Chemically Tunable Ionic Liquids with Aprotic Heterocyclic Anion (AHA) for Post-Combustion Carbon Dioxide Capture

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Non-volatility, good thermal stability and high CO_2 solubility make Ionic Liquids (ILs) a promising replacement for current volatile solvents used in post-combustion CO_2 capture. One of the most attractive advantages is that the physiochemical properties can be varied by tuning cation/anion combinations and their chemical substituents. The reaction enthalpy of ILs with CO_2 is directly related to the CO_2 capacity and regeneration energy, and this binding energy can also be tuned. In a recent paper, aprotic heterocyclic anions, or "AHAs", have been introduced to bind CO_2 with reaction energies that are suitable for gas separations, without suffering large viscosity increases [1]. First, the CO_2 absorption isotherms were obtained at a total of five temperatures (22, 40, 60, 80 and 100 °C) for trihexyltetradecylphosphonium pyrrolide ([P_{66614}][2-CNpyr]). From these isotherms, the enthalpy and entropy of absorption are determined. Since a wide range of tunability of the reaction enthalpy is possible for these AHAs, we have synthesized and characterized ILs bearing a phosphonium cation and indolide, imidazolide, pyrrolide, pyrazolide and triazolide-based anions that span a wide range of predicted reaction enthalpies with CO_2. The capacity of CO_2 in each AHA-based IL was experimentally measured at pressures between 0 and 1 bar at 22 °C. The experimental results are in good agreement with computed enthalpies of IL-CO_2 reaction products from computational simulation. As water vapor would be naturally present in a post-combustion CO_2 capture process, the behavior of H_2O in an IL/CO_2 system and the effect of water on CO_2 absorption by ILs will also be discussed.

[1] Gurkan, B.; Goodrich, B. F.; Mindrup, E. M.; Ficke, L. E.; Massel, M.; Seo, S.; Senftle, T. P.; Wu, H.; Glaser, M. F.; Shah, J. K.; Maginn, E. J.; Brennecke, J. F.; Schneider, W. F. *J. Phys. Chem. Lett.* **2010**, *1*, 3494–3499.