

Thermodynamic modelling of CO₂ solubility in ionic liquids

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Ionic liquids are salts that exist as liquids at ambient temperature, and have negligible vapor pressure. Since its first synthesis in the early 20th century, ionic liquids have been studied to a large extent, owing to the fact that they have unique properties which could be useful in various processes. Recently, using supercritical CO₂ to separate reaction products dissolved in an ionic liquid was proposed, and many researches have carried out experiments and measured the solubility of CO₂ in different ionic liquids. However, there has been only a few researches going on regarding the prediction of CO₂ solubilities in ionic liquids. In this study, a thermodynamic model involving quantum mechanics to predict CO₂ solubility in different ionic liquids will be made and compared to experimental data.