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# Insights into Ionic Liquid/Aromatic Systems from NMR Spectroscopy: How Water Affects Solubility and Intermolecular Interactions

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Hydrocarbon solubility and chemical interactions in ten imidazolium- and pyridinium-based ionic liquids (ILs) with four different anions (thiocyanate $[SCN]^-$, dicyanamide $[DCA]^-$, tricyanomethanide $[TCM]^-$, and bis(trifuoromethylsulfonyl)imide $[NTf_2]^-$) have been studied by $^1H$ and $^{13}C$ NMR spectroscopy. The anion structure has the main influence on the anion–aromatic chemical interaction strength; it is directly correlated to the NMR chemical shift deviations but not to the hydrocarbon solubility. The $[TCM]^-$ anion shows the largest chemical shift deviations, but the $[NTf_2]^-$ anion has the highest hydrocarbon solubility due to steric effects. Higher water contents decrease the hydrocarbon solubility in ILs. Ion-water solvation mainly occurs until 1 $mol_{water}/mol_{IL}$ with the saturation limit at 10 $mol_{water}/mol_{IL}$. Toluene-ion interactions are stronger than water–ion interactions in $[DCA]^-$ and $[TCM]^-$-based ILs, but they have a similar or even lower strength in $[SCN]^-$-based ILs.

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