

<b>PB 02</b>
<b>CO<sub>2</sub>/hydrocarbon selectivity of phosphonium based ionic liquids</b>
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Abstract (less than 300 words)
<p>Carbon dioxide (CO<sub>2</sub>) separation is critical in the petrochemical industry for natural gas purification and coal gasification. Chemical/physical absorption, adsorption, and membrane separation have been attempted for CO<sub>2</sub> separation from CO<sub>2</sub>-hydrocarbon gas mixtures. The conventional physical absorbents such as Selexol and Rectisol absorb a large amount of CO<sub>2</sub> and a significant amount of hydrocarbons such as methane (CH<sub>4</sub>), therefore, their CO<sub>2</sub>/hydrocarbon selectivities are not so high. Ionic liquids (ILs) are expected to be a promising alternative to the conventional physical absorbents because of their comparable CO<sub>2</sub> solubilities and high CO<sub>2</sub>/CH<sub>4</sub> selectivities ranging from 10 to 20 [1].</p> <p>In the previous study, trihexyl(tetradecyl)phosphonium bis(trifluoromethanesulfonyl)amide ([P<sub>66614</sub>][TFSA]) and trihexyl(tetradecyl)phosphonium perfluorooctanesulfonate ([P<sub>66614</sub>][PFOS]) were chosen as the ILs with superior CO<sub>2</sub> absorption by predicting Henry's law constants of CO<sub>2</sub> in 68775 ILs using conductor like screening model for realistic solvation (COSMO-RS) method [2]. Based on the prediction results, CO<sub>2</sub> solubilities of the selected phosphonium based ILs were measured at 313.15 K and 333.15 K [3].</p> <p>In the present study, hydrocarbon such as CH<sub>4</sub>, ethane (C<sub>2</sub>H<sub>6</sub>), and ethylene (C<sub>2</sub>H<sub>4</sub>) solubilities in [P<sub>66614</sub>][TFSA] or [P<sub>66614</sub>][PFOS] were measured at 313.15 K and 333.15 K by using a magnetic suspension balance. Henry's law constants of CO<sub>2</sub> or hydrocarbon were calculated from the experimental solubility data at pressures lower than 0.4 MPa. Furthermore, CO<sub>2</sub>/hydrocarbon selectivities of ILs were obtained from the ratio of CO<sub>2</sub> and hydrocarbon experimental solubility data.</p>
References
<p>[1] L.M.C. Pereira <i>et al.</i>, <i>J. Supercrit. Fluids</i>, 110 (2016) 56-64.</p> <p>[2] N. Kuroki <i>et al.</i>, <i>J Comput. Chem. Jpn.</i>, 18(5) (2019) 217-220.</p> <p>[3] D. Kodama <i>et al.</i>, <i>Preprints of SCEJ 51st Autumn Meeting</i>, Morioka, (2020) Y216.</p>
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