-imidazolium bis (trifluoromethyl-sulfonyl) imide (C8H12S2O4F6N3) were studied by using the transpiration method. An extended version of this technique is presented, which allows to determine the composition of the vapor phase of high boiling mixtures and to calculate activity coefficients in the liquid phase. The measurements were carried out over the whole concentration range at different temperatures between 298 K and 323 K. Activity coefficients of these solvents in the ionic liquid have been derived and from their temperature dependence partial molar excess enthalpies of the solutes in the ionic liquid have been estimated.

653595: Density functional investigation of ionic liquid cation-anion ratios in the catalysis of Diels-Alder reactions

IEC 0 [653595]: Density functional investigation of ionic liquid cation-anion ratios in the catalysis of Diels-Alder reactions

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Room temperature ionic liquids are a novel class of solvents that influence the chemical reactivity and stereoselectivity of a vast range of organic reactions, but the molecular factors that

give ionic liquids their great potential are largely unknown. Our computational study targets the understanding of the local microscopic interactions of ion pairs at the transition structure. The focus is to examine the possibility that 1-ethyl-3-methylimidazolium cation (EMI^+) acts as a Lewis acid and how it is modulated by the surrounding chloroaluminate counterions. The local effects of different cation-to-anion ratios upon chemical reactivity are investigated using density functional theory at the B3LYP/6–31G(d) level of theory. The isolated ions that form in the melts ($AlCl_4^-$, $Al_2Cl_7^-$ and EMI^+) along with their 1:1 complexes ($AlCl_4^- \cdots EMI^+$ and $Al_2Cl_7^- \cdots EMI^+$) and 2:1 anion-cation complexes ($Cl^- \cdots EMI^+ \cdots AlCl_4^-$, $AlCl_4^- \cdots EMI^+ \cdots AlCl_4^-$, $Al_2Cl_7^- \cdots EMI^+ \cdots AlCl_4^-$ and $Al_2Cl_7^- \cdots EMI^+ \cdots Al_2Cl_7^-$) have been computed with the correct experimental trend. A new conceptual model has been formulated.

654277: Spectroscopic studies of biomolecular stability and activity in ionic liquids

IEC 0 [654277]: Spectroscopic studies of biomolecular stability and activity in ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy*
Invited: *Y*
Comments to Organizer: *invited for: SPECTROSCOPY session of the Ionic Liquid symposium*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Key issues relevant to the exploitation of biocatalysis within ionic liquids will be discussed. We will also present recent findings from our group and highlight important hurdles to the broader implementation of ionic liquids in this area.

654724: Criticality in C4mimBF4 + water mixture

IEC 0 [654724]: Criticality in C4mimBF4 + water mixture

Claudio A. Cerdeirina[1], J. Troncoso[1], L. Romani[1], V. Najdanovic-Visak[2], J.M.S.S. Esperanca[2], and L.P.N. Rebelo[2]. (1) Departamento de Física Aplicada, Universidad de Vigo, As Lagoas s/n, Ourense 32004, Spain, Fax: 988-387227, calvarez@uvigo.es, (2) Instituto de

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Critical point universality in liquid mixtures (3D-Ising universality class) originates from the long-range nature of the concentration fluctuations. Close enough to the critical point, the correlation length of concentration fluctuations becomes so large that microscopic details of intermolecular interactions are of vanishing importance. This is so for simple mixtures, however, 3D-Ising-type criticality is not obvious a priori in complex fluids such as ionic solutions. The increased interest in room temperature ionic liquids (RTIL) has promoted their thermodynamic study in both basic and applied thermodynamic grounds. A study on the criticality of the binary mixture containing the RTIL, C4mimBF4, and water is presented. Both the isobaric heat capacity and density in the immediate vicinity of the critical point as well as the slope of the critical line were experimentally determined. The results thus obtained were interpreted from excess volumes and enthalpies on the basis of Prigogine & Defay's equation.

654729: Halide determination in Ionic Liquids

IEC 0 [654729]: Halide determination in Ionic Liquids

Christopher Hardacre[1], Maggel Deetlefs[2], William R. Pitner[2], and Constanza Villagran[2]. (1) School of Chemistry, Queen's University Belfast, David Keir Building, Stranmillis Road, BT9 5AG Belfast, United Kingdom, Fax: 44 28 90 382117, c.hardacre@qub.ac.uk, (2) Queen's University Ionic Liquid Laboratories, Queen's University Belfast

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *LCD projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Halide contamination of ionic liquids can be problematic when utilising them as a reactive medium particularly in catalytic reactions. The concentration of halide can be determined using a

number of methods, for example titrimetric, electrochemical and ion chromatography. The detection limits, advantages and disadvantages of each method will be compared for both water miscible and water immiscible ionic liquids. In particular, this paper will focus on the use of ion chromatography as a flexible and effective method for the determination halide in ionic liquids. As a further example of its use, recent results on the rate of decomposition of fluorine containing anions will be presented.

655349: Effects of ionic liquid structure on gas solubilities

IEC 0 [655349]: Effects of ionic liquid structure on gas solubilities

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Previously we have reported the solubilities of a wide range of gases including carbon dioxide, ethylene, ethane, methane, oxygen, argon, carbon monoxide, hydrogen, and nitrogen in the ionic liquid [bmim][PF_6]. Here we explore the effects that changing the structure of the cation and anion can have on the solubilities of the gases in the ionic liquids (ILs). The additional ionic liquids considered include imidizolium-based ILs such as [bmmim][PF_6], [bmim][BF_4], [bmmim][BF_4], [bmim][Tf_2N], [emim][Tf_2N], and [emmim][Tf_2N], tetraalkylammonium-based ILs such as [$MeBu_3N$][Tf_2N] and [$HeBu_3N$][Tf_2N], and the pyrrolidinium-based IL [MeBuPyrr] [Tf_2N]. We will also compare our experimental results with molecular dynamics simulations of gas solubilities in ILs. Based on these results, we can begin to determine what factors control gas solubilities in ionic liquids.

655563: High lithium metal cycling efficiency in a room temperature ionic liquid

IEC 0 [655563]: High lithium metal cycling efficiency in a room temperature ionic liquid

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
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Last Modified: *2003-05-10*

Abstract

A novel room temperature ionic liquid (RTIL) electrolyte, 0.5 mol/kg lithium bis (trifluoromethylsulfonylamide) (LiTFSA) in N–methyl, N–alkyl pyrrolidinium bis (trifluoromethylsulfonylamide) (P1xTFSA), has been investigated to assess its suitability for use with lithium metal electrodes for rechargeable lithium batteries. In this electrolyte it is found that lithium can be cycled with a high degree of reversibility. A coulombic cyclic efficiency >99.5% is observed for more than 300 cycles, and an average cycling efficiency of greater than 99% is achieved when cycling at a current density of 1.0 mAcm-2 (Idep=Idiss) on a platinum substrate. At deposition rates up to 1.75 mAcm-2 optical micrographs indicate that the lithium deposit is uniform and non-dendritic. Above 1.75 mAcm-2, the lithium deposit becomes dendritic and cycling efficiency rapidly decays. At low rates (0.1 mAcm-2) high cycling efficiency (>99%) can be obtained on a copper substrate. In this case, the deposition/cycling history influences the cycling behaviour of the deposit.

655702: Deep Desulphurization of Fuels by Extraction with Ionic Liquids

IEC 0 [655702]: Deep Desulphurization of Fuels by Extraction with Ionic Liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Fuels & Applications*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *LCD projector, lapel microphone and laser pointer*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The classical process for desulphurization of fuels is catalytic hydrogenation of sulphur

compounds into hydrogen sulfide. However this process requires high operating and investment costs when producing ultra-low sulphur gasoline and diesel fuels.

An alternative concept is liquid-liquid-extraction by ionic liquids. Novel developments on the use of (halogen-free) ionic liquids will be presented.

656150: Solvent strength of the ionic liquids/carbon dioxide mixtures

IEC 0 [656150]: Solvent strength of the ionic liquids/carbon dioxide mixtures

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
Previously we have shown that organic solutes can be extracted from ionic liquids (ILs) with supercritical CO_2 and that ILs can be induced to separate from organic and aqueous mixtures by applying gaseous CO_2 pressure. Thus, we are interested in the solvent strength of CO_2/IL mixtures. Here we use 4-nitroaniline, *N,N*-diethyl-4-nitroaniline, and Reichardts dye 33 to determine the Kamlet-Taft parameters for several ILs and their mixtures with CO_2. The effect of temperature and carbon dioxide concentration on these parameters was determined. The polarizability parameter depends weakly on the CO_2 concentration. However, the hydrogen bond donating ability and the hydrogen bond accepting ability are virtually independent of CO_2 pressure. The implications of these results on the use of IL/CO_2 mixtures as green solvents will be discussed.

656321: New ionic liquids

IEC 0 [656321]: New ionic liquids

Gregory W. Drake[1], Tommy W. Hawkins[1], Kerri Tollison[2], Leslie Hall[1], Greg Kaplan[2], and Ashwani Vij[1]. (1) AFRL/PRSP, Air Force Research Laboratory, 10 East Saturn Boulevard, Building 8451, Edwards Air Force Base, CA 93524, Fax: 661-275-5471, gregory.drake@edwards.af.mil, (2) PRSP, ERC, Inc

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications*
Invited: *Y*
Comments to Organizer: *We were invited to speak by Robert Mantz a session organizer*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

New Ionic Liquids

Greg Drake; Tommy Hawkins; Kerri Tollison#; Leslie Hall; Greg Kaplan#; Ashwani Vij

AFRL/PRSP and #ERC, Inc. Air Force Research Laboratory Edwards Air Force Base, CA 93524

In our laboratories we have been designing and synthesizing new salts that have low melting points. Using shape and packing issues, we have mimicked the well known class of ionic liquids based on 1,3-dialkylsubstituted imidazolium systems with a similar shaped ring of 4-amino-1,2,4-triazole. This new class of 1-substituted-4-amino-1,2,4-triazolium cation based salts have higher densities and heats of formation than their corresponding imidazole based systems and they can be paired with well known anions resulting in several new large arrays of ionic liquids. The synthesis and physical properties of these new salts as well as discussions on single crystal x-ray diffraction study results of several of the new materials will be overviewed.

656672: Performance enhancing electrolytes:The impact of Ionic liquids on artificial muscle development

IEC 0 [656672]: Performance enhancing electrolytes:The impact of Ionic liquids on artificial muscle development

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*

Last Modified: *2003-05-10*

Abstract

Electrolytes play a critical role in determining the performance characteristics of both naturally occuring and synthetic systems.As we attempt to make electrochemical devices more sophisticated such as in the development of electromechanical actuators (artificial muscles) the requirements we place on electrolytes become demanding. Ionic liquids are proving to be particularly useful in this area. The use of ionic liquids as electrolytes has resulted in dramatically improved performance for inherently conducting polymer based artificial muscles. This presentation will discuss the effect of ionic liquids on the electrochemical and mechanical properties of inherently conducting polymers and detail some practical applications of artificial muscles that have become possible through the use of these performance enhancing electrolytes.

656913: Ionic liquids as sources of heavy-ion beams for electrical propulsion

IEC 0 [656913]: Ionic liquids as sources of heavy-ion beams for electrical propulsion

Juan Fernandez de la Mora, Department of Mechanical Engineering, Yale University, 9 Hillhouse Avenue, New Haven, CT 06520-8286, Fax: 203-432-7654, juan.delamora@yale.edu

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications*
Invited: *Y*
Comments to Organizer: *The specific session (organized by Paul Trulove)will be called: Novel Applications of Ionic Liquids*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

When a liquid meniscus is charged to a sufficiently high voltage with respect to neighboring grounded electrodes, the liquid surface deforms into a so-called Taylor cone, whose apex ejects a thin jet. Its diameter D can be controlled through the liquid's electrical conductivity K. When K ~ 1 S/m, D may be as small as 10-20 nm, with associated surface electric fields of the order of 1 V/nm, at which ions evaporate directly into the surrounding. Use of this phenomenon for ion beam generation requires operation under vacuum, hence highly conducting liquids of low volatility. Ionic liquids are unmatched in both respects. The characteristics of drop vs. ion emissions, the purely ionic regime, the production of ion beams of very high mass and rich range of chemical composition and applications to electrical propulsion and mass spectrometry will be discussed.

656932: Developments of ionic liquids applications for ATOFINA processes

IEC 0 [656932]: Developments of ionic liquids applications for ATOFINA processes

Philippe Bonnet, Department of catalysis, ATOFINA / Rhone Alpes Research Center, rue Henri Moissan, PIERRE BENITE cedex 69493, France, philippe.bonnet@atofina.com

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
futher information is not possible at this early stage due to Industrial property reasons

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657017: Ionic Liquids: Fundamental research and applied technology

IEC 0 [657017]: Ionic Liquids: Fundamental research and applied technology

T. Mark McCleskey, Chemistry Division, C-SIC, Los Alamos National Lab, MS J514, Los Alamos, NM 87544, Fax: 505-667-9905, tmark@lanl.gov, Anthony K Burrell, C-SIC, Los Alamos National Laboratory, Gary A. Baker, Bioscience Division, Michelson Resource, Los Alamos National Laboratory, and Sheila N. Baker, Chemistry Division, Los Alamos National Laboratory

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
We will report on a wide range of activities at Los Alamos National Laboratory. Results on basic research including biomolecules and electron transfer will be discussed. Recent applications of ionic liquids in the areas of sensors and electro-optic devices will also be presented.

