

Screening of Metal Chloride Anion-based Ionic Liquids for Direct Conversion of Hydrogen Sulfide by COSMO-RS

Authors : Muhammad Syahir Aminuddin, Zakaria Man, Mohamad Azmi Bustam Khalil

Abstract : In order to identify the best possible reaction media for performing H₂S conversion, a total number of 300 different ILs from a combination of 20 cations and 15 anions were screened via COSMO-RS model simulations. By COSMO-RS method, thermodynamic and physicochemical properties of 300 ILs, such as Henry's law constants, activity coefficient, selectivity, capacity, and performance index, are obtained and analyzed. Thus, by comparing the performance of ILs via COSMO-RS, a series of TSILs containing cation of [P66614] with metal chloride anions such as Fe, Ga, and Al were chosen and selected for synthesis based on their performance predicted by COSMO-RS and their economic values. Consequently, the physiochemical properties such as density, viscosity, thermal properties, as well as H₂S absorptive oxidation performances in those TSILs will be systematically investigated.

Keywords : conversion of hydrogen sulfide, hydrogen sulfide, H₂S, sour natural gas, task specific ionic liquids

Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development

Conference Location : Chicago, United States

Conference Dates : December 12-13, 2020