## 167b Gas Solubilities in Tunable Ionic Liquids

*Jessica L. Anderson, JaNeille K. Dixon, Mark J. Muldoon, Edward J. Maginn, and Joan F. Brennecke* We are interested in how ionic liquids (ILs) can be tuned for specific and selective gas separations, as well as solvents for reactions involving permanent gases like O2. Selection of different combinations of anions and cations allow the IL to be tuned for specific purposes. We and others have shown previously that the properties of an IL, including gas solubilities, are affected most strongly by the anion, and less strongly by the cation. Thus, using systematic changes in the anion and cation, the goal of this work is to measure the solubility of gases in various ILs in order to understand the structure property relationships of ILs for gas solubility.

The pure gas solubilities were measured in various imidazolium- and pyridinium-based ILs making use of both physical and chemical absorption. In all cases, solubility increased with an increase in pressure, measured up to 400 bar at temperatures ranging between 10 to 60 oC. The solubility of CO2 was found to be the greatest in all ILs, followed by hydrocarbons such as CH4, C2H6, and C2H4, then subsequently by O2 and N2. Physical absorption of gas increased with increased fluorination; the effect was most pronounced with fluorination on the anion, i.e. moving from the tris(pentafluoroethyl)trifluorophosphate to the tris(heptafluoropropyl)-trifluorophosphate, but also occurred with fluorination on the cation, i.e. the 1-methyl-3-(nonafluorohexyl)-imidazolium versus the 1-methyl-3-(tetradecylfluorooctyl)-imidazolium. Chemical absorption by ILs containing amine, acetate and other functional groups, was found to be superior to physical absorption. However, desorption of the gas was much slower with the chemically absorbed gas than that of the physically absorbed gas. Not only will this slow down the rate at which the absorbent can be regenerated, the higher binding energy will also increase regeneration energy costs. Thus, we will show that we are able to measure the gas solubility in various ILs using both physical and chemical absorption, furthering knowledge of property-structure relationships between the gas and IL.