Predicton of CO_2 solubility in ionic liquids using a quantum mechanical method

김지은, 강정원*
고려대학교
(jwkang@korea.ac.kr*)

The non-volatility of ionic liquids has opened up a possibility to replace conventional solvents with them in CO_2 absorption, an important separation technique. Many experiments have already been carried out to measure the solubility of CO_2 in different ILs. However, the number of ILs that can be made is too large to test them all experimentally. Therefore an effective simulation approach is appreciated.

In this work, the solubility of CO_2 in various ILs was predicted using a quantum mechanical method, namely the COSMO-RS approach. First, the Henry's law constants were calculated using the quantum mechanical method for a number of ILs. These values were correlated with the energy parameters in group-contribution hydrogen-bonding non-random lattice fluid equation of state (GC NLF-HB EoS). This correlation was used to predict the solubility of CO2 in some other ILs from their Henry's law constants. Finally, the results were compared with experimental data for the evaluation.