657198: Ionic Liquids: Highly Effective medium for Enatiopure Amino Acid

Esters via Enzymatic Resolution

IEC 0 [657198]: Ionic Liquids: Highly Effective medium for Enatiopure Amino Acid Esters via Enzymatic Resolution

Sanjay V. Malhotra, and Hua Zhao, Chemistry & Environmental Science, New Jersey Institute of Technology, 384 Teirnan Hall, University Heights, Newark, NJ 07102-1982, Fax: 973-596-8436, sanjay.malhotra@njit.edu

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Abstract text not available.

657377: Phase behavior of mixtures containing ionic liquids

IEC 0 [657377]: Phase behavior of mixtures containing ionic liquids

Sudhir N.V.K. Aki, Jennifer L. Anthony, Jacob M Crosthwaite, Aaron M. Scurto, and **Joan F. Brennecke**, Department of Chemical and Biomolecular Engineering, University of Notre Dame, 182 Fitzpatrick Hall, Notre Dame, IN 46556, Fax: 574-631-8366, asudhir@nd.edu, jfb@nd.edu

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The phase behavior of ionic liquids with gases, organic liquids and solids is vital for evaluating their use as solvents for reactions and as media for separations. We will present information on multicomponent phase behavior, as well as binary measurements such as gas solubilities in ionic liquids and liquid/liquid equilibrium. We will focus on our work that has shown that one can use gases, such as CO_2, to separate ionic liquid/organic mixtures. In particular, we will explore how phase separation temperatures and pressures depend on the nature of the solute and the choice of cation and anion of the ionic liquid. We quantify the degree of separation possible using a new high pressure sampling apparatus.

657381: The road to partition: Mechanisms of metal ion transfer into ionic liquids (ILs) and their implications for the application of ILs as extraction solvents

IEC 0 [657381]: The road to partition: Mechanisms of metal ion transfer into ionic liquids (ILs) and their implications for the application of ILs as extraction solvents

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
The rational design of ionic liquid-based metal ion separation systems requires either that the ion transfer properties of these systems be predictable from the known behavior of conventional organic solvents or that the mechanism(s) of ion transfer be understood at a fundamental level. With this in mind, we have examined the transfer of selected metal ions (*e.g.*, alkaline earths and lanthanides) from acidic aqueous media into a series of *N,N'*-dialkylimidazolium-based room-temperature ionic liquids (RTILs) , either alone or in the presence of crown ethers or b-diketones . The results obtained indicate that although certain aspects of metal ion extraction into RTILs parallel the behavior of conventional solvents, ionic liquids frequently play a more active role in the partitioning process, with ion exchange involving the cationic or anionic constituents of the ionic liquid comprising an important mode of ion transfer.

657402: Nonlinear optical ionic liquids

IEC 0 [657402]: Nonlinear optical ionic liquids

John S. Wilkes[1], Rico E. Del Sesto[1], Fassil Ghebremichael[1], Norman E. Heimer[2], Douglas S. Dudis[3], and A. Todd Yeates[4]. (1) Department of Chemistry, US Air Force Academy, 2355 Fairchild Drive, Suite 2N225, USAF Academy, CO 80840-6230, Fax: 719-333-2947, john.wilkes@usafa.af.mil, (2) Department of Chemistry, United States Air Force Academy, (3) AFRL/MLBP, Wright-Patterson AFB, (4) Materials & Manufacturing Directorate, Air Force Research Laboratory

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Molecular orbital calculations indicate that molecules with a high electron density diffused over a large volume will have third order nonlinear optical activity. Anions often have higher second hyperpolarizability values (gamma) than similar neutral molecules. Also, molecules or ions containing higher row elements have higher gammas. Salts with cations that have their positive charge only weakly interacting with the anion also enhance the third order nonlinear optical activity. That looks like the recipe for ionic liquids. A number of sulfur-containing mono- and dianion salts were synthesized and characterized through Z-scan measurements. Most were ionic liquids, and some showed significant third order nonlinear optical behavior. The general features of ionic liquids such as wide liquidus range, good thermal stability, and low vapor pressure are particularly advantageous for applications of nonlinear optical materials. Potential applications are in optical limiting and other all-optical devices.

657590: Investigation of the structure of ionic liquids and their interactions with water by nuclear Overhauser effect

IEC 0 [657590]: Investigation of the structure of ionic liquids and their interactions with water by nuclear Overhauser effect

Andrea Mele[1], Chieu D. Tran[2], and Silvia De Paoli Lacerda[2]. (1) Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano, Via L. Mancinelli, 7, Milano I-20131, Italy, Fax: +39-02-23993080, andrea.mele@polimi.it, (2) Department of Chemistry, Marquette University

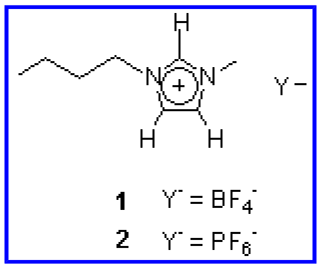
ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy*
Invited: *Y*
Comments to Organizer: *Invited talk. For information please refer to Prof. Chieu D. Tran*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *pc, MS-PowerPoint, Windows 2000*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The strict relationship between ionic liquid structure and their behavior as reaction media

stimulated studies with a broad repertoire of techniques (FT-IR, Near-IR, fluorescence, viscosimetry, conductivity etc.) [1]. Unfortunately, these techniques cannot provide direct information on molecular level of structure of RTILs and their interactions with water. In this communication we report on some results of an NMR study via intermolecular nuclear Overhauser enhancements (NOEs) on model compounds 1-*n*-butyl-3-methylimidazolium tetrafluoborate ($[BMIm]^+$ $[BF_4]^-$, **1**) and 1-*n*-butyl-3-methylimidazolium hexafluorophosphate ($[BMIm]^+$ $[PF_6]^-$, **2**). The NOEs patterns observed with and without known amounts of water indicated that the presence of water changes the structure of the pure ionic liquid by introducing water-cation interactions. Further structural details on the type and site of water-imidazolium ion interactions are obtained by the quantitation of water-cation NOEs.

[1] C. D. Tran, S. H. D. P. Lacerda and D. Oliveira, *Appl. Spectrosc.* **2003**, *57*, 152-157 and references therein.



657927: Ruthenium and uranium halide complexes in ionic liquids

IEC 0 [657927]: Ruthenium and uranium halide complexes in ionic liquids

Maggel Deetlefs[1], Denise Appleby[2], Paul A. Barnard[3], Christopher A. Bowlas[4], Peter B. Hitchcock[2], Charles L. Hussey[3], Thamer J. Mohammed[2], T. Anthony Ryan[5], Kenneth R. Seddon[1], Janet E. Turp[2], Edmund H. Ward[3], and Jalal A. Zora[2]. (1) QUILL Research Centre, David Keir Building, Stranmillis Road, Belfast BT9 5AG, United Kingdom, Fax: +44 28 90661462, m.deetlefs@qub.ac.uk, (2) School of Chemistry and Molecular Sciences, University of Sussex, (3) Department of Chemistry, University of Mississippi, (4) School of Chemistry, Queen's University of Belfast, (5) Polymer Chemistry Group, ICI Chemicals and Polymer Group

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Ionic liquids have recently reached industrial fruition with BASF's BASIL (Biphasic Acid Scavenging utilising Ionic Liquids) process [1], and interest in these neoteric solvents as "green" alternatives to traditional solvents continues to grow at an astounding rate in a diversity of research fields [2 – 8]. However, within the variety of research interests, the main recent emphasis remains on organic and catalytic aspects, with limited attention being paid to their physical properties, and even less to inorganic chemistry in these solvents [9]. This is despite the fact that ionic liquids have proven to be excellent solvents for studying electrochemical and spectroscopic characteristics of a variety of inorganic compounds [10]. Therefore, to redress the balance, we have prepared and examined the spectroscopic and electrochemical properties of a range of pyridinium- and imidazolium-based ruthenium(IV), uranium(VI) and uranium(IV) halide salts. Single crystal diffraction studies of a number of these salts also provide evidence for the factors governing the structural assemblies of the salts. References [1]. Freemantle, M. Chem. Eng. News, March 31, 2003, 81, p9. [2]. Welton, T. Chem. Rev. 1999, 99, 2071-2083. [3]. Holbrey, J. D.; Seddon, K. R. Clean Prod. Proc. 1999, 1, 223-236. [4]. Wasserscheid, P.; Keim, W. Angew. Chem. Int. Ed. Engl. 2000, 39, 3772-3789. [5]. Sheldon, R. Chem. Commun. 2001, 2399-2407. [6]. Gordon, C. M. Appl. Catal. A. 2001, 222, 101-117. [7]. Zhao, D.; Wu, M.; Kou, Y.; Min, E. Catalysis Today. 2002, 2654, 1-33. [8]. Olivier-Bourbigou. H.; Magna, H. J. Mol. Catal. A. 2002, 164, 1-19 [9]. Seddon, K. R. Green Chem. 2002, 4, G25-G26. [10]. Hussey, C. L. Adv. Molten Salt Chem. 1983, 5, 185-230.

658035: Interactions of gases with ionic liquids: Experimental approach

IEC 0 [658035]: Interactions of gases with ionic liquids: Experimental approach

Margarida F. Costa Gomes, Pascale Husson, Johan Jacquemin, and Vladimir Majer, Laboratoire de Thermodynamique des Solutions et des Polymères, CNRS/Université Blaise Pascal, 24, avenue des Landais, 63177 Aubière, France, Fax: +33473407185, margarida.c.gomes@univ-bpclermont.fr

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The interactions between gaseous molecules and room temperature ionic liquids are investigated by studying their solubility as a function of temperature. Original experimental data were obtained for atmospheric gases (oxygen, nitrogen and carbon dioxide), a rare gas (argon) and a low molecular weight hydrocarbon (methane) in two commonly used ionic liquids (1-butyl-3-methylimidazolium tetrafluoroborate and 1-butyl-3-methylimidazolium hexafluorophosphate). The experimental technique used is based on an isochoric saturation method and involves the equilibration of known amounts of dry gas and degassed solvent. The quantity of dissolved gas is calculated from the measurement of the equilibrium pressure of the saturated solution at each

temperature. From the variation of the solubility with temperature, partial molar quantities of solvation such as free energy and enthalpy were derived, providing an insight on the molecular mechanisms involved in the dissolution process.

658042: Interactions of gases with ionic liquids: Molecular simulation

IEC 0 [658042]: Interactions of gases with ionic liquids: Molecular simulation

Agílio A. H. Pádua, and Johnny Deschamps, Laboratoire de Thermodynamique des Solutions et des Polymères, CNRS/Université Blaise Pascal, 24, avenue des Landais, 63177 Aubière, France, Fax: +33473407185, agilio.padua@univ-bpclermont.fr

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The interactions of different gaseous solutes with room temperature ionic liquids were studied by molecular simulation. The solutes considered were argon, oxygen, nitrogen, carbon dioxide and methane, interacting with 1-butyl-3-methylimidazolium tetrafluoroborate and with 1-butyl-3-methylimidazolium hexafluorophosphate. The gases were represented by Lennard-Jones plus charges multi-site models, and the ionic liquids were modeled using all-atom force fields including specific electrostatic and intramolecular terms describing the conformations of the cation. Henry's law constants were calculated via the chemical potential of the gases at infinite dilution, and compared with experimental results. This allowed an investigation of the significance of the different contributions present in the solute-solvent interactions (repulsive, electrostatic, dispersion) and of the role of structural properties of the solvents (distribution of cavities).

658059: Monte Carlo simulations of gas solubility in ionic liquids

IEC 0 [658059]: Monte Carlo simulations of gas solubility in ionic liquids

Jindal K. Shah[1], Jennifer L. Anthony[1], Timothy I. Morrow[2], Joan F. Brennecke[1], and Edward J. Maginn[1]. (1) Department of Chemical and Biomolecular Engineering, University of Notre Dame, B2 Fitzpatrick Hall of Engineering, Notre Dame, IN 46556, Fax: 574-631-8366, jshah@nd.edu, (2) Department of Chemical Engineering, University of Notre Dame

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry &*

Engineering and Separation Science & Technology subdivisions): General Contributions
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Ionic liquids (ILs) have been studied in great detail for their potential applications as reaction media. Many of these reactions are conducted with gases as one of the reactants. Subsequent extraction of reactants and products with supercritical carbon dioxide is a promising green technology as it minimizes cross contamination and prevents loss of solvent. The effectiveness of the entire process heavily depends on the solubility of gases in the IL. In this study, we assess the feasibility of predicting solubility of water, argon and carbon dioxide in the widely studied IL, 1-butyl-3-methlyimidazolium hexafluorophosphate [bmim][PF_6] with Monte Carlo simulations. We develop a molecular mechanics force field for the IL that enables accurate prediction of the thermophysical properties such as molar volumes as a function of temperature. We report the Henry's constants for water, carbon dioxide and argon. The simulation results for the absorption isotherms, heats and entropies of absorption are compared with experimental data.

