

Abstract Submitted
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Nanoscale heterogeneity in alkyl-methylimidazolium bromide ionic liquids DAVID PRICE, BACHIR AOUN, MARIE-LOUISE SABOUNGI, ANDREAS GOLDBACH, MIGUEL A. GONZÁLEZ, SHINJI KOHARA — High-energy x-ray diffraction measurements on 1-alkyl-3-methylimidazolium bromide ionic liquids with ethyl, butyl and hexyl alkyl chains reveal a peak at low scattering vector Q that rises and moves to lower Q with increasing chain length. Atomic molecular dynamics simulations, which give results in excellent agreement with the x-ray data, show that this behavior is most pronounced in the partial structure factor for the tails of the alkyl chains but is also seen in those for the imidazolium ring centers and anions. The heterogeneity with a length scale of 1.9 nm established for the liquid with the hexyl chain is quantified by a density heterogeneity order parameter that shows a clustering of the tails. Our results are consistent with explanations in the literature of the increase in viscosity with alkyl chain length in terms of nanoscale segregation.

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