

Report on IACT/IUPAC Project – Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the Development of Standardized Systems

By

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Presented at Thermodynamics 2005,
Sesimbra, Portugal

6 – 8 April 2005

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There has been considerable scatter in the literature data
on measured properties of ionic liquids.

AIM OF TASK GROUP

- ❑ To establish reliable results for reference systems of IL's and IL + liquid mixtures using IL with known purity and well characterized water content
- ❑ To encourage systematic studies on the thermodynamic and thermophysical properties of Ionic Liquids (IL) based on the needs of industrial chemical processes

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Task Group Members

- Ken Marsh (Canterbury)
 - Ken Seddon (Queens, Belfast)
 - Luis Rebelo (Universidade Nova de Lisboa),
 - Cor Peters (Delft),
 - Michael Frenkel (NIST),
 - Andreas Heintz (Rostock),
 - Joseph Magee (NIST)
 - Joan Brennecke (Notre Dame)
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- Reference ionic liquid is 1-hexyl-3-methylimidazolium bistriflate amide (CF₃SO₂)₂N. A single 1.5 L sample was prepared at Notre Dame and sealed samples were distributed by NIST to the participants.
 - All samples have known purity and water content and water will be determined by investigators during each measurement

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NIST Boulder/Gaithersburg

Joseph Magee, Jason Widegren, Richard Perkins, and
Donald Archer

- Viscosity and density measurements have been measured from (238.15 to 373.15) K. Anton Parr viscodensimeter agrees with Ubbelohde to 0.5 %.
- Thermal conductivity measurements are planned for April/May 2005
- Heat capacity measurements are planned for May/June 2005
- Electrolytic conductivities have been measured at (288, 293, 298, 308, and 323) K

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Andreas Heintz, University of Rostock

- Gamma infinity measurements with [hmim][Tf2N] + hexan-1-ol and + butan-1-ol at (25, 40 and 60) °C have been completed.
- Enthalpies of dilution measurements for [hmim][Tf2N] in hexan-1-ol and butan-1-ol will be completed by end of June.
- LLE measurements with the same systems have begun and will be finished in April.

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Gas Solubility Measurements

To be made on a variety of gases with a variety of methods (H₂, CO₂, CH₄, O₂, C₃H₈)

- Margarida Costa Gomes, University Blaise Pascal. Measurements on H₂, CO₂, and C₂H₆ at low pressures at (5 to 70) C up to 2 bar underway
- Cor J. Peters, Delft University of Technology. High pressure measurements are scheduled for the period of March to May.
- Gerd Maurer, University of Kaiserslautern. High pressure measurements in progress. Measurement on CO₂ at 293.15 K complete.

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Joan Brennecke, University of Notre Dame

- T_g , T_m , T_f , have been measured by DSC.
- T_{decomp} has been measured by TGA in N_2 and air
- Densities have been measured from (20 to 70) °C.
- Viscosities have been measured from (10 to 70) °C.
- LLE with hexan-1-ol and octan-1-ol has been measured by the cloud point technique..

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Joan Brennecke, University of Notre Dame (continued)

- Solubilities of CO_2 , O_2 and CH_4 have been measured at (10, 25, and 50) °C and pressures to 13 bar.
- Solubility of CO_2 has been measured to 100 bar at (25, 40 and 60) °C.
- LLE with water at room temperature is also planned.

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Luis Paulo N. Rebelo, Universidade Nova de Lisboa

- Density measurements (20 to 60) °C to 700 bar done
- Speed of sound (20 to 60) °C to 1500 bar begun
- LLE butan-1-ol, pentan-1-ol, and hexan-1-ol and pressure effect of UCST begun
- Excess volume with ethanol and propan-1-ol to be done

Tooru Atake, Tokyo Institute of Technology

- Heat capacity measurements 75 % complete

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Ken Marsh, University of Canterbury, NZ

- Viscosity measurements with vibrating wire instrument.
- Density measurements will be made with a vibrating tube instrument with allowance for viscous effects
- Relative permittivity will be made with a reentrant cavity.
- Thermal conductivity with Hotdisk apparatus (tentative)

Ken Seddon, Queen's University, Belfast

- Density and viscosity measurements started

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Gennady Kabo, Belarusian State University

- Adiabatic heat capacity measurements 90 % completed

Carlos Nieto de Castro, Universidade de Lisboa

- Viscosity measurements by capillary viscometry (May) and oscillating cup viscometer (June).
- Relative permittivity measurements with a new cell (late spring).
- Thermal conductivity measurements (hot wire) are tentatively planned

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Summary and Publication

- All measurements should be completed by the end of July 2005
- All data will be collected by one of the investigators and analyzed. All investigators will contribute to paper and be authors
- Will include recommended values and/or equations
- Finalize and report at Thermo International 2006 Boulder
- This is a unique exercise in international cooperation
- Special thanks to Jason Widegren, NIST, who has done most of the organization for this project and Mark Muldoon, University of Notre Dame, who synthesized the sample

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