Mutual and Self-Diffusion Coefficients of Binary Mixtures of 1-Ethyl-3-methylimidazolium Tetracyanoborate with Dissolved Gases by Using Dynamic Light Scattering and Molecular Dynamics Simulations

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Ionic liquids (ILs) based on the tetracyanoborate ($[B(CN)_4]^-$) anion are potential working fluids for the separation of carbon dioxide (CO_2) from flue gas. For a selective separation of CO_2 from other flue gas components, reliable mutual diffusivity and solubility data are required for mixtures of ILs with dissolved gases. In the present study, dynamic light scattering (DLS) and molecular dynamics (MD) simulations were used for the characterization of the molecular transport in binary mixtures of the IL 1-ethyl-3-methylimidazolium tetracyanoborate ($[EMIM][B(CN)_4]$) with the dissolved gases CO_2, nitrogen, carbon monoxide, hydrogen, methane, oxygen, and hydrogen sulfide at temperatures from 298.15 to 363.15 K and pressures up to about 60 bar. For the binary mixtures of the IL with gases, the mutual diffusivities measured by DLS can be compared with self-diffusivities of the corresponding gases calculated by MD. At infinite dilution of the dissolved gas, mutual diffusivity and self-diffusion coefficients should match, which was confirmed by our study. Furthermore, experimental mutual diffusivities and simulated self-diffusion coefficients are in good agreement with literature. The results from DLS and MD reveal that for the IL hydrogen mixtures distinctly larger diffusion coefficients are obtained in comparison to mixtures with all other gases. This behavior might be caused by the quantum characteristics of hydrogen and results in the failure of a correlation of the mutual diffusivities with the molar volume of the gas at its normal boiling point.