658187: X-ray and Raman spectroscopic studies of the structure of [bmim]X, where X=Cl, BF4, PF6

IEC 0 [658187]: X-ray and Raman spectroscopic studies of the structure of [bmim]X, where X=Cl, BF4, PF6

Hiro-o Hamaguchi, Ryosuke Ozawa, Stoshi Hayashi, and Satyen Saha, Department of Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan, Fax: 3-3818-4621, hhama@chem.s.u-tokyo.ac.jp

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Structure of [bmim]X, where X=Cl, BF4, PF6, has been studied by x-ray diffraction and Raman spectroscopy. We found that [bmim]Cl shows crystal polymorphism, having two crystal forms, Crystal (1) and Crystal (2), characterized by distinct x-ray powder patterns and Raman spectra. Two sets of characteristic Raman bands of Crystals (1) and (2), which are mutually exclusive with each other, are observed simultaneously in the spectrum of liquid [bmim]Cl, suggesting that two distinct structures of the [bmim]+ ion, one corresponding to that in Crystal (1) and the other

to that in Crystal (2), coexist in the ionic liquid state. It is most likely that these two forms of the [bmim]+ ion are the "hydrogen-bonding" isomers. Raman spectra suggest that these two distinct structures are also coexisting in [bmim]BF4 and [bmim]PF6 in their ionic liquid states.

658237: Investigations on the stability and aggregate formation of an ionic liquid

IEC 0 [658237]: Investigations on the stability and aggregate formation of an ionic liquid

Sandra Dorbritz, Wolfgang Ruth, and Udo Kragl, Department of Chemistry, Rostock University, Albert-Einstein-Strasse 3a, 18059 Rostock, Germany, Fax: 0049-381-4986452, Sandra.Dorbritz@chemie.uni-rostock.de

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Last Modified: *2003-05-10*

Abstract

Elementary for an optimized reaction procedure in an ionic liquid is a fundamental knowledge on its stability and configuration. We have analyzed 1-Butyl-3-methyl-imidazolium-tetrafluoroborate using mass spectrometry and ion chromatography.

Dissolved ionic liquids do not exist as discrete ions. Depending on the solvent they form aggregates with different sizes. The aggregate sizes were identified by mass spectrometry. Thus, it can be said ionic liquids adapt to their environment. While larger aggregates with a small charge density are generated in less polar solvents, small aggregates with a higher charge density are built in polar solvents. The described observations can be supported by conductivity measurements.

The stability of $[BMIM][BF_4]$ can be investigated by the changing fluoride – and tetrafluoroborate – concentration with time using ion chromatography for analysis. In an aqueous solution at room temperature about one fourth of the ionic liquid decomposes within two weeks. Similar investigations were carried out in a non-diluted $[BMIM][BF_4]$ – melt and at higher temperatures.

658438: Bronsted acid-base ionic liquids as fuel cell electrolytes under non-humidifying conditions

IEC 0 [658438]: Bronsted acid-base ionic liquids as fuel cell electrolytes under

non-humidifying conditions

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry*
Invited: *Y*
Comments to Organizer: *Electrochemistry session of the symposium*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The realization that the constraints, associated with the use of water at temperatures higher than 100 oC, place a stumbling block on the widespread use of proton exchange membrane fuel cells, has resulted in an upsurge of interest in the option of ubiquitous ionic liquids. Here, we report that novel Bronsted acid-base ionic liquids, derived from a simple combination of a wide variety of organic amines with bis(trifluoromethanesulfonyl) amide (HTFSI), are proton conductors under an anhydrous condition. The proton conduction follows a combination of Grotthuss and vehicle mechanisms, depending on the composition of the ionic liquids. Some of the neutral salts as well as base rich compositions are electroactive for H2 oxidation and O2 reduction at a Pt electrode under non-humidifying conditions, which shows the prospect of the use of protic ionic liquids as new materials for anhydrous proton conductors at elevated temperatures.

658457: Ionic liquids and ion gels as new electrolytes for electrochemical systems

IEC 0 [658457]: Ionic liquids and ion gels as new electrolytes for electrochemical systems

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications: Polymers & Gels*
Invited: *Y*
Comments to Organizer: *The session of polymers and gels in this symposium*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
Ionic liquids are of great interest as new electrolyte materials. We have directed our attention to the combination of ionic liquids and polymers as new polymer electrolytes. In situ radical polymerization of common vinyl monomers in these ionic liquids affords compatible combinations of the ionic liquids and the resulting network polymers. Completely compatible combinations are new polymer electrolytes and named ion gels, which exhibit high ionic conductivities (typical room temperature conductivity: 10-2 Scm-1). The high conductivities are caused by self-dissociating and ion-transporting abilities of the ionic liquids and by the decoupling of the ion transport from polymer segmental motion. If specific properties such as lithium ion conduction are molecularly designed in the ionic liquids, the scope of the utility of ionic liquids and ion gels may greatly expand. In this talk, I shall present our research on the design of Li+-conducting and electron-transporting ionic liquids and ion gels.

658476: Use of ionic liquids in oil shale processing

IEC 0 [658476]: Use of ionic liquids in oil shale processing
Mihkel Koel, Institute of Chemistry, Tallinn Technical University, Akadeemia tee 15, Tallinn 12618, Estonia, vmihkel@chemnet.ee

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Fuels & Applications*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *overhead projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
The world's vast reserves of oil shale will play an important role in energy supply for the future, and conversion of solid fuels to chemicals feedstock and cleaner-burning liquid or gaseous fuels is becoming more desirable. Containing sufficient amount of organic matter, oil shale utilization to produce petroleum-like oils and gaseous products could be under certain conditions feasible. Liquid products could be as an alternative synthetic fuel source or even more valuable feedstock for chemical industry. Processing of oils and gaseous products is a place for utilization of ionic liquids either as solvents for extraction or reaction media with very good properties for catalyst solubilization. In this paper under the consideration are possibilities of extraction of shale oil with ionic liquids and problems of recycling of them.

658525: Control of the phase-boundary potential across the interface between room-temperature molten salt and water

IEC 0 [658525]: Control of the phase-boundary potential across the interface between room-temperature molten salt and water

Takashi Kakiuchi, Norihiro Tsujioka, and Fumiko Shigematsu, Department of Energy and Hydrocarbon Chemistry, Kyoto University, Yoshida Honmachi, Sakyoku, 606-8501 Kyoto, Japan, Fax: +81-75-753-3360, kakiuchi@scl.kyoto-u.ac.jp

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Room temperature molten salts, also called ionic liquids, that are immiscible or partially miscible with water can form either electrochemically polarizable or nonpolarizable interface with an aqueous electrolyte solution. The polarizability depends on the solubility of the molten salt in water. When there is a common ion between the two adjacent phases, the phase-boundary potential is determined by the Nernst equation for the distribution of the common ion in the two phases and the interface is nonpolarized. When the solubility of the salt in water is low, the interface maybe polarized externally by applying the potential across the interface.

658530: Eu(III) luminescence spectroscopy in 1-methyl-3-butylimidazolium bistriflimide

IEC 0 [658530]: Eu(III) luminescence spectroscopy in 1-methyl-3-butylimidazolium bistriflimide

Clotilde Gaillard[1], Isabelle Billard[1], Soufiane Mekki[1], Gilles Moutiers[2], Clarisse Mariet[2], Alexandre Labet[2], Peter Hesemann[3], and Jean-Claude Bünzli[4]. (1) Chimie Nucléaire, Institut de Recherches Subatomiques (IReS), B. P. 28, 67037 Strasbourg Cedex 2, France, Fax: 33388106431, clotilde.gaillard@ires.in2p3.fr, (2) INSTN, CEA, (3) Laboratoire de Chimie Organométallique, (4) laboratory of lanthanide supramolecular chemistry, Swiss federal Institute of Technology

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Invited: *Y*
Comments to Organizer: *no comments*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *LCD projector and labtop computer*
Conforms to Bylaw 6: *Y*

Last Modified: *2003-05-10*

Abstract

The spectroscopic characteristics (excitation, emission and lifetime) of Eu(III) dissolved in BumimTf2N has been studied. In a first series of experiments, the effect of the water absorption with time has been examined. It appears that non-degassed solutions are most probably inhomogeneous, displaying large water clusters that lead to an intense diffusion of the red light of a He:Ne laser. In these samples, the Eu emission spectrum is close to that observed in slightly acidic aqueous solutions. When the samples are degassed, by contrast, the solution appears homogeneous and water is to be considered as a competitive ligand for the first coordination sphere of Eu. In a second step, the complexation of Eu(III) with tetrabutylammonium chloride (TBACl) dissolved in BumimTf2N has been studied. The presence of an antenna effect gives insight onto the Eu coordination sphere and possible structures will be discussed.

658557: Catalysis in ionic liquids: towards the detection of reactive intermediates

IEC 0 [658557]: Catalysis in ionic liquids: towards the detection of reactive intermediates

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Last Modified: *2003-05-10*

Abstract

There are countless examples of catalytic reactions that are run in a matching ionic liquid. These media often provide a substantial enhancement in reactivity and selectivity as compared to conventional solvents. What is the reason for this behavior? What are the properties of ionic liquid solvent systems that promote catalytic activity? How should an “ideal” ionic liquid be designed? Or is there something like an overlooked unique “ionic liquid effect”? In combination with conventional screening experiments (directed towards anion and cation effects), we are establishing a set of in situ spectroscopic methods that will allow mechanistic investigations in situ in ionic liquid systems. To that end, we are combining the in situ spectrometer ReactIR with a purpose-built high-pressure autoclave (e.g. for monitoring hydrogenation reactions). Additionally, we are reporting our first experiences with a specialized NMR probe for in situ NMR spectroscopy in ionic liquids.

658775: New, Functionalized Ionic liquids from Michael-type Reactions - a Chance for Combinatorial Ionic Liquid Development

IEC 0 [658775]: New, Functionalized Ionic liquids from Michael-type Reactions - a Chance for Combinatorial Ionic Liquid Development

Peter Wasserscheid[1], Birgit Drießen-Hölscher[2], Roy van Hal[1], and Christian Steffens[1]. (1) ITMC, Universität Aachen, Worringer Weg 1, Aachen D-52074, Germany, Fax: +49 241 8022177, wasserscheid@itmc.rwth-aachen.de, (2) Technische Chemie und Kunststoffe, Universität Paderborn

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis*
Invited: *Y*
Comments to Organizer: *This paper should show up in the organic synthesis session since it describes a new synthetic methodology for the synthesis of functionalized ILs*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Ionic liquids with functionalized alkyl groups at the cation have only described in a few papers up to now. So far, the synthesis of these materials has been rather complicated and multi-step procedures were used. These included the synthesis of a functionalized alkylating agent followed by the alkylation of the amine, some further modification of the obtained salt to obtain the desired functional group and finally - in most cases - an anion exchange reaction. In our contribution, we describe for the first time an alternative and far more efficient method to synthesise functionalised ionic liquids in a simple, straight-forward, two-step synthesis. Our approach includes a protonation step of an amine or phosphine followed by conversion with a Michael-acceptor in presence of a suitable base. It is important to note that the overall reaction sequence proceeds with perfect atom effiency since no by-product is formed. Furthermore no ion-exchange, extraction or filtration step is necessary. This allows for the first time the rapid synthesis of libraries of functionalized ionic liquids in a combinatorial fashion.

659185: Ionic liquids as green solvents: Engineering new bio-based materials

IEC 0 [659185]: Ionic liquids as green solvents: Engineering new bio-based materials

Richard P. Swatloski, John D. Holbrey, Scott K. Spear, and Robin D. Rogers, Department of Chemistry and Center for Green Manufacturing, The University of Alabama, Tuscaloosa, AL 35487, Fax: 205-348-0823, tubarick@aol.com

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry &*

Engineering and Separation Science & Technology subdivisions): Novel Applications
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
The ideas and concepts of green chemistry were established in order to facilitate the development and implementation of innovative sustainable non-polluting chemical technologies in an economically feasible manor. Not only is it important to lower process emissions, it is also imperative that a shift be made to the development of sustainable resources to complement, or replace diminishing petroleum-based feed-stocks. We have recently utilized 1-butyl-3-methylimidazolium chloride for the dissolution of nature's most abundant renewable resources--cellulose. Because ionic liquids can dissolve a wide range of materials, it can be anticipated that they will offer a route for incorporation of many functional molecules for sensing, recognition, or molecular binding into modified cellulose materials that have not been accessible in other traditional cellulose solvent systems. In this presentation we will examine the physical properties of these new materials, as well as their possible application.

659696: Coordination chemistry and electrochemical behavior of actinide and transition metal complexes in room temperature ionic liquids

IEC 0 [659696]: Coordination chemistry and electrochemical behavior of actinide and transition metal complexes in room temperature ionic liquids

Warren J. Oldham[1], D. Bridget Williams[2], Michael E. Stoll[2], Brian L. Scott[3], and David A. Costa[2]. (1) Chemistry Division (C-INC), Los Alamos National Laboratory, Mail Stop J-514, Los Alamos, NM 87545, woldham@lanl.gov, (2) Nuclear Materials Technology (NMT-15), Los Alamos National Laboratory, (3) Chemistry Division (C-SIC), Los Alamos National Laboratory

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations*
Invited: *Y*
Comments to Organizer: *This paper is submitted in the chemical separations section of the RTIL symposium. I was contacted by Bill Tumas to give this talk.*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
Room temperature ionic liquids are interesting solvents to consider in the development of advanced actinide purification and processing schemes. Because a detailed understanding of the coordination chemistry and electrochemical behavior of actinide and transition metal complexes

is a necessary foundation on which to develop novel separations technology, we have recently initiated a comprehensive program to study these issues. This presentation will outline a series of structural, spectroscopic, and electrochemical studies undertaken to obtain detailed characterization of the primary coordination sphere of electrophilic metal ions dissolved in $^{-}N(SO_2CF_3)_2$ based ionic liquids. We demonstrate that the $^{-}N(SO_2CF_3)_2$ anion can behave as a competent ligand, coordinating to metal ions through direct metal–nitrogen or metal–oxygen bonds. The consequences of $^{-}N(SO_2CF_3)_2$ coordination on the properties and electrochemical behavior of metal species in these novel chemical environments is highlighted.

