

## 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 H<sub>2</sub>S gas. In this work, it is attempted to predict the solubility of hydrogen sulfide (H<sub>2</sub>S) in ILs by COSMO-RS method. Since H<sub>2</sub>S 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 H<sub>2</sub>S in 140 ILs with various combinations of cations and anions. It is found by the screening that more H<sub>2</sub>S can be absorbed in ILs with [Cl] and [Ac] anion. The solubility of H<sub>2</sub>S in ILs with different alkyl chain at the cations not much affected and with different type of cations are slightly influence H<sub>2</sub>S capture capacities. Even though the cations do not affect much in solubility of H<sub>2</sub>S, 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 H<sub>2</sub>S need to be consider chemically to get high capacity of absorption of H<sub>2</sub>S.

**Keywords :** H<sub>2</sub>S, hydrogen sulfide, ionic liquids, COSMO-RS

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