

IUPAC Partnership Develops Standards and a Data Retrieval System for Ionic Liquids

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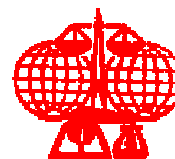
Ionic liquids, a class of organic salts that are liquid at or near room temperature, have been proposed as solvents for *Green Processing*. In spite of the many advantages that these fluids are predicted to offer, fundamental data on their physical and chemical properties, property measurement methodology, high quality data on reference systems, standards for reporting thermodynamic data, and creation of a comprehensive database infrastructure for ionic liquids are needed to provide US industry with a knowledge base to exploit these solvents.

To achieve these goals in the shortest time possible and reach an international consensus on the central issues, two IUPAC projects have been initiated with NIST/CSTL involvement. The first of these IUPAC projects is *Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the Development of Standardized Systems*. The lack of consistent requirements for the publication of

This IUPAC task group has convened international discussion of the issues by conducting two IUPAC workshops on ionic liquids, held at the 17th IUPAC Conference on Chemical Thermodynamics (Rostock, Germany) at the 18th IUPAC Conference on Chemical Thermodynamics (Beijing, China) and a 3rd Workshop will be convened in Boulder as part of the 19th IUPAC Conference on Chemical Thermodynamics in 2006

thermodynamic data for ionic liquids has led to major barriers to an unambiguous interpretation of the data and a critical evaluation with regard to their uncertainties. This drastically diminishes the value of the reported numerical data for use in a variety of engineering applications. To address these issues, a standardization in reporting thermodynamic data for ionic liquids could be accomplished by an expansion of the Guided Data Capture (GDC) software developed by the NIST's TRC Group, formerly known as the Thermodynamic Research Center (TRC).

NIST works with the international community to address the lack of consistent requirements for reporting thermodynamic data for ionic liquids by employing the Guided Data Capture software developed in CSTL.



International Union of Pure and Applied Chemistry

Outcomes of the first workshop were reported in a special section of the *Journal of Chemical and Engineering Data*. In Beijing, the IUPAC Task Group planned an international round robin study of a reference substance, 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide, abbreviated as [hmim][Tf₂N]. Using NIST-supplied reagents, 1.5 kg of [hmim][Tf₂N] was synthesized at the University of Notre Dame and then was shipped to NIST.

After drying and chemical characterization at NIST, samples were packaged under an inert atmosphere and were shipped to the participating laboratories. NIST will coordinate round robin studies of density, heat capacity, and viscosity, and will participate in measurements of those properties plus thermal conductivity, electrolytic conductivity and industrial gas solubility.

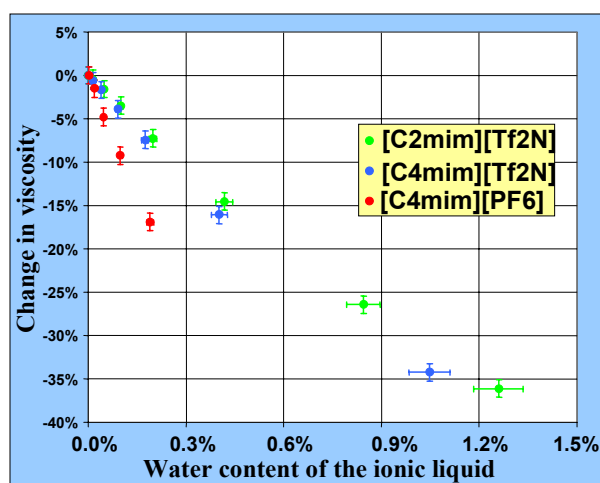
Preface to Special Section: Papers Presented at the Workshop on Ionic Liquids, ICCT, Rostock, Germany, July 28 to August 2, 2002. J. W. Magee, *J. Chem. Eng. Data* 2003 48, 445.

The second IUPAC project *Ionic Liquids Database* is addressing the need for an open-access, public-domain data storage system scoped to cover information pertaining to ionic liquids. The vision for this project is to create a distributed-access data retrieval system for ionic liquids and their mixtures that encompasses chemical structure, solvent properties, ionic liquids use in synthesis, reviews, reactions and catalysis, manufacturer information, benchmark properties and models, and thermophysical and thermochemical data. During FY 2004, the task group met to share a common vision and to divide the data collection effort among the participants.

The NIST measurement program continues to provide benchmark physical properties data for selected ionic liquids that are liquid-phase at room temperature and both air- and moisture- stable. For 1-butyl-3-methylimidazolium hexafluorophosphate, considered to be the archetypal ionic liquid, we have published the first reports of thermodynamic properties of the ideal gas state at temperatures to 1500 K and high-accuracy thermodynamic properties in condensed states (crystal, glass, and liquid) covering a range of temperatures from 5 K to 550 K. A study of the viscosity of three hydrophobic ionic liquids and the effect of a dilute water impurity has been completed.

Y.U. Paulechka, G.J. Kabo, A.V. Blokhin, O.A. Vydrov, J.W. Magee, and M. Frenkel, *“Thermodynamic Properties of 1-Butyl-3-methylimidazolium Hexafluorophosphate in the Ideal Gas State”* J. Chem. Eng. Data 2003, 48, 457-462.

G. J. Kabo, A. V. Blokhin, Y.U. Paulechka, A.G. Kabo, M.P. Shymanovich, and J.W. Magee, *“Thermodynamic Properties of 1-Butyl-3-methylimidazolium Hexafluorophosphate in the Condensed State”* J. Chem. Eng. Data 2004, 49, 453-461.



Anomalously high sensitivity of transport properties (in this case kinematic viscosity) to water content has been revealed by recent NIST measurements on ionic liquids.

In the future, properties studies will continue with new measurements of thermodynamic density, heat capacity, enthalpy of solution, gas solubility, and also expanded transport property measurements, such as thermal conductivity and electrolytic conductivity, a key electrical characteristic. Structure-property relationships for physical properties will be explored by analyzing evaluated data in our database. Modifications that support ionic materials will be applied to the TRC Source Database at NIST and to the Guided Data Capture application to facilitate the storage and retrieval of ionic liquids property data.