659730: Highly Enantioselective Asymmetric Catalysis in Ionic Liquids

IEC 0 [659730]: Highly Enantioselective Asymmetric Catalysis in Ionic Liquids

Wenbin Lin[1], Helen L Ngo[2], and Aiguo Hu[2]. (1) Department of Chemistry, CB#3290, University of North Carolina, Chapel Hill, NC 27599, Fax: 9199622388, wlin@unc.edu, (2) Department of Chemistry, University of North Carolina

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Room temperature ionic liquids (RTILs) have recently received a great deal of attention as alternative reaction media. RTILs are non-volatile, and thermally and oxidatively stable, and typically immiscible with both water and nonpolar solvents. They contain poorly coordinating ions and thus will not interfere with most catalytic processes. RTILs are also easy to prepare and modify to impart desirable polarity and solubility characteristics. These features make RTILs ideal solvents for the synthesis of high-value chiral organic compounds via catalytic processes. We have investigated asymmetric hydrogenation of a variety of unsaturated substrates using custom-designed polar derivatives of Ru-BINAP and Rh-BINAP catalysts. Extremely high enantioselectivity was observed for all the reactions examined, and more importantly, these polar derivatives of Ru-BINAP and Rh-BINAP catalysts have been effectively immobilized in the RTIL phase and were reused several times without the loss of catalytic activity and enantioselectivity. RTIL thus represents an ideal media for the immobilization of expensive asymmetric catalysts that also prevents the leaching of toxic group 8 metals into the organic products, and should be highly desirable for the production of pharmaceutical intermediates that are free from metal contaminants.

659826: Electrochemical polymerisation of polypyrrole in ionic liquids

IEC 0 [659826]: Electrochemical polymerisation of polypyrrole in ionic liquids

Jennifer M. Pringle[1], John Efthimiadis[2], Patrick Howlett[1], Gordon G. Wallace[3], Jim Efthimiadis[2], Douglas R. MacFarlane[1], and Maria Forsyth[2]. (1) School of Chemistry, Monash University, Wellington Road, Clayton, Melbourne, Victoria 3800, Australia, Fax: 613 9905 4597, j.pringle@sci.monash.edu.au, (2) School of Physics and Materials Engineering, Monash University, (3) Intelligent Polymer Research Institute, University of Wollongong

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Inherently conducting polymers (ICPs), such as polypyrrole, are used in a wide range of applications, including chemical and biological sensors, mechanical actuators, LEDs and advanced battery systems. Electrochemical polymerisation and cycling of ICPs is traditionally performed in an electrolyte/molecular solvent system, and the processing parameters, such as the chemical nature of the solvent and electrolyte, can have a marked influence on the properties of the resultant polymer film. We report the use of ionic liquids as both a growth medium and as an electrolyte for the electrochemical cycling of ICP films. Use of the ionic liquid as the growth medium results in significantly altered film morphologies and greatly improved electrical and mechanical properties.

659957: New catalysts for hydroamination reactions - transition metal complexes in supported ionic liquids

IEC 0 [659957]: New catalysts for hydroamination reactions - transition metal complexes in supported ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *Y*
Special Equipment Needs: *beamer*

Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

A concept for the immobilization of homogeneous catalysts in ionic liquids (IL), here 1-ethyl-3-methyl-imidazolium trifluoromethanesulfonate, and their use as stationary phase in fixed bed reactors is presented. Based on this concept a new catalyst system for the direct addition of amines to alkynes and dienes (hydroamination) was developed. The addition of aliphatic and aromatic amines to phenyl-acetylene and 1,3-cyclohexadiene were explored in detail. Lewis acidic metal complexes, such as Zn(CF3SO3)2 and [(C6H5Me)(CuCF3SO3)2] were employed as catalytically active species. It is particularly noteworthy that the intrinsic catalytic activity of the supported metal complexes was much higher than of the corresponding homogeneous catalysts. Explanations for this observation are (i) the stabilization of a polar transition state in the presence of the IL and (ii) favorable partitioning coefficients of products and reactants in the solvent pair heptane/IL.

659975: Structural investigation of $[C_n mim]_2[\{(UO_2)(NO_3)_2\}_2(\mu_4\text{-}C_2O_4)]$ and $[C_n mim][(UO_2)(NO_3)_3]$ complexes

IEC 0 [659975]: Structural investigation of $[C_n mim]_2[\{(UO_2)(NO_3)_2\}_2(\mu_4\text{-}C_2O_4)]$ and $[C_n mim][(UO_2)(NO_3)_3]$ complexes

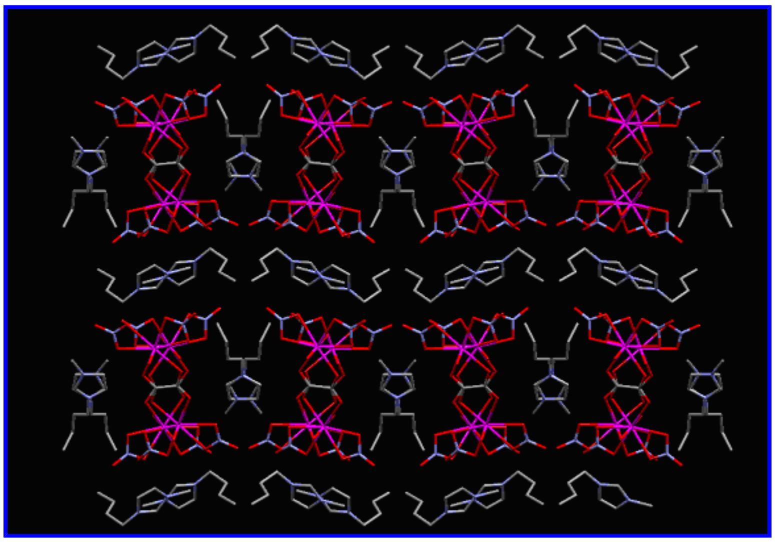
M. Nieuwenhuyzen[1], A. E. Bradley[2], C Hardacre[1], William R. Pitner[3], R. C. Thied[4], Kenneth R. Seddon[3], and David Sanders[5]. (1) School of Chemistry, The Queen's University of Belfast, David Keir Building, Stranmillis Road, BT9 5AG Belfast, United Kingdom, woody.m@qub.ac.uk, (2) School of Chemistry, Queen's University Belfast, (3) QUILL Research Centre, The Queen's University of Belfast, (4) Research and Technology, British Nuclear Fuels (BNFL), (5) School of Chemistry, Queens University Belfast

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

In this paper we describe the EXAFS investigation of the structure of 1-butyl-3-methylimidazolium μ_4-(O,O,O',O'-ethane-1,2-dioato)-bis[bis(nitrato-O,O)dioxouranate(VI) both as a solid and dissolved in $[C_4mim][NO_3]$ media. EXAFS has become an increasingly important technique for the identification of both the oxidation state and coordination sphere of uranium

species both in solid state compounds and in solution. The coordination chemistry of uranium in aqueous solutions has been extensively studied by EXAFS due to its importance both for the nuclear fuel recycling and waste clean up industries. The properties of the dimeric 1-butyl-3-methylimidazolium μ_4-(O,O,O',O'-ethane-1,2-dioato)-bis[bis(nitrato-O,O)dioxouranate(VI)] compound have been investigated using single crystal x-ray crystallography and EXAFS. EXAFS spectroscopy of the complex in solid state and solution were in good agreement with the single crystal structure determined by x-ray crystallography (1). In addition we describe the effects of changes to the length of the 1-alkyl group on the composition and structure of the dioxouranium(VI) complexes formed.



660048: Force field development and liquid state simulations on ionic liquids

IEC 0 [660048]: Force field development and liquid state simulations on ionic liquids

Hubert Stassen[1], Elvis S. Böes[1], and Jones de Andrade[2]. (1) Instituto de Química/Grupo de Química Teórica, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves, 9500, 91540-000 Porto Alegre - RS, Brazil, Fax: +55-51-33167304, gullit@iq.ufrgs.br, (2) School of Mathematics & Physics/Atomistic Simulation Group, Queens University Belfast

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Comments to Organizer: *I have received the invitation to present as a key speaker our recent results.*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *standard equipment*
Conforms to Bylaw 6: *Y*

Last Modified: 2003-05-10

Abstract

Performing quantum mechanical computations and molecular mechanics calculations, an all-atom force field compatible with the AMBER methodology has been developed for ionic liquids containing 1,3-dialkylimidazolium cations. The force field was employed in extensive molecular dynamics simulations on the condensed phase of several ionic liquids. The influence of the alkyl chain length and the anion size on equilibrium properties has been investigated. We present results for the densities, internal energies, and structural features in terms of radial and angular distribution functions for several ionic liquids based on the 1,3-dialkylimidazolium cation. In addition, the diffusion coefficients and electric conductivities were computed for these ionic liquids. The good agreement between the computed data and experimental findings demonstrates that the obtained force field is able to represent the liquid phase of the considered ionic liquids.

660148: Photolytic destruction of organic compounds in room temperature ionic liquids

IEC 0 [660148]: Photolytic destruction of organic compounds in room temperature ionic liquids

Qiaolin Yang, and **Dionysios D. Dionysiou**, Department of Civil and Environmental Engineering, University of Cincinnati, 765 Baldwin Hall, B.O. Box 0071, Cincinnati, OH 45221-0071, Fax: 513-556-2599, yangql@email.uc.edu, dionysios.d.dionysiou@uc.edu

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Photodegradation of organic compounds in room temperature ionic liquids (RTILs) using UV radiation and the feasibility of recycling the ionic liquids are investigated. Two RTILs, 1-butyl-3-methylimidazolium hexafluorophosphate and 1-ethyl-3-methylimidazolium bis (perfluoroethylsulfonyl)imide are studied as solvent media in the UV photolytic process. Chlorophenols and polycyclic aromatic hydrocarbons in the ionic liquids are degraded by 253.7 nm UV radiation. The ionic liquids in their pure form do not significantly absorb photons of the incident light and exhibit resistance for degradation under the experimental conditions applied in this study. Therefore, the destruction of the compounds results in the simultaneous regeneration of the ionic liquids. This technique can be further developed into a two-step process for the extraction and in-situ photodegradation of organic compounds from soils, sediments or other media using RTILs. This approach can also be utilized for the purification of ionic liquids contaminated by organic compounds in chemical and electrochemical applications.

660359: Development of Ionic Liquids containing environmentally acceptable and sustainable components

IEC 0 [660359]: Development of Ionic Liquids containing environmentally acceptable and sustainable components

John D. Holbrey, W. Matthew Reichert, Megan B. Turner, Keith Green, and Robin D. Rogers, Department of Chemistry and Center for Green Manufacturing, The University of Alabama, Tuscaloosa, AL 35487

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *Y*
Preferred Presentation Format: *Poster*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
There are issues with end-of-life disposal and environmental impact of some ionic liquid (IL) components, particularly perfluorinated anions. Although a solvent does not have to be green to be part of a green process, there is an understandable desire to develop green processes that utilize green components. We are actively investigating approaches to the synthesis of ILs with the aims of achieving atom efficiency, elimination of undesirable metathesis steps, and incorporation of application-enhancing functionality in the ionic liquid core. One area of particular interest is in reducing the requirement for anions that are environmentally hazardous, or for which, there are significant disposal issues. The potential to prepare new ionic liquids using range of pharmaceutically acceptable anions and the utilization of clean syntheses of imidazolium-based ionic liquids will be presented.

660451: Application of novel oxime-deriviatized task-specific ionic liquid for the solvent extraction of copper

IEC 0 [660451]: Application of novel oxime-deriviatized task-specific ionic liquid for the solvent extraction of copper

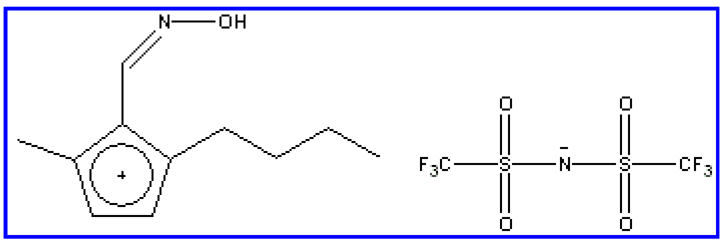
Peter M Smith, and Katie A Krone, Chemistry Department, Westminster College, S. Market St., New Wilmington, PA 16172, Fax: 724-946-7158, smithpm@westminster.edu

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations*
Invited: *N*
Preferred Presentation Format: *Oral*

Consider for Sci-Mix: *Y*
Special Equipment Needs: *projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The task-specific ionic liquid (TSIL) 1-butyl-2-hydroxyiminomethyl-3-methylimidizaolium bis (trifluoromethylsulfonyl)imide, [1-C_4-2-oxime-3-mim][Tf_2N], has been synthesized. This TSIL can be used as a ligand for transition metal ions. Specifically, this TSIL is used as an extractant, with [C_4mim][Tf_2N] as the diluent, for the solvent extraction of Cu^{2+} ions from an aqueous phase into the water-immiscible room-temperature ionic liquid phase. The distribution ratio of the Cu^{2+} ion is measured at various TSIL concentrations, pH values, and Cu^{2+} ion concentrations. The distribution ratios are compared to standard industrial methods for the solvent extraction of copper.



