

## Estimation of Vapor Pressures and Vaporization Enthalpies of Ionic Liquids

Yong Huang<sup>S</sup> and Joan Brennecke<sup>C</sup>

University of Notre Dame, Chemical and Biomolecular Engineering, Notre Dame, IN, U.S.A.

*jfb@nd.edu*

Ionic liquids (ILs) are organic salts with low melting points (below 100 °C). Due to extremely low vapor pressure, relatively high thermal stability and other tunable properties, ILs are being investigated for a variety of applications, including solvents for reactions and separations and as heat transfer fluids. Since 2003, there have been several reports of successful thermal vaporization of ILs<sup>1-3</sup>. This work focuses on vapor pressures and vaporization enthalpies of thermally stable imidazolium and pyridinium ILs with the bis(trifluorosulfonyl)amide anion by isothermal thermogravimetric analysis (TGA, Mettler Toledo) under an inert environment. All experiments were performed at five temperatures between 240 and 320 °C for 16 hours under a nitrogen or helium environment. The data was evaluated by using a pseudo zero-order vaporization mechanism because the weight loss as a function of time is highly linear. Methyl paraben was used as a calibration standard to calculate the TGA vaporization constant, and then vapor pressures of several organic compounds, as well as the ILs, were analyzed by the Langmuir and Antoine equations. Vaporization enthalpies and  $T_{1\%/1\text{day}}$  (the temperature at which 1% weight loss occurs in 1 day) of the ILs were calculated with the Clausius-Clapeyron equation. Furthermore, several ILs were studied by chromatoprobe gas chromatography/mass spectrometry (GC/MS, Varian) under a helium environment in both EI and CI modes to confirm vaporization or decomposition products at same high temperatures. GC/MS spectra results showed that most ILs could be vaporized at high temperature, although dealkylation of the imidazolium or pyridinium ring may occur for a very small fraction of the IL samples.

(1) Paulechka, Y.; Kabo, G.; Blokhin, A.; Vydrov, O.; Magee, J.; Frenkel, M. *J. Chem. Eng. Data* **2003**, *48*, 457-462.

(2) Earle, M. J.; Esperanca, J. M. S. S.; Gilea, M. A.; Lopes, J. N. C.; Rebelo, L. P. N.; Magee, J. W.; Seddon, K. R.; Widegren, J. A. *Nature* **2006**, *439*, 831-834.

(3) Heym, F.; Etzold, B. J. M.; Kern, C.; Jess, A. *Green Chem.* **2011**, *13*, 1453-1466.