

Enhanced CO₂ Solubility in Aromatic and Alkyl Chain Substituted Imidazolium-based Room Temperature Ionic Liquids

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Room-temperature ionic liquids (RTILs) are molten organic salts that possess a number of desirable properties for gas separations applications. Their high thermal and chemical stability, negligible vapor pressures, and tunable chemistry make them great candidates to replace less environmentally friendly materials such as volatile organic compounds. The versatile functionality of RTILs allows for their potential usage for gas separations as a bulk fluid, a supported liquid membrane, or as a polymerized RTIL solid membrane. Gas separations in these materials are driven by large solubility differences between gases, rather than by diffusion differences. Therefore, it is important to investigate the gas transport properties in RTILs to better understand their gas separation capabilities.

This study focuses on the solubility (S), diffusivity (D), permeability (P), and selectivity behaviors of CO₂, CH₄, and N₂ gases in bulk fluid RTILs at constant temperature (22C). The bulk fluid RTILs tested are 1-methyl, 3-tolyl imidazolium bis(trifluoromethanesulfonyl)imide ([c₁tim][Tf₂N]), 1-ethyl, 3-paraxylyl imidazolium bis(trifluoromethanesulfonyl)imide ([c₂pxim][Tf₂N]), 1-butyl, 3-paraxylyl imidazolium bis(trifluoromethanesulfonyl)imide ([c₄pxim][Tf₂N]), 1-hexyl, 3 paraxylyl imidazolium bis(trifluoromethanesulfonyl)imid ([c₆pxim][Tf₂N]), 1-octa, 3 paraxylyl imidazolium bis(trifluoromethanesulfonyl)imid ([c₈pxim][Tf₂N]), and 1-deca, 3 paraxylyl imidazolium bis(trifluoromethanesulfonyl)imid ([c₁₀pxim][Tf₂N]). Our initial results show that gas solubility increases, diffusivity has a small variance, and permeability slightly increases with increasing alkyl chain length. Solubility and permeability selectivity decreases while diffusion selectivity remains relatively unchanged with increasing chain length. The addition of the aromatic ring substitution shows enhanced solubility over analogous alkyl-chain only substituted RTILs. Also, our work demonstrates that regular solution theory is valid for these RTILs.