660457: Metal ion transfer into room-temperature Ionic Liquids: The role of anionic complexes

IEC 0 [660457]: Metal ion transfer into room-temperature Ionic Liquids: The role of anionic complexes

Mark Jensen, Jörg Neuefeind, James V. Beitz, S. Skanthakumar, and Lynne Soderholm, Chemistry Division, Argonne National Laboratory, 9700 S. Cass Avenue, bldg 200, Argonne, IL 60439, Fax: 630-252-7501, mjensen@anl.gov

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Invited: *Y*
Comments to Organizer: *please check whether this has been previously submitted as abstract #657827*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The structure and stoichiometry of the lanthanide(III) (Ln) complexes with the ligand 2-thenoyltrifluoroacetone (Htta) formed in a biphasic aqueous-room-temperature ionic liquid system have been studied by equilibrium thermodynamics, optical absorption and luminescence spectroscopies, high-energy X-ray scattering, EXAFS, and molecular dynamics simulations. The results show that anionic $Ln(tta)_4^-$ complexes form in $[C_4mim][Tf_2N]$ phases under conditions that favor the formation of weak, cationic Ln-tta complexes in the aqueous phase or the formation of neutral $Ln(tta)_3$ complexes in molecular organic solvents. The net metal-ion extraction equilibrium can be considered an anion exchange reaction where the partitioning of the $Ln(tta)_4^-$ anion into $[C_4mim][Tf_2N]$ is driven by displacement of the $[Tf_2N]^-$ anion into the aqueous phase. Work supported by the Office of Basic Energy Science, U.S. Department of Energy under contract number W-31-109-ENG-38

660485: Electronic spectroscopy of rhenium dioxo complexes within ionic liquids

IEC 0 [660485]: Electronic spectroscopy of rhenium dioxo complexes within ionic liquids

Ryan E. Da Re[1], Sheila N. Baker[1], Gary A. Baker[2], David E. Morris[1], and David A. Costa[3]. (1) Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM 87545, ryandare@lanl.gov, (2) Bioscience Division, Michelson Resource, Los Alamos National Laboratory, (3) Nuclear Materials Technology (NMT-15), Los Alamos National Laboratory

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy*
Invited: *Y*
Comments to Organizer: *Invited for the SPECTROSCOPY session of the Ionic Liquid Symposium (Siddharth Pandey presiding over this session).*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Relatively few studies have appeared dealing specifically with transition-metal complexes in room temperature ionic liquids. In view of the dearth of studies of this type, current interest in our group lies in probing the influence of ionic liquid media on the ligand-field and charge-transfer excited states of several transition-metal complexes using electronic spectroscopy. Recent results from our spectroscopic investigation into the electronic structures of rhenium dioxo complexes in ionic liquids will be reported.

660526: Nanocomposite design & biomimetic approaches using ionic liquids

IEC 0 [660526]: Nanocomposite design & biomimetic approaches using ionic liquids

Sheila N. Baker[1], Gary A. Baker[2], Ryan E. Da Re[1], and T. Mark McCleskey[1]. (1) Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM 87545, sbaker@lanl.gov, (2) Bioscience Division, Michelson Resource, Los Alamos National Laboratory

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy*
Invited: *Y*
Comments to Organizer: *invited for the "SPECTROSCOPY" session of the Ionic Liquid Symposium (Siddharth Pandey presiding)*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
Growing interest in ionic liquids arises from the fact that they increasingly show improved performance in niche areas relative to conventional solvents. Although ionic liquids posses a range of unique properties suitable for incorporation into advanced materials, efforts to date have flagged relative to their use as solvents for extraction and synthesis. In this contribution, we offer current results from our group in the design of functional materials using ionic liquids and suggest further avenues for consideration.

660587: Photovoltaic applications of ionic liquids

IEC 0 [660587]: Photovoltaic applications of ionic liquids

Shaik M Zakeeruddin, Department of Chemistry, Swiss Federal Institute of Technology, Laboratory for Photonics and Interfaces, Ecublens, Lausanne, Switzerland, Fax: +41 21 693 4111, shaik.zakeer@epfl.ch

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
The development of clean and sustainable energy resources is a worldwide quest. During the last decade dye-sensitized solar cells (DSC) have attracted much attention as low-cost alternatives to conventional inorganic photovoltaic devices. One of the key factors that limit practical

applications of flexible DSC is the organic electrolyte usage. The reason for this is that the organic solvent reacts or evaporating through the plastic based current collector. A viable solution to this drawback is replacement of organic solvent electrolytes by ionic liquid electrolytes, whose vapor pressure is negligible. Ionic liquids with good chemical, thermal stability and wide electrochemical window have been recently pursued as alternative electrolytes for DSC. This lecture will summarize the most recent developments in the use of ionic liquid electrolytes for DSC in competing with conventional organic liquid electrolytes. These ionic liquid electrolytes should foster widespread application of flexible DSC.

660589: Predicting infinite dilution activity coefficients of organic solutes in ionic liquids using quantitative structure-property relationships

IEC 0 [660589]: Predicting infinite dilution activity coefficients of organic solutes in ionic liquids using quantitative structure-property relationships

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Fuels & Applications*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
Ionic liquids have shown great potential as reactions and separations media. Such applications require knowledge of how solutes interact with ionic liquids. Infinite dilution activity coefficients provide this sort of information; however, these data have been gathered for only a few solutes in even fewer ionic liquids. To expand the usefulness of ionic liquids, methods are needed which allow predictions to be made based on existing data. We describe how the Quantitative Structure-Property Relationship (QSPR) method can be used to relate thermodynamic properties of ionic liquids to their chemical structures. Specifically, details of how infinite dilution activity coefficients can be correlated and predicted from chemical structure are discussed. In addition, the structural and chemical features that most influence infinite dilution activity coefficients will be considered with respect to the underlying mechanisms that relate structure to properties.

660612: Short-time local dynamics of ionic liquids: Neutron scattering and Molecular Dynamics simulations

IEC 0 [660612]: Short-time local dynamics of ionic liquids: Neutron scattering and Molecular Dynamics simulations

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
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Abstract

Ionic liquids (ILs) show great promise as potential green solvents for industrial processes. While there have been a few computational studies and numerous experimental studies of the thermophysical properties of ILs, little is known about the short-time dynamics of the ions and how the local motion of the cations and anions is affected by their molecular structure. We present the results of a study of the hydrogen dynamics in imidazolium-based ILs, and examine the effect of cation structure and temperature on the short-time, local motion of the H-atoms. We present the van Hove correlation function, *G(r,t)*, and intermediate incoherent scattering function, *I(q,t)* over a 100 picosecond time range as computed from molecular dynamics simulations in the microcanonical ensemble. The predicted *I(q,t)* curve for [bmim][PF_6] agrees very well with the experimental curve over the 30-70 ps time range.

660972: Biphasic hydroformylation catalysis in ionic liquid media

IEC 0 [660972]: Biphasic hydroformylation catalysis in ionic liquid media

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Fuels & Applications*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
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Abstract

The separation of homogeneous hydroformylation catalysts from reaction mixtures has been a

big challenge and continues to be the focus of intense research. Over the last three decades, several elegant approaches have been explored to overcome this limitation, for example, aqueous and fluorous biphase catalysis, reactions in supercritical media, and catalyst immobilization onto solid support materials. More recently, ionic liquids have been used as alternative reaction media for homogeneous catalysis. Based on their highly charged nature, ionic liquids are well suited for biphasic reactions with organic substrates. While the first hydroformylation reaction in an ionic liquid was performed by Parshall as earlier as 1972, Chauvin et. al. used for the first time water-soluble phosphine ligands like tri(m-sulfonyl)triphenyl phosphine trisodium salt (tppts) to retain active rhodium complexes in ionic liquid phases and used them successfully in biphasic hydroformylation catalysis. Since then, a variety of different metal complexes have been investigated for biphasic hydroformylation reactions in ionic liquid media. As the production of aldehyde is one of the largest volume processes in the chemical industry we have investigated the potential of ionic liquids for hydroformylation reactions. Here, we report our findings of the biphasic hydroformylation catalysis using conventional rhodium catalysts in ionic liquid media. Following the initial report by Chauvin et. al. we have studied the reactivity of HRh(CO)(P)3 (P=phosphine ligand) hydroformylation catalysts in 1-butyl-3-methyl-imidazolium ionic liquid derivatives of tetrafluoroborate and hexafluorophosphate. In addition, we have complimented our investigation with a high-pressure NMR study of the reaction mixture containing the active rhodium species in ionic liquids.

661044: Synthesis, characterization, and applications of new hydroxyl-appended ionic liquids

IEC 0 [661044]: Synthesis, characterization, and applications of new hydroxyl-appended ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*
Preferred Presentation Format: *Poster*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
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Abstract

New ionic liquids containing 2-hydroxypropyl-functionalized imidazolium cations have been synthesized by the atom-efficient reaction of 1-methylimidazole with propylene oxide and an acid, which provides the anion for the resulting ionic liquid. Introduction of the hydroxyl-group causes significant rheological changes in the properties of the ionic liquids through the introduction of both hydrogen-bond donor and acceptor positions. These new ionic liquids have been fully characterized and have been investigated as solvents for a range of biocatalytic

reactions, where the incorporation of hydroxyl-groups may be of use in stabilizing enzymatic catalysts in these non-aqueous environments.

661056: Molecular modeling of the thermodynamic and transport properties of ionic liquids

IEC 0 [661056]: Molecular modeling of the thermodynamic and transport properties of ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *LCD projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Ironically, one of the great difficulties associated with the development of ionic liquids for industrial applications stems from one of the strengths of this class of fluids: the fact that a huge number of different compounds can be made to function as ionic liquids. The search for new ionic liquids with desirable properties can be enhanced through an understanding of the way in which physical properties are related to chemical constitution and structure. We describe our efforts at making this link through use of molecular-based modeling efforts. Using techniques of varying sophistication, including first principles quantum calculations of gas phase ions, classical molecular dynamics and Monte Carlo simulations of the condensed phase, and empirical quantitative structure-property relations, we show how thermodynamic and transport properties of a range of different ionic liquids can be accurately calculated.

Pure component properties such as density, isothermal compressibility, volume expansivity, melting point, local structure and dynamics and self-diffusivity are computed and compared against experiment. Mixture properties, such as gas absorption isotherms and activity coefficients are also computed for a range of different solutes and ionic liquids, and shown to agree quantitatively with experiment. The applicability of these methods for computing other properties, as well as their limitations, is also discussed.

661065: Cellulose films regenerated from ILs and their role as scaffolding for enzyme attachment via glutaraldehyde

IEC 0 [661065]: Cellulose films regenerated from ILs and their role as scaffolding for enzyme attachment via glutaraldehyde

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Poster*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
Immobilization of enzymes in a wide range of matrices has been widely studied. Immobilization can increase enzyme stability and thus activity, and also enable simple recovery and recycling of catalysts. Here we describe the investigation of cellulose films containing encapsulated laccase, from Rhus vernificera, prepared by dissolution and casting from 1-butyl-3-methylimidazole chloride ionic liquid solution. Laccase can be successfully immobilized in cellulose films prepared in this way, while maintaining enzymatic activity, and the activity can be controlled by pretreatment and processing methodologies. A comparison between the methods of film preparation, as well as their respective activies will be presented.

661277: Refractive Indices of Ionic Liquids

IEC 0 [661277]: Refractive Indices of Ionic Liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *Overhead projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
All nontoxic substances that are both liquid at room temperature and transparent in visible light

have refractive indices less than 1.82. Higher refractive index liquids that are nontoxic would find many uses in optical applications. In addition, precise measurements of refractive index could be a useful tool in identifying ionic liquids. For these reasons we have measured the refractive indices of a series of carefully designed ionic liquids. We report on trends seen as we vary both cation and anion, and on future prospects for high index ionic liquids.

661283: Enhanced Ion Dissociation in Polyelectrolyte Gel Electrolytes

IEC 0 [661283]: Enhanced Ion Dissociation in Polyelectrolyte Gel Electrolytes

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications: Polymers & Gels*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Single ion conduction is an important feature required in some electrolyte applications, including the lithium and lithium ion cells. One approach to single ion conduction is to use a polyelectrolyte material in which one of the ions is tethered to the polymer backbone and the counter ion is free in principle to dissociate. Traditional polyelectrolytes in solvents of interest tend not to fully dissociate and hence their conductivities are limited. By copolymerising the charged monomer with a compatible neutral monomer some of this dissociation problem can be overcome. In this work we have applied two approaches to further improve the dissociation and conductivity of poly(lithium 2-acrylamido-2-methyl-1-propanesulfonic acid-co-dimethyl acrylamide). In one case the addition of up top 10% TiO2 nanoparticles was found to enhance Li ion transport properties. In the other, the use of ionic liquids and zwitterionic materials has been found to produce a substantial increase in conductivity.

