

Pyridinium-based ionic liquids bearing a thiocyanate anion for the selective extraction of aromatics from aliphatic hydrocarbon mixtures

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The performance of N-alkylpyridinium-based ionic liquids with a SCN anion (PyILs) was evaluated for the selective extraction of aromatics from aliphatic hydrocarbons. The aromatic extraction ability of PyILs was greatly enhanced by the presence of a methyl group on the pyridinium ring at the 3- or 4-position, whereas the solubility of the aromatics in the PyILs decreased with increasing number of methyl groups on the benzene ring. The FT-IR studies revealed that the solubility of an aromatic compound in a PyIL is closely correlated with the degree of aromatic C-H bending frequency shift observed during the dissolution of the aromatic compound in the PyIL: the larger the shift, the higher the solubility. The computational calculations on the dispersion interactions between aromatics and PyILs demonstrated that the anion-aromatic interaction is much more important than the cation-aromatic interaction in determining the aromatic solubility in PyILs, and such anion-aromatic interaction can be enhanced by introducing a methyl group at the carbon atom of the pyridinium ring.