

**Importance of Hydrogen Bonds on the Structure of Neat DES, their Solvation Properties and the Nature of their Liquid-Liquid interface with Water.
A Molecular Dynamics Study.**

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Deep Eutectic Solvents (DES) are gaining increasing attention as potential “environmentally friendly” alternatives to volatile organic solvents (VOCs). However, so far very little is known on the microscopic structure of these solvents and even less on their solvation properties or on their nature of their liquid – liquid interface. We report here results obtained from molecular dynamics (MD) studies on menthol - thymol mixtures of various compositions which can be seen as a prototype for hydrophobic type V DES. In particular we have investigated the importance of H-bonds for the formation of neat DES, but also on their solvation properties as well as on the nature of their liquid-liquid interface with water. In particular we describe how the formation of H-Bond networks evolves a) with the exact composition of the mixture and b) with temperature. Furthermore, we show how solvation properties of these mixtures vary as a function of the molar fraction of thymol in the mixture. Finally, we discuss how H-Bonds structure the interface between the menthol-thymol 1:1 mixture and water.

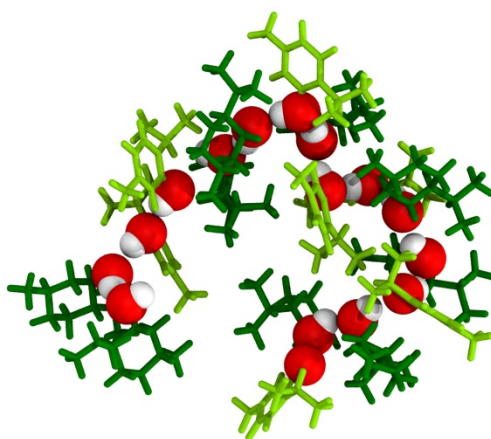


Figure: Snapshot extracted from the MD trajectory showing of a H-Bond network formed by 9 Menthol (*dark green*) and 7 Thymol (*light green*) in the Menthol – Thymol 1:1 mixture.