

Meeting of Task Group, IUPAC project 2002-005-1-100: Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems, Snowbird May 2004 (during PPEPPD Conference)

Attendees: Ken Marsh, Joan Brennecke, Cor Peters, Michael Frenkel

It was agreed:

1. We would recommend that 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, hmimTf₂N be the reference compound.
2. Joe Magee, Joan Brennecke, and Ken Seddon would be responsible for the obtaining of the starting materials and the preparation of the material. It is probably that NIST could purchase the materials (1-chlorohexane, 1-methylimidazole, and Lithium Tf₂N) and send to Joan for making. NIST would be asked to distribute the material. A small amount of the material would be purchased from Merck and a property sensitive to impurity (e.g. viscosity) be measured and compared with the prepared material.
3. Responsibility for contacting various researchers to organize particular property measurements would be distributed amongst the members in the following way:

Pure fluid properties:

- a. Heat capacity, viscosity, and density: Joe Magee
- b. Thermal conductivity, electrical conductivity, relative permittivity: Ken Marsh
- c. TGA (in nitrogen and air), DSC, melting point, Ken Seddon

Mixture properties:

- a. Gas solubility (low, medium and high solubility gases): Joan Brennecke
- b. Supercritical:: Cor Peters
- c. LLE: Luis Rebelo
- d. VLE, gamma infinity (and possibility enthalpy of mixing but this could require a lot of fluid): Andreas Heintz

various members of the Project can work with the responsible member for specific property measurements.

The following needs to be considered in asking research groups to make measurements:

- a. a maximum of three groups to measure a particular property and if significant differences additional groups might be asked to make measurements
- b. Each group should have access to Karl Fischer to determine water content before and after the measurements
- c. Each group should require at a maximum 100 ml. This should be returned to NIST or Ken Seddon after the measurements
- d. If measurements made at high temperature the sample purity should be checked by NMR before reuse.

- e. Water content must be < 100 ppm in order to make any measurement
- f. guide on how to dry and recover the sample will be distributed to each measurement group
- g. guide on how to do a Karl Fischer titration will be distributed

Please send any comments, additional suggestions for property measurements, etc. ASAP

There will be a meeting of the committee at the IACT/IUPAC International Conference on Chemical Thermodynamics in Beijing, August 15 to August 20. Date and meeting place to be finalized. There will be an open discussion at the ionic liquid workshop at the .ICCT meeting.

It would be good if the groups that would be willing to contribute to the various measurements be finalized by that date.