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Senior Project Title: Simulations of AOT Reverse Micelles with Chloride Salts

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## Abstract

Aqueous reverse micelles have been utilized as proxies for atmospheric aerosols. They are composed of a water core held together by surfactant molecules in a hydrophobic solvent. Such reverse micelles were composed of surfactant dioctyl sodium sulfosuccinate (AOT), water represented by TIP3P model and isooctane solvent in several MD simulations. They were created using Packmol and constant pressure-temperature simulations were conducted using GROMACS molecular dynamics package. These fully atomistic simulations were carried out using the CHARMM36 force field and the reverse micelle was unconstrained and allowed to move freely during the simulation. Specifically, the simulated reverse micelles had w 0 values of 10, 15, and 20. For each w 0 value the reverse micelles were simulated with either KCl, MgCl2, or CaCl2 at concentration values of 0 M, 0.25 M, 0.5 M, 0.8 M, and 1.0 M. The results indicate that the ions tend to form well defined layers in the interfacial region. Specifically, the cations reside near the anionic surfactant head groups and even replace the Na+ counter-ion of the surfactant while the Cl- anion prefers the water core. Density calculations suggest that the interfacial region of the reverse micelles are structured as follows: R-SO3- > Na+ ≥ cation > Cl- (Core). Other measurements calculated include mass distribution in the simulation box, radial distribution, and the distance of ions from the center of the water core. The impact of ionic concentration on shape and size of reverse micelles was also calculated. Ultimately, it was concluded that the connection between ionic concentration and shape of reverse micelle depends on the composition of the reverse micelle.