661375: New task-specific ionic liquids (TSIL) in separations of petrochemical relevance

IEC 0 [661375]: New task-specific ionic liquids (TSIL) in separations of petrochemical relevance

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Fuels & Applications*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Separations (gas-gas, liquid-gas and liquid-liquid) are vital elements of petrochemical processing. Many of these separation types involve the use of volatile organic solvents (e.g., amines, amides, sulfoxides), and the vapor pressures and substrate miscibility properties of these solvents play a major role in the breadth of utility of any particular separation in which they are used. In the present paper we will discuss the synthesis of several new ionic liquids with appended functional groups and their potential utility as replacements for VOCs in certain types of petrochemically relevant separations.

661403: New applications of ionic liquids: Task-specific ionic liquids (TSIL) as alternatives to functionalized resins as scavengers for solution phase synthesis

IEC 0 [661403]: New applications of ionic liquids: Task-specific ionic liquids (TSIL) as alternatives to functionalized resins as scavengers for solution phase synthesis

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*
Preferred Presentation Format: *Poster*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Modern solution phase syntheses, especially those using combinatorial approaches, often involve the use of excess reactants in order to maximize the conversion of valuable substrates. Doing so creates a new difficulty, namely separation of the modified substrate from unused excess reagent. Current approaches to this separation dilemma stress the use of functionalized scavenger resins

to remove the reagent. These resins tend to be expensive and can require the use of relatively large volumes of solvent to mechanically swell the resin to facilitate access to functional sites. We report here on some early successes in using functionalized ionic liquids to accomplish similar separations, and several advantages of using ILs to do so.

661420: Thioether, sulfoxide and sulfone-incorporating task-specific ionic liquids

IEC 0 [661420]: Thioether, sulfoxide and sulfone-incorporating task-specific ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
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Preferred Presentation Format: *PosterOnly*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

We report on the synthesis, characterization and properties of several new ionic liquids that incorporate thioether, sulfoxide or sulfone functional groups. Several of these syntheses involve the interconversion of an existing ionic liquid into a new one containing a different functional group.

661425: New applications of ionic liquids: Preparation of functionalized resins by ion exchange with task-specific ionic liquids

IEC 0 [661425]: New applications of ionic liquids: Preparation of functionalized resins by ion exchange with task-specific ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*
Preferred Presentation Format: *PosterOnly*
Consider for Sci-Mix: *Y*

Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Over the past five years, we have prepared a large number of functionalized ions for use in formulating functionalized or "task-specific" ionic liquids. In this paper, we report on the use of these salts in conjunction with conventional ion-exchange resins to form functionalized resins in which the resin functionality originates in the coulombically-tethered functional ion.

661437: Enthalpy change determinination of BMIC using DTA

IEC 0 [661437]: Enthalpy change determinination of BMIC using DTA

Mingming Zhang, Venkateswarulu Kamavaram, and Ramana G. Reddy, Department of Metallurgical and Materials Engineering, The University of Alabama, P.O. Box 870202, Tuscaloosa, AL 35487, zhang028@bama.ua.edu

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *overhead projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The enthalpy change of 1-butyl-3-methylimidazolium chloride (BMIC) was quantitatively determined using TG/DTA equipment. A new method of baseline determination was used to precisely detect the overall enthalpy change of BMIC over certain temperature range. The enthalpy of melting and vaporizing were determined to be 5.71 KJ/mol and 44.05 KJ/mol. The measured results were compared with those determined by DSC and other methods to ensure the accuracy. Based on measured enthalpy values, the entropy and Gibbs energy change of BMIC were then calculated within the temperature range from 25 to 180 Celsius degree.

661506: New synthetic routes, scale-up and technical applications of the ECOENG^{TM}-family

IEC 0 [661506]: New synthetic routes, scale-up and technical applications of the ECOENG^{TM}-family

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Halogen-free Ionic Liquids have recently gained significant interest in academic and industrial research alike. So far the synthesis of some compounds was restricted by complicated anion-exchange reactions and sophisticated purification procedures were necessary in order to obtain the desired quality. In our contribution we present a new, far more efficient and sustainable synthetic approach to ECOENG(TM)-Ionic-Liquids. It combines an alkylation step with a chemical transformation of the obtained anion that opens the door to a wide variety of new halogen-free Ionic Liquids. By this approach, customized synthesis of task-specific examples is possible. Remarkably, the new approach is free of halogen-containing reactants and water and thereby the achievable quality is always high. In our presentation the new synthesis will be described in detail. Furthermore the scale-up-options and some potential technical applications will be presented.

661554: Supported ionic liquid phase (SILP) catalysis - heterogenization of homogeneous catalysts

IEC 0 [661554]: Supported ionic liquid phase (SILP) catalysis - heterogenization of homogeneous catalysts

Anders Riisager[1], Rasmus Fehrmann[1], Roy van Hal[2], and Peter Wasserscheid[2]. (1) Department of Chemistry and ICAT, Technical University of Denmark, Building 207, Lyngby DK-2800, Denmark, ar@kemi.dtu.dk, (2) Institut für Technische Chemie und Makromolekulare Chemie, RWTH Aachen

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
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Abstract

Ionic liquids have attracted significant academic interest as reaction medium for two-phase homogeneous catalysis of organic substrates, e.g. olefin hydroformylation. In contrast, a strong preference of using heterogeneous catalyst systems predominate in chemical industry due to the ease of separation and the possibility to use fixed-bed reactors leading to advantageous process design, e.g. continuous operation mode, avoidance of large amount of solvent, applicability to gas-phase reactions. Nevertheless, only very recently heterogenized homogeneous catalyst systems comprised of neutral, weakly-coordinating ionic liquids containing active transition metal catalysts on the surface of a porous high-area support, i.e. supported ionic liquid phase (SILP) catalysts, have been examined. In this work the concept of supported ionic liquid phase (SILP) catalysis will be addressed and results obtained from catalytic applications using SILP catalysts will be presented, e.g. olefin hydroformylation.

661792: Adiponitrile synthesis in room temperature ionic liquids

IEC 0 [661792]: Adiponitrile synthesis in room temperature ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Fuels & Applications*
Invited: *N*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *Y*
Last Modified: *2003-05-10*

Abstract

Adiponitrile is a key intermediate for nylon 6-6 and nylon 6 productions and is industrially prepared by hydrocyanation of butadiene with homogeneous phosphite-nickel catalysts. Previous attempts to use phosphane-nickel catalysts under biphasic conditions with water as the catalyst co-phase solvent are well-documented in the patent literature. Room temperature ionic liquids have proven to be excellent new green media for a wide variety of catalytic organic reactions under homogeneous and biphasic conditions. The effect of several ionic liquids on this reaction was investigated with neutral and ionic ligands. The immobilisation of the catalyst and the possibility to recycle the catalyst phase will be discussed.

661888: Charge transfer polymerization of acrylic monomers in ionic liquid solvents

IEC 0 [661888]: Charge transfer polymerization of acrylic monomers in ionic

liquid solvents

Douglas R MacFarlane, and R Vijayaraghavan, School of Chemistry, Monash University, Clayton, Australia, d.macfarlane@sci.monash.edu.au

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications: Polymers & Gels*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Charge Transfer (CT) initiated and Hydroquinone (HQ) promoted polymerization of acrylate monomers and has been successfully carried out in a variety of room temperature ionic liquids as solvents. Enhanced polymer yields and rates of reaction are obtained. Molecular weight of the product is similar to traditional solvents. For example the polymerization of methyl methacrylate in a methyl butyl pyrrolidinium TFSA ionic liquid proceeds readily at room temperature. The use of the ionic liquid (IL) allowed replacement of solvents such as dimethylsulfoxide (DMSO) which are used in the conventional CT polymerization. The polymer is separated from the ionic liquid by precipitation. It is shown the ionic lqiuid can then be recycled.

661943: Physicochemical Properties of Ionic Liquids used in Aluminum Electrorefining at Low Temperatures

IEC 0 [661943]: Physicochemical Properties of Ionic Liquids used in Aluminum Electrorefining at Low Temperatures

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Physicochemical properties such as viscosities, densities, electrical conductivities, decomposition temperatures and electrochemical windows of ionic liquid electrolytes were determined. The ionic liquid electrolytes used in the present study are 1-Butyl-3-

methylimidazolium chloride (C4mimCl) + AlCl3 and 1-Hexyl-3-methylimidazolium chloride (C6mimCl) + AlCl3. An empirical expression was developed to describe the variation of density, viscosity and conductivity of these liquids as a function of both temperature and composition. Electrorefining of aluminum alloys in ionic liquids via low temperature electrolysis was the principal objective of this research. The applicability of different ionic liquids such as C4mimCl+AlCl3 and C6mimCl+AlCl3 in the electrorefining process was studied. The effect of physical properties of the electrolytes on the electrorefining process was investigated using the data obtained from the above study. Density and viscosity showed a marked effect on the effective rates of deposition (current density) and the microstructure of the deposits. The electroefining process has the advantages of low energy consumption, low temperature and no pollutants emission compared to the current industrial processes.

661987: Rate constants for solvent displacement from [$C_6H_6Cr(CO)_2$Solv] complexes; ionic liquids compared to conventional solvents

IEC 0 [661987]: Rate constants for solvent displacement from [$C_6H_6Cr(CO)_2$Solv] complexes; ionic liquids compared to conventional solvents

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Several [$C_6H_6Cr(CO)_2$Solv] complexes have been generated via pulsed laser photolysis of [$C_6H_6Cr(CO)_3$] in a variety of solvents including imidazolium cation based ionic liquids. The peak maximum of the UV/VIS absorption spectrum of the parent [$C_6H_6Cr(CO)_3$] complex was essentially independent of solvent. However that of the [$C_6H_6Cr(CO)_2$Solv] complexes was solvent dependent allowing us to determine the following spectrochemical series; Cyclohexane< [bmim][PF_6]< dichloroethane< methanol=[bmim][Tf_2N]=dioxane < acetonitrile. The temperature dependence of the bimolecular rate constant, k_q, for the displacement of solvent by a new ligand, L, from the [$C_6H_6Cr(CO)_2$Solv] complex forming [$C_6H_6Cr(CO)_2L$] has also been investigated. It was found that k_q decreased as follows; cyclohexane>[bmim][PF_6]

>dichloroethane. It has not been possible to displace methanol, [bmim][Tf_2N], dioxane or acetonitrile over the available timescales accessible to our apparatus. Further studies using [bmim][SbF_6] and [bmim][BF_4] are currently underway and the results will be presented in full.

662062: Structure and dynamics of ionic liquids

IEC 0 [662062]: Structure and dynamics of ionic liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

In this paper we report the application of a range of complementary techniques (notably small and wide angle X-ray scattering (S-WAXS), quasi-elastic neutron scattering (QENS), Raman spectroscopy and conductivity measurements) to investigate the structural properties of ionic liquids. The salts under investigation include those that are molten at room temperature, for example 1-butyl-3-methylimidazolium hexafluorophosphate, and those that are crystalline solids at room temperature but form liquid crystal phases on melting, for example 1-hexadecyl-3-methylimidazolium hexafluorophosphate. Where possible, both the cation and anion have been varied in order to determine the influence of each on the properties of the salts. The QENS results on liquid salts have been used to provide information on ultrafast dynamic processes. These are compared with information gained from other sources, notably optical Kerr effect studies and molecular dynamics calculations. Such information is extremely valuable in understanding the nature of ionic liquids as solvents and their liquid phase structures. The variable temperature S-WAXS data provide detailed information regarding the structure of both crystalline and liquid crystalline phases of long alkyl chain substituted salts. In combination with QENS, Raman spectroscopy and conductivity data we have been able to characterise a hitherto unobserved low temperature phase in a series of $[PF_6]^-$ salts.

662209: Application of task specific ionic liquids (TSILs) in the acid gas separation processes of supported ionic liquid membranes (SILMs) and electrochemical modulated complexation (EMC)

IEC 0 [662209]: Application of task specific ionic liquids (TSILs) in the acid gas separation processes of supported ionic liquid membranes (SILMs) and electrochemical modulated complexation (EMC)

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Previously, we reported on SILMs and RTILs in EMC for acid gas separations. In the later, the dissolving of complexation agents into the RTILs is critical; while in the former, dissolving agents facilitates the separation. While the agents were different, low solubility of the agents limited the efficiency of both processes. We used TSILs to address the low complexation-agent solubility in RTILs. The anion was [Tf_2N-], while an imidazolium cation contained the complexation-agent as a functional group. A factor in optimizing TSILs for a separation process is the effect of functionalization on the physical gas solubility, in addition to the gas complexation. The comparison of EMC vs. SILMs explores this factor, since EMC requires low physical gas solubility while SILMs are optimal with high solubility. We explore the physical gas solubilities of TSILs in light of our proposal that heats-of-vaporization and molar volumes govern gas solubilities in unfunctionalized RTILs.

662669: Modeling ionic liquids using an extended OPLS-AA force field

IEC 0 [662669]: Modeling ionic liquids using an extended OPLS-AA force field

José Nuno A. Canongia Lopes[1], Agílio A. H. Pádua[2], and Johnny Deschamps[2]. (1) Centro de Química Estrutural, Instituto Superior Técnico, Av. Rovisco Pais, 1049 001 Lisboa, Portugal, jnlopes@ist.utl.pt, (2) Laboratoire de Thermodynamique des Solutions et des Polymères, CNRS/Université Blaise Pascal

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*

Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

In this contribution we introduce a force field capable of addressing three main issues. i) Auto-consistency: Ab-initio calculations can provide essential data to the development of an auto-consistent force field, including molecular geometry optimization, the adequate description of the electronic density, the determination of any missing force field parameters and the correct attribution of point charges on the interaction centers. ii) Additivity: parameterization of a particular ionic liquid is not the correct approach if one wants to deal with a family of similar compounds. The proposed IL field will concentrate on the parameterization of molecular residues that are common to an entire family of cations, with rules to add specific side-chains; and iii) Tranfereability: the model is based on the OPLS-AA force field. This means that any other molecule or residues already in the OPLS database can be "combined" with the new IL force field. The proposed force field is tested against relevant experimental and simulation data.

662738: Property of Ionic Liquids and Additions for Deposition:- Performance Pertaining to Their Viability

IEC 0 [662738]: Property of Ionic Liquids and Additions for Deposition:- Performance Pertaining to Their Viability

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Ionic liquids (ILs), a new class of green solvents, have many beneficial properties. This work looks at ILs role in the electrochemical deposition of metals by commonly used scientific physical characterisation techniques. Elucidation of the experimental data obtained is used to determine the viability of the ionic liquid and additives in the proposed application. A model was developed from the chemical/physical understanding of the molecular processes involved based on the experimental data. This model was used as a predictive tool for determining the viability of electrolytes based on ionic liquids quickly.

662772: Densities of ionic liquids as a function of temperature

IEC 0 [662772]: Densities of ionic liquids as a function of temperature

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*
Preferred Presentation Format: *PosterOnly*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

We studied the effect that changing the temperature, anion, or cation has on the density of the ionic liquid. Densities for a few of the ionic liquids and temperatures considered in this work have been previously reported and our results are consistent with those in the current literature. Here, we report the effect of various cations, including tetraalkylammonium-based, imidazolium-based, and pyrrolidinium-based, with the bis(trifluorosulfonyl)imide anion and the effect of various anions, including bis(trifluorosulfonyl)imide, tetrafluoroborate, and trifluorosulfonate, with the 1-butyl-3-methylimidazolium cation. We found the structure of the IL did have a large effect on the density. We also found that the IL densities decreased with increasing temperature. However, there was no significant effect of the structure on the temperature dependence.

662886: Thermal and kinetic studies of tri-alkyl-imidizaolium salts

IEC 0 [662886]: Thermal and kinetic studies of tri-alkyl-imidizaolium salts

Douglas M. Fox[1], Walid Awad[2], Thomas E. Sutto[3], Jeffrey W. Gilman[4], Paul C. Trulove[5], and Hugh C. De Long[5]. (1) Chemistry Division, Naval Research Laboratory, Code 6170, Building 207, 4555 Overlook Ave. SW, Washington, DC 20375, Fax: (202) 767-3321, dmfox@ccs.nrl.navy.mil, (2) Materials Fire Research Group, Fire Science Division, National Institute of Standards and Technology and NIS Egypt, (3) Code 6170, Chemistry Division, Naval Research Laboratory, (4) Building and Fire Research Laboratory, National Institute of Standards and Technology, (5) Air Force Office of Scientific Research

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Oral*

Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

The thermal properties of tri-alkyl-imidazolium room temperature ionic liquids (RTILs) have been determined using the techniques of thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC). Using a Setaflash flashpoint analyzer, all the salts studied were found to have flashpoints above 200ºC. TGA was utilized to study the decomposition of both neat RTILs and polymer-clay nanocomposites modified with tri-alkyl-imidazolium cations. The effects of alkyl chain length, anion, gas type, and pan composition will be discussed. DSC was utilized to measure the phase change temperatures and enthalpies between –70ºC and 400ºC. All the RTILs studied show significant super-cooling before freezing. The larger chain tri-alkyl-imidazolium hexafluorophosphates show both solid-solid phase transitions and liquid crystalline behavior. The decomposition kinetics of 1,2-dimethyl-3-butylimidazolium hexafluorophosphate was investigated using TGA. The kinetic model and Arrhenius parameters have been determined by employing both non-isothermal and isothermal programs.

662893: Surface chemistry and tribological behavior of ionic liquid boundary lubrication additives in water

IEC 0 [662893]: Surface chemistry and tribological behavior of ionic liquid boundary lubrication additives in water

Jeffrey S. Zabinski[1], Benjamin S. Phillips[2], Robert A. Mantz[1], and Paul C. Trulove[3]. (1) AFRL/MLBT, Air Force Research Laboratory, Wright Patterson Air Force Base, Ohio, Bldg. 654, Rm 136, 2941 P Street, Wright Patterson AFB, OH 45433, Fax: 937 255 2176, jeffrey.zabinski@wpafb.af.mil, (2) Systran Corporation, (3) Air Force Office of Scientific Research

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Ionic liquids (IL) are studied to determine their potential as boundary lubrication additives for water. There are a number of applications where water may be used as a lubricant; for example, in steam engines designed to quietly and economically provide electricity and heat. ILs are environmentally friendly, thermally stable, and have negligible vapor pressure. It has recently been reported that they can also lubricate steel and ceramic surfaces. In this presentation, ILs with hexafluorophosphate and tetrafluoroborate anions are evaluated as boundary lubrication

additives. Friction and wear properties are determined using a ball-on-disk tribometer operated in steam and water. The surface chemistry and forces controlling IL tribology on Al_2O_3 and Si_3N_4 are studied using XPS, FTIR, and SPM. As little as two weight percent IL dramatically lowers friction and wear. Evidence for tribologically formed boundary layer films and electric double layer mediated surface protection is discussed.

662968: Abraham solvent parameters for ionic liquid/organic two-phase systems

IEC 0 [662968]: Abraham solvent parameters for ionic liquid/organic two-phase systems

W. Matthew Reichert, Jonathan G. Huddleston, John D Holbrey, and Robin D. Rogers, Department of Chemistry and Center for Green Manufacturing, The University of Alabama, Tuscaloosa, AL 35487

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
The solvent properties of a range of room temperature ionic liquids (ILs) have been investigated, and are compared to those of traditional molecular solvents. Tracer-level partitioning of organic solutes between an organic phase (e.g., hexane, toluene, t-butyl methyl ether) and different ILs has been investigated and the results will be discussed. Analysis of the partitioning data using an LSER approach yields Abraham solvent parameters for each liquid-liquid system. Comparison of the data from different biphasic systems allows a more complete description of the solvent nature of ILs to be made.

662971: X-Ray crystallography of novel ionic liquids based on N-alkylmorpholinium salts

IEC 0 [662971]: X-Ray crystallography of novel ionic liquids based on N-alkylmorpholinium salts

Richard P. Swatloski[1], Robin D. Rogers[1], Charles R. Lea[2], Isaac A. Miller[2], and David M. Brown[2]. (1) Department of Chemistry and Center for Green Manufacturing, The University of Alabama, Tuscaloosa, AL 35487, Fax: 205-348-0823, tubarick@aol.com, (2) Department of Chemistry, Davidson College

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*
Preferred Presentation Format: *PosterOnly*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

From commercially-available starting materials, two new classes of ionic liquids based on N-methylmorpholine were synthesized, characterized, and their properties evaluated against those of existing ionic liquids. Starting materials for these new N-morpholinium-based ionic liquids cost 60% less than starting materials for ionic liquids based on N-methylimidazole. Exhibiting interesting properties due in part to their non-planar structures, these new ionic liquids serve to expand the current offering available to scientists seeking to tailor a particular set of solvent properties to a particular problem. Several of these new ionic liquids have been crystallographically characterized. Results from structural studies, as well as important solubility data, toxicity, and viscosities will be presented.

663178: Liquid-liquid equilibria of imidazolium-based ionic liquids and alcohols

IEC 0 [663178]: Liquid-liquid equilibria of imidazolium-based ionic liquids and alcohols

Jacob M Crosthwaite, Sudhir N.V.K. Aki, Edward J. Maginn, and Joan F. Brennecke, Department of Chemical and Biomolecular Engineering, University of Notre Dame, 182 Fitzpatrick Hall, Notre Dame, IN 46556, jcrosthw@nd.edu

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Ionic liquids have been suggested as replacements solvents in liquid-liquid extraction processes. Even though the effectiveness of this process has been demonstrated, very little information regarding the phase behavior of ionic liquids with organic solvents is available. Here we will present liquid-liquid equilibrium data for imidazolium based ionic liquids with alcohols. The influence that alkyl chain length and branching in the alcohol have on the phase behavior will be discussed. In addition, we will show that the choice of anion can have a dramatic effect on the liquid-liquid equilibrium. Systems examined include alcohols such as 1-propanol, 1-butanol, 1-

hexanol, 2-propanol, *tert*-butanol and imidazolium salts with anions including $[BF_4]$, $[(CF_3SO_2)_2N]$, $[CF_3SO_3]$, and $[NO_3]$.

663321: The Application of Trialkyl-Imidazolium Ionic Liquids and Salts to the Preparation of Polymer Clay Nanocomposites

IEC 0 [663321]: The Application of Trialkyl-Imidazolium Ionic Liquids and Salts to the Preparation of Polymer Clay Nanocomposites

Paul C. Trulove[1], Walid Awad[2], Jeffrey W. Gilman[3], Rick D. Davis[3], Thomas E. Sutto[4], Douglas M. Fox[4], Paul H. Maupin[5], and Hugh C. De Long[1]. (1) Air Force Office of Scientific Research, 4015 Wilson Blvd., Rm 713, Arlington, VA 22203, Fax: 703-696-8449, (2) Materials Fire Research Group, Fire Science Division, National Institute of Standards and Technology and NIS Egypt, (3) Building and Fire Research Laboratory, National Institute of Standards and Technology, (4) Chemistry Division, Naval Research Laboratory, (5) Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Polymer melt intercalation is a promising approach to the synthesis of polymer-layered silicate nanocomposites. Increasing the thermal stability of the organically modified layered silicates used in this process is one of the key points in the successful application of these nanocomposites on the industrial scale. Tri-alkyl imidazolium ionic liquids and salts provide a unique and more thermally stable alternative to the quaternary alkyl ammonium salts currently used as clay modifiers. In this presentation we will discuss our recent efforts to characterize the thermal properties of tri-alkyl imidazolium treated clays. We will discuss the effect of counter ion, alkyl chain length and structural isomerism on the treated clay thermal stability. Furthermore, we will present results from the application of these tri-alkyl imidazolium treated clays to the preparation of polymer-layered silicate nanocomposites with polymers such as polystyrene (PS) and poly(ethylene terephthalate) (PET).

663570: Nanostructured materials based on room-temperature ionic liquids

IEC 0 [663570]: Nanostructured materials based on room-temperature ionic liquids

Millicent A. Firestone[1], Amanda Wolf[1], Julie Dzielawa[2], Soenke Seifert[3], and Mark L. Dietz[2]. (1) Materials Science Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, firestone@anl.gov, (2) Chemistry Division, Argonne National Laboratory, (3) Advanced Photon Source Division, Argonne National Laboratory

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

A major area of current interest in the field of nanoscience is the use of self-assembly to prepare functional materials in a spontaneous, yet controlled fashion. Of particular interest has been the development of means to direct molecular organization and to generate novel supramolecular structures in soft condensed matter phases. Recently, we have demonstrated that addition of a small amount of water to certain room-temperature ionic liquids (e.g., 1-decyl-3-methylimidazolium halides) can trigger their self organization and the concomitant formation of a liquid-crystalline gel phase (ionogel). Small-angle X-ray scattering (SAXS) studies have shown that further increasing the water content of these systems leads not only to lamellar structures, but also to highly ordered cubic phases. These soft nanostructures, which feature a highly anisotropic environment and segregated aqueous and organic domains, can be used as templates to photochemically generate inorganic nanoparticles of controlled size and shape. Anomalous SAXS studies on ionogel-nanoparticle composites also indicate that highly ordered arrays of nanoparticles can be prepared.

663749: Redox chemistry of polyoxometalates in ionic liquids

IEC 0 [663749]: Redox chemistry of polyoxometalates in ionic liquids

Ming-Hsi Chiang, Julie A. Dzielawa, Mark L. Dietz, and **Mark R. Antonio**, Chemistry Division, Argonne National Laboratory, 9700 South Cass Avenue, Building 200, Argonne, IL 60439, Fax: 630-252-4225, mchiang@anl.gov, mantonio@anl.gov

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry*
Invited: *N*
Comments to Organizer: *This is submitted for the proposed session on Electrochemistry (MacFarlane)*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *Standard*

Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Although often overlooked, the impact of countercations on the redox activity of polyoxometalate (POM) anions is now known to drive critical phenomena in catalysis and aggregation behavior. Specific to our investigations of the effects of interionic associations between POM anions and cations on redox processes in aprotic media, we are using ionic liquids (ILs) as solvents and electrolytes for electrochemical studies of heteropolyoxoanions. We will describe the results of cyclic voltammetry measurements of the Keggin anion obtained in ILs and conventional organic media. The comparison provides insights to the remarkable electrochemical activity of the Keggin anion. With ILs, the access to redox behaviors that are otherwise unattainable is of significance to a number of issues with regard to electrochemical phenomena, especially electro-chromic and -catalytic applications as well as redox-switchable systems for separations science. This work is supported by the U.S. DOE, OBES–Chemical Sciences under contract No. W-31-109-ENG-38.

663961: Metal Ion Extraction by Crown Ethers in Ionic Liquids

IEC 0 [663961]: Metal Ion Extraction by Crown Ethers in Ionic Liquids

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

To further explore the features of room temperature ionic liquids (RTILs) in separation processes, the selectivity and efficiency of competitive metal ion extraction from aqueous media into solutions of crown ethers in RTILs have been investigated. Effects of structural variation in the crown ether and changing the identities of the anion and cation for both the RTIL diluent and the metal salts have been examined.

664008: Opportunities for membrane processing using ionic liquids

IEC 0 [664008]: Opportunities for membrane processing using ionic liquids

Joao G. Crespo, Thomas Schaefer, Pavel Izak, Raquel Fortunato, Luis Branco, and Carlos A. M. Afonso, CQFB-Dept. Chemistry, FCT/Universidade Nova de Lisboa, Campus de Caparica, 2829-516 Caparica, Portugal, Fax: 351-21-2948385, jgc@dq.fct.unl.pt

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations*
Invited: *N*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

This paper discusses the use of membrane processes for the selective recovery of solutes from ionic liquids, namely using supported liquid membranes and pervaporation. The use of ionic liquids immobilised in porous membranes was evaluated for the selective transport of solutes. The role of the water content in the supported liquid phase was elucidated allowing us to understand the transport of small ions. The recovery of target solutes from organic media was also studied: an extremely high selective transport of secondary amines against tertiary amines was achieved (up to a 55:1 molar ratio), and explained. This paper also demonstrates that pervaporation is capable of quantitatively recovering volatile solutes: 1- water, whose removal shifts the reaction equilibrium toward higher product yields; 2– ethyl hexanoate, as a product from a heat sensitive biotransformation; 3– chlorobutane as a residue stemming from the synthesis of the ionic liquid; 4– naphthalene as a low-boiling compound.

664030: Formation of aqueous biphasic systems with hydrophilic ionic liquids via the addition of water-structuring salts: applications to nuclear tank wastes

IEC 0 [664030]: Formation of aqueous biphasic systems with hydrophilic ionic liquids via the addition of water-structuring salts: applications to nuclear tank wastes

Keith E. Gutowski[1], Grant A. Broker[1], Nicholas J. Bridges[1], Jonathan G. Huddleston[1], Heather D. Willauer[2], John D. Holbrey[1], and Robin D. Rogers[1]. (1) Department of Chemistry and Center for Green Manufacturing, The University of Alabama, Tuscaloosa, AL 35487, gutow001@bama.ua.edu, (2) Chemistry Division Code 6180, Naval Research Laboratory

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session*
Invited: *N*
Preferred Presentation Format: *Poster*
Consider for Sci-Mix: *Y*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
The use of Ionic Liquids (ILs) in aqueous/IL biphasic separation systems is currently limited to examples in which the IL contains anions that are fluorinated, expensive, and environmentally non-benign. However, ILs are very appealing for use in liquid-liquid separations due to their very low vapor pressure, wide liquidus range, and tunable physical properties. We have recently shown that hydrophilic 1-butyl-3-methylimidizolium chloride forms an aqueous biphasic systems with K_3PO_4, a kosmotropic salt. This salting-out phenomenon occurs with a variety of other such salts providing access to a much wider range of aqueous biphase forming systems, leading us to investigate the applicability to partitioning systems using nuclear tank waste simulants for separation of fission products and transuranic species. Here we present results which attempt to characterize the phases according to composition and speciation as well as the partitioning of various organic/inorganic solutes between the phases with emphasis on using extractant molecules for metal ion separations.

664093: Reactivity of solvated and pre-solvated electrons in alkylammonium bistriflylimide ionic liquids

IEC 0 [664093]: Reactivity of solvated and pre-solvated electrons in alkylammonium bistriflylimide ionic liquids

Alison M. Funston[1], James F. Wishart[1], Pedatsur Neta[2], Sharon I. Lall[3], Robert Engel[3], and Joan F. Brennecke[4]. (1) Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973, Fax: 631-344-5815, afunston@bnl.gov, (2) National Institute of Standards and Technology, (3) Department of Chemistry and Biochemistry, Queens College and the Graduate Center of CUNY, (4) Department of Chemical and Biomolecular Engineering, University of Notre Dame

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract
Pulse radiolysis of [R4N][NTf2] ionic liquids produces solvated electrons that persist for hundreds of nanoseconds. Systematic cation variation shows that solvated electron spectroscopic properties depend strongly on the lattice structure of the ionic liquid. The rate constants of solvated electron reactions with O2, CO2 and aromatic acceptors (e.g.; pyrene) were measured in several liquids. The diffusion rate for the solvated electron in these ionic liquids is significantly lower than those of small neutral molecules, in contrast to the situation in molecular solvents. Pre-solvated electron scavenging is a significant facet of overall radiation sensitivity of ionic liquids, possibly due to slower electron solvation processes. Ionic liquid solvation dynamics, as

measured by emission Stokes shifts and polarization anisotropy decays, will be applied to the understanding of the electron solvation process. Supported in part by the U.S. Department of Energy, Division of Chemical Sciences, Office of Basic Energy Sciences, under contract DE-AC02-98-CH10886.

664377: In Situ Multi Nuclei NMR Spectroscopy Studies of polymerization Process of Styrene and MMA in Ionic Liquid Mediate

IEC 0 [664377]: In Situ Multi Nuclei NMR Spectroscopy Studies of polymerization Process of Styrene and MMA in Ionic Liquid Mediate

M. M. Guo, Polymer Science Institute, The University of Akron, Akron, OH 44325-3909, Fax: 330-972-5290, mguo@uakron.edu

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications: Polymers & Gels*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *power pointer*
Conforms to Bylaw 6: *N*
Last Modified: *2003-05-10*

Abstract

The real time solution 1H, 13C, 19F and 31P NMR spectroscopy was performed to monitor: 1) the thermal stability of the ionic liquids IMIP 4, IMIP6, IMIP8 with different amount of water at 60, 70, 80, and 90 °C; 2) the decomposition kinetics of AIBN in ionic liquid IMIP4, 6,8; 3) polymerization kinetic of St and MMA in ionic liquid IMIP4, 6,8. The results indicates that: 1) while there is no reaction happen for IMIP8 with no residue water, for IMIP4 and IMIP6 with residue water there are HF, carbine type imidazole ring and the complexes of the imidazole with PF6 formed during the isothermal heat at 60,70,80, and 90 °C; 2) the thermal decomposition rate of the free radical initiator AIBN is much faster in the ionic liquids that in toluene and methanol; 3) the polymerization rate of St and MMA are much faster in the ionic liquids that in toluene and methanol. Although the two monomer can dissolved in the ionic liquids, the polymers formed can not, this indicates that the reactions are precipitation polymerization. While the 1H NMR signal of PS and PMMA are escaped from the NMR spectra, the PMMA ionic solution is transparent and the PS ionic liquid solutions are milk like colloids.

664580: Surface tension of ionic liquids

IEC 0 [664580]: Surface tension of ionic liquids

Telma Cordeiro[1], **Eduardo J. M. Filipe**[1], José M. S. S. Esperança[2], Henrique J. R. Guedes[2], and Kenneth R. Seddon[2]. (1) Instituto Superior Técnico, Centro de Química Estrutural, Lisbon 1049-001, Portugal, Fax: +351-21-8464455, te_cordeiro@yahoo.com, efilipe@ist.utl.pt, (2) QUILL, The Queen's University of Belfast

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

Room temperature ionic liquids (IL) are emerging as novel replacements for volatile organic compounds traditionally used as industrial solvents. IL are thermally stable, non-corrosive and non-flammable. Without measurable vapour pressure, IL have the ability to dissolve a considerable variety of organic, inorganic and polymeric materials, up to very high concentrations. In this work the surface tension and density of two families of ionic liquids, [Cnmim][X], where [Cnmim] represents the 1-alkyl-3-methylimidazolium cation and [X] the hydrophobic anions, X=PF6- and N(SO2CF3)2-, have been measured as a function of temperature, between 24ºC and 65ºC. The results allow a discussion on the influence of both the alkyl chain length of the cation and the nature of the anion on the surface tension of ionic liquids.

664619: Getting started with Ionic Liquids: An experience-based tutorial

IEC 0 [664619]: Getting started with Ionic Liquids: An experience-based tutorial

John D. Holbrey[1], Richard P. Swatloski[1], W. Matthew Reichert[1], Joan F. Brennecke[2], Kenneth R. Seddon[3], Ullastina Hakala[3], Maggel Deetlefs[4], M. Nieuwenhuyzen[5], Thomas Welton[6], Philip Mawdsley[6], James Vallance[6], Oonagh Sheppard[5], and Robin D. Rogers[1]. (1) Department of Chemistry and Center for Green Manufacturing, The University of Alabama, Tuscaloosa, AL 35487, (2) Department of Chemical and Biomolecular Engineering, University of Notre Dame, (3) Queen's University Ionic Liquid Laboratories, Queen's University of Belfast, (4) Queen's University Ionic Liquid Laboratories, Queen's University Belfast, (5) School of Chemistry, The Queen's University of Belfast, (6) Department of Chemistry, Imperial College

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Experienced Based Tutorials; Question & Answer Session*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*

Last Modified: *2003-05-10*

Abstract

Synthesis of a wide range of ILs is relatively straightforward. However, with a range of synthetic methods available, an appreciation of some of the potential pit-falls and traps that can inadvertently lead to problems and the introduction of undesirable contaminants is necessary. Students and staff from The University of Alabama, The Queen's University of Belfast, Imperial College, and The University of Notre Dame will be on hand to give case studies from their experience with ionic liquids, with particular attention to potential problems that can be encountered during synthesis, handling, clean up and characterisation. There will short presentations on the synthesis and characterisation of ionic liquids, and their design and use for green synthesis. This is planned as an introductory session for novices, and question and answer periods will be central.

671422: Ionic liquids by proton transfer, ΔpKa, and the ionic liquid fuel cell

IEC 0 [671422]: Ionic liquids by proton transfer, ΔpKa, and the ionic liquid fuel cell

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ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2003-05-10*

Abstract

We describe the behavior of the conductivity, viscosity, and vapor pressure of various binary liquid systems in which proton transfer occurs to form salts of varying stabilities. We find a simple relation between the temperature at which the vapor pressure reaches one atm. and the difference in pK_a value for the acid and base in dilute aqueous solution, despite the fact that there is no water in the present systems. For ΔpK_a values above 10, the boiling point elevation becomes so high (>300ºC) that pre-emptive decomposition prevents its measurement. In these liquids we find a special stability for the hydrogen bonded di-anion species $(AHA)^-$, which can serve as a proton-transporting agent and can participate in electrode processes. Low vapor pressure proton transfer ionic liquids of this type (**PTILs**) constitute an interesting class of non-corrosive proton-exchange electrolyte, that we have shown can serve well in high temperature

(T=100-250^{o}C) fuel cell applications. Simple H_2(g)/Pt/**PTIL**/Pt /O_2(g) fuel cells have been tested. For favorable choices of PTIL, these outperform their standard phosphoric acid cell equivalents. They equal the phosphoric acid cell voltage output and, when special additives are included in the electrolyte, more than double their short circuit currents in much of the temperature range.

675768: Intermission

0 [675768]: Intermission

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Preferred Presentation Format: *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675774: Introductory Remarks

0 [675774]: Introductory Remarks

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties*
Preferred Presentation Format: *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675775: Break

0 [675775]: Break

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry &*

Engineering and Separation Science & Technology subdivisions): Physical/Thermo Properties
Preferred Presentation Format: *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675777: Introductory Remarks

0 [675777]: Introductory Remarks

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Fuels & Applications*
Preferred Presentation Format: *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675778: Intermission

0 [675778]: Intermission

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Fuels & Applications*
Preferred Presentation Format: *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675787: Introductory Remarks

0 [675787]: Introductory Remarks

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract

Abstract text not available.

675788: Intermission

0 [675788]: Intermission

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Catalysis/Synthesis* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract

Abstract text not available.

675791: Introductory Remarks

0 [675791]: Introductory Remarks

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract

Abstract text not available.

675792: Intermission

0 [675792]: Intermission

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Separations* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675803: Introductory Remarks

0 [675803]: Introductory Remarks

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675804: Intermission

0 [675804]: Intermission

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675812: Introductory Remarks

0 [675812]: Introductory Remarks

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675813: Intermission

0 [675813]: Intermission

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Spectroscopy* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675814: Introductory Remarks

0 [675814]: Introductory Remarks

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications: Polymers & Gels* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675815: Intermission

0 [675815]: Intermission

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Novel Applications: Polymers & Gels* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675829: Introductory Remarks

0 [675829]: Introductory Remarks

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675830: Intermission

0 [675830]: Intermission

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Electrochemistry* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract

Abstract text not available.

675836: Introductory Remarks

0 [675836]: Introductory Remarks

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Preferred Presentation Format: *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675837: Intermission

0 [675837]: Intermission

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Inorganic/Materials*
Preferred Presentation Format: *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675850: Introductory Remarks

0 [675850]: Introductory Remarks

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Preferred Presentation Format: *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675851: Intermission

0 [675851]: Intermission

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): General Contributions*
Preferred Presentation Format: *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675857: Panel Discussion

0 [675857]: Panel Discussion

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Experienced Based Tutorials; Question & Answer Session* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2003-05-10*

Abstract
Abstract text not available.

675858: Poster Author Introductions

0 [675858]: Poster Author Introductions

ACCEPTED
Topic Selection: *Ionic Liquids: Progress and Prospects (sponsored by Green Chemistry & Engineering and Separation Science & Technology subdivisions): Poster Session Discussion*
Preferred Presentation Format: *Break*
Consider for Sci-Mix:

Last Modified: *2003-05-10*

Abstract
Abstract text not available.