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Solvation properties of C60 fullerene in water-DMSO mixtures
CLEITON MACIEL, Universidade Federal do ABC, EUDES FILETI, Universidade Federal de São Paulo — Binary solvent mixtures present important properties that allow their use in wide field of applications. For instance, aqueous solutions of dimethyl sulfoxide have been use in biological systems due to the properties that can reach varying on the concentration of the compounds. Solvation properties in these mixtures have been explored but have never been reported investigations of solvation properties of large non polar solutes in that system. In this work, molecular dynamics simulations were employed to investigate the solvation properties of C60 fullerene immersed in water-DMSO binary mixtures. The role of DMSO as a cosolvent was studied modeling fullerene solutions varying the DMSO molar fraction from 0 to 1.0. Partial structural results showed a dense concentration of DMSO molecules around C60 at low DMSO content solutions. In high DMSO concentrations ($\sim$ 0.70) the average number of hydrogen bonds between DMSO and water molecules and the lifetime of these interactions were smaller and higher than poor DMSO solutions, respectively. Additionally, free energy calculations were performed and an increasing hydrophobic behavior of C60 was observed in DMSO rich solutions.

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