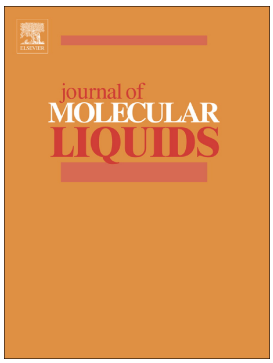

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Molecular dynamics simulation of aqueous 1-dodecyl-3-methylimidazolium chloride: Emerging micelles

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Abstract

In this computational study, we investigate the morphology and dynamics of nanostructures formed by the ionic liquid 1-dodecyl-3-methylimidazolium chloride $[C_{12}mim]Cl$ dissolved in water. Recent works emphasize the positive impact of this additive on various catalytic transformations. The assembling process revealed by molecular dynamics simulation is discussed in detail. For verification, small-angle X-ray scattering diffractograms and dielectric relaxation spectra are calculated from the trajectories and compared to experimental ones. For the latter, we offer an alternative hypothesis to the contemporary interpretation based on our component analysis.

Keywords: molecular dynamics simulation, ionic liquid, micelle, self-assembly, SAXS, dielectric spectroscopy

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