Understanding the Conformational Preferences of Tenside Surfactants

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Surfactants are chemical agents that lower the surface tension of a liquid or the interfacial tension between two liquids. Often, they are amphiphilic molecules that form micelles in solution at a critical concentration. These events are often characterized by changes in physical properties of the amphiphiles. Cationic surfactants have found an increasing role in a number of applications including liquid crystals, oil recovery, road repair, and prevention of metal corrosion. Alkyldimethylbenzylammonium compounds have been shown to display germicidal properties in addition to acting as traditional surfactants. This has been important in the development of novel cleaning and cosmetic agents. Because much of their behavior is mediated by solvent effects, it is important to computationally investigate these molecules by including solvent effects. Here, we attempt to understand the ensemble conformational properties of each of six amphiphilic, cationic surfactants through the use of conformational searching in conjunction with an implicit solvent model. We further elucidate the potential energy surfaces of these molecules through the use of density functional theory (DFT), also in conjunction with an implicit solvent model.