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Screening of Ionic Liquids for Hydrogen Sulfide Removal Using COSMO-RS

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Abstract : The capability of ionic liquids in various applications makes them attracted by many researchers. They have potential to be developed as “green” solvents for gas separation, especially H2S gas. In this work, it is attempted to predict the solubility of hydrogen sulfide (H2S) in ILs by COSMO-RS method. Since H2S is a toxic pollutant, it is difficult to work on it in the laboratory, therefore an appropriate model will be necessary in prior work. The COSMO-RS method is implemented to predict the Henry’s law constants and activity coefficient of H2S in 140 ILs with various combinations of cations and anions. It is found by the screening that more H2S can be absorbed in ILs with [Cl] and [Ac] anion. The solubility of H2S in ILs with different alkyl chain at the cations not much affected and with different type of cations are slightly influence H2S capture capacities. Even though the cations do not affect much in solubility of H2S, we still need to consider the effectiveness of cation in different way. The prediction results only show their physical absorption ability, but the absorption of H2S need to be consider chemically to get high capacity of absorption of H2S.

Keywords : H2S, hydrogen sulfide, ionic liquids, COSMO-RS
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