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## Molecular interactions between betaine monohydrate-glycerol deep eutectic solvents and palmitic acid: Computational and experimental studies

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### Abstract

Recently, deep eutectic solvents (DES) have received great attention as green media, thus suitable for use for several different applications, such as reactions, separations and purifications. DES are formed by mixing the quaternary ammonium salt and the hydrogen bond donor (HBD) compound. Previous work studied the deacidification of palm oil using a betaine monohydrate-glycerol based DES as the solvent, and the results indicated that the ability of this DES to extract palmitic acid depends on the molar ratio of the salt to the HBD compound. Therefore, molecular interactions between betaine monohydrate-glycerol DES and palmitic acid at the different molar ratios of betaine monohydrate to glycerol were investigated by molecular dynamics simulation and experiments (FT-IR and NMR) in this work. The number of H-bond interactions between betaine monohydrate and glycerol molecules depends on the molar ratio of betaine monohydrate to glycerol in the DES. Based on the computational and experimental studies, the hydrogen bonding interactions between molecules were present. Palmitic acid interacts with the betaine monohydrate, and it can also possibly interact with glycerol molecules. The presence of palmitic acid in the mixtures induces an increase in the H-bond interactions between betaine and glycerol molecules.

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