

Supercritical Fluid Chromatography as a Source of Solute Partition Coefficients in Room-Temperature Ionic Liquid-scCO₂ Systems

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Systems involving supercritical carbon dioxide (scCO₂) form a specific segment in rapidly growing applications of room-temperature ionic liquids (RTILs) in green chemistry and technology. Biphasic RTIL-scCO₂ solvent systems can be employed in biphasic catalysis, enzymatic processes, or in extractions of organic nonelectrolytes from a RTIL environment with scCO₂. In such applications, partition coefficients are needed of the organic compounds between the RTIL-rich phase and the CO₂-rich phase.

In this contribution, the pros and cons are discussed of supercritical fluid chromatography (SFC) as a prospective source of thermodynamic information on partitioning of a dilute solute between both phases in a RTIL-scCO₂ system. Apart from infinite-dilution partition coefficients of organic nonelectrolyte solutes of diverse volatilities, estimates of solubility parameters of CO₂-loaded RTILs can also be obtained from solute retention times in SFC. The previous results with 1-butyl-3-methylimidazolium tetrafluoroborate ([bmim][BF₄]) indicate that the limiting partition coefficients of solutes in RTIL-scCO₂ systems can be described and possibly predicted with linear solvation energy relationships employing solute descriptors of Abraham et al. In application-oriented part of this contribution, limiting partition coefficients are presented of several sulfur-containing aromatic heterocycles between both phases in 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide-scCO₂ system.

Practical concerns and precautions in preparing wall-coated, open tubular capillary columns are also mentioned. While capillary columns with [bmim][PF₆] and [bmim][BF₄] are relatively stable, a [hmim][Tf₂N] column showed significant bleeding of the RTIL from the column, with the bleeding rate dependent on the density of CO₂.

Our previous data on solute partition coefficients in alkylmethylimidazolium-based RTIL-scCO₂ systems are compared with preliminary results for systems containing a phosphonium-based RTIL.