

Physical and Chemical Absorption of Carbon Dioxide in Room-Temperature Ionic Liquids

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Gaseous solubilities (vapor-liquid equilibria) of carbon dioxide (CO₂) in 18 room-temperature ionic liquids (RTILs) have been measured using a gravimetric microbalance. [1-5] The observed pressure-temperature-composition (*PTx*) data have been analyzed by use of an equation-of-state (EOS) model. Henry's law constants have been obtained from the observed (*PTx*) data directly and/or from the EOS correlation. Ten RTILs among the present ionic liquids results in the physical absorption and eight RTILs show the chemical absorption. The classification of whether the absorption is the physical or chemical type is based on the excess Gibbs and enthalpy functions as well as the magnitude of the Henry's constant. In the chemical absorption cases, the ideal association model has been applied in order to interpret those excess thermodynamic functions. Then, two types of the chemical associations (AB and AB₂, where A is CO₂ and B is RTIL) have been observed with the heat of complex formation of about -11 (for AB) and from -27 to -37 (for AB₂) kJ mol⁻¹, respectively. The present EOS has also predicted partial immiscibility at the CO₂-rich side solutions and vapor-liquid-liquid equilibrium experiments using a mass-volume method have confirmed our predictions. Quantitative predictions for the separation of CO₂ and hydrogen (H₂) have been made using our EOS model and indicate high selectivity (CO₂/H₂: 30-300) can be obtained using RTILs.

- [1] M. B. Shiflett and A. Yokozeki, *Ind. Eng. Chem. Res.* 44 (2005) 4453-4464.
- [2] M. B. Shiflett and A. Yokozeki, *J. Phys. Chem. B* 111 (2007) 2070-2074.
- [3] A. Yokozeki and M. B. Shiflett, *Appl. Energy* 84 (2007) 351-361.
- [4] M. B. Shiflett, D. J. Kasprzak, C. P. Junk, and A. Yokozeki, *J. Chem. Thermodyn.* 40 (2008) 25-31.
- [4] A. Yokozeki, M. B. Shiflett, C. P. Junk, L. M. Grieco, and T. Foo, *J. Phys. Chem. B*, (2008) in press.
- [5] M. B. Shiflett and A. Yokozeki, *J. Chem. Eng. Data* (2008) in press.