Measurement and Prediction of Solubility of CO_2 in the Ionic Liquids [bmim][PF_6], [bmim][BF_4], and [bmim][Tf_2N]

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Among their many unique properties, the non-volatility of ionic liquids has opened up a possibility to replace conventional solvents with them in CO_2 absorption processes. An enormous number of experiments have been carried out to measure the solubility of CO_2 in over 200 different ionic liquids. [bmim][PF_6], [bmim][BF_4], and [bmim][Tf_2N] are three well-known examples of ILs studied.

In this work, these ILs have been selected to evaluate a method which predicts their capacity to dissolve CO_2 at given temperatures. The solubility of CO_2 in these ILs was predicted based on their structures using a quantum mechanical method, namely the COSMO-RS approach. The Henry's law constants calculated using the COSMOthermX program for the above ILs were correlated with the energy parameters in group-contribution non-random lattice fluid equation of state (GC-NLF EoS). These correlations were used to predict the solubility of CO_2 in each ionic liquid at temperatures 278 K, 288 K, and 298 K. Then the results were compared with experimental solubility data obtained using a closed phase equilibrium cell in water bath.