Self-Diffusion Coefficients of Gases in Ionic Liquids [EMIM][B(CN)₄] and [HMIM][B(CN)₄]

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The removal of harmful gases from industrial flue gas streams originating from the combustion of fossil fuels has attracted tremendous attention as a consequence of the impact of such gases on global warming. At present, task-specific ionic liquids (ILs) are intensively discussed regarding their capabilities as gas separation media. For the selective absorption of CO₂, ILs based on the tetracyanoborate anion are attractive agents due to their high solubility for this gas. In addition to solubility data, gas diffusion coefficients are of practical importance for process design. In general, there is a lack of such data for mixtures of ILs with absorbed gases. In the present study, molecular dynamics (MD) simulation is used to calculate self-diffusion coefficients for the gases CO₂, H₂S, H₂, CO, CH₄, N₂, and O₂ in the tetracyanoborate-based ILs [EMIM][B(CN)₄] (1-ethyl-3-methylimidazolium tetracyanoborate) and [HMIM][B(CN)₄] (1-hexyl-3-methylimidazolium tetracyanoborate) at atmospheric pressure in dependence on temperature from 298.15 K to 363.15 K. The investigations for the two homologous ILs allow studying the influence of the cationic chain length on the diffusion coefficients. Based on newly developed force fields for both ILs, diffusivity data were obtained solving the Einstein equation. For each IL, the computed diffusivities for CO₂, H₂S, CO, CH₄, N₂, and O₂ are all in the same range, apparently due to their similar molar liquid volumes. Yet, the values for H₂ with comparable molar volume are almost one order of magnitude larger. Comparison with experimental data was only possible for the system CO₂ and [EMIM][B(CN)₄] at 298.15 K. Here, the deviation of the simulated from the measured datum is less than 10%.