

Abstract Submitted
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Study on the Surfactant in the Dishwasher Detergent Using Chemical and Computational Analysis SEBIN LEE, SUNHEE LEE, CRG-NJ
— All the surfactants, the active agents in detergent consist of a hydrophobic group coupled to a hydrophilic group which has variations such as a negative or positive charge, no charge or a variable charge according to pH. In this research, computational methods employing quantum chemistry were used to model various surfactants in the linear alkyl groups and alkyl benzene sulphonates(ABS). The molecules were assessed for thermodynamic stability, reactivity and polarization. Certain number of Alkyl group based detergent and Alkyl benzene sulfate (ABS) molecules were tested for their thermodynamic stability which were measured through the optimized energy. Also the reactivity and conductivity were measured through the dipole moments to calculate the level of activity the molecule could have with other nearby molecules. Lastly