Molecular Dynamics Simulations of Heterogeneous Hydrogen Bond Environment in Hydrophobic Deep Eutectic Solvents

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Abstract

Hydrophobic deep eutectic solvents (DESs) have emerged as excellent extractants. Their performance depends on the heterogeneous hydrogen bond environment formed by multiple hydrogen bond donors and acceptors. An understanding of this heterogeneous hydrogen bond environment can be used to develop principles for designing high-performance DESs for extraction and other separation applications. We investigate the structure and dynamics of hydrogen bonds in eight hydrophobic DESs formed by decanoic acid, menthol, thymol, and Lidocaine using molecular dynamics simulations. The results show the diversity of hydrogen bonds in the eight DESs and their impact on diffusivity and molecular association. Each DES possesses four-six types of hydrogen bonds and one or two of them overwhelm the others in quantity and lifetime. The dominating hydrogen bonds determine whether the DESs are governed by intra- or inter-component associations. The component diffusivity presents an inverse relationship with the hydrogen bond strength.

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