

# IUPAC Project on Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and Standardized Systems

Meeting Notes

August 17, ICCT-2004, Beijing, China

**In attendance:** Joan F. Brennecke, John Dymond, Michael Frenkel, Anthony R. H. Goodwin, Andreas Heintz, Kenneth N. Marsh, Cornelis J. Peters, Jason A. Widegren. **Apologies:** Ken Seddon, Luis Paulo Rebelo, Joseph Magee

**Summary of discussion:** The first item considered was whether or not to include [bmim][Tf<sub>2</sub>N] in the project. Previously it had been decided that [hmim][Tf<sub>2</sub>N] would be the primary ionic liquid (IL) for this project because of a patent covering [bmim][Tf<sub>2</sub>N] in the USA. However, in the e-mail discussion prior to this meeting it was suggested that groups outside the USA could make measurements on [bmim][Tf<sub>2</sub>N] as well. After a brief discussion it was decided that the IUPAC project would only cover work on the [hmim][Tf<sub>2</sub>N]. While work on the [bmim][Tf<sub>2</sub>N] is not discouraged, it is not an official part of the IUPAC project.

J. Brennecke reported that the synthesis and purification of the approximately 1 liter of [hmim][Tf<sub>2</sub>N] for this project would be complete around the end of August. (We should all remember to acknowledge Mark Muldoon in any publications that result from the use of this IL.) At that point, the IL will be shipped to NIST for distribution. The IL will be dried at NIST and the water content determined by coulometric Karl Fischer titration. Unless otherwise arranged, the IL will be shipped dry in vacuum (Schlenk) tubes.

For the pure fluid, J. Magee will coordinate measurements of density, heat capacity and viscosity. K. Marsh will coordinate measurements of thermal conductivity, dielectric constant, electrolytic conductivity, surface tension and speed of sound. For mixtures of the ionic liquid, J. Brennecke will coordinate measurements of gas solubility, A. Heintz will coordinate measurements of VLE,  $\gamma_i^E$  and  $H_i^{E,8}$ , and L. Rebelo will coordinate LLE and density measurements on mixtures ( $V^E$ ). While measurements should be made over as wide a temperature range as possible, they must include 298 K. Gas solubility measurements will be made for CO<sub>2</sub> (high solubility), ethane (medium solubility), and H<sub>2</sub> (low solubility). Other mixture data will be collected for an alcohol, probably hexanol since butanol is totally miscible with [hmim][Tf<sub>2</sub>N] at room temperature. There is no restriction on the publication of data collected for this project.

Although not discussed at this meeting, Ken Seddon will coordinate measurements of  $T_g$ ,  $T_m$ , and  $T_{decomp}$  in both air and N<sub>2</sub>, at both fast and slow heating rates (perhaps 10 K/min and 2 K/min).

There was a discussion of the scientists that will be recruited to measure each property, along with estimates of the amount of IL required for each measurement. Final decisions about participants will be left up to the coordinators for each category of set of measurements. The names and addresses of each participant should be e-mailed to J. Widegren by September 15<sup>th</sup> (now end of November) J. Widegren will coordinate the shipping date and the amount of material to be shipped to each participant. Samples will be mailed by the end of October (now end of November) unless otherwise arranged. The experimental portion of the project should be completed by July 31, 2005.

## PARTICIPANTS IN THE MEASUREMENT PROGRAM:

### GAS SOLUBILITY (J. Brennecke, Coordinator)

Joan Brennecke  
Margarida Costa Gomez  
Gerd Maurer  
Cor Peters

### VLE, GAMMA INFINITY, AND EXCESS ENTHALPY (A. Heintz, Coordinator)

Andreas Heintz (VLE, gamma infinity, excess enthalpy)  
Trevor Letchor (gamma infinity)

### DENSITY, VISCOSITY, HEAT CAPACITY (J. Magee, Coordinator)

Ken Marsh (density and viscosity)  
Jason Widegren (viscosity)  
Don Archer (heat capacity)  
Joan Brennecke  
Ken Seddon  
Tooru Atake (heat capacity)  
Luis Paulo Rebelo (density)

### THERMAL CONDUCTIVITY, RELATIVE PERMITTIVITY, ELECTROLYTIC CONDUCTANCE, SURFACE TENSION, SPEED OF SOUND (K. Marsh, Coordinator)

Ken Marsh (thermal conductivity, relative permittivity, electrolytic conductance)  
Andreas Heintz (surface tension)  
Luis Rebelo (speed of sound)  
Richard Perkins (thermal conductivity)  
Jason Widegren (electrolytic conductance)

### LIQUID-LIQUID EQUILIBRIA, EXCESS VOLUMES (Luis Paulo Rebelo, Coordinator)

Luis Paulo Rebelo (LLE and VE)  
Andreas Heintz (LLE)

### DECOMPOSITION TEMPERATURE, THERMAL ANALYSIS (Ken Seddon, Coordinator)

Ken Seddon (decomposition temperature, T<sub>g</sub>, T<sub>m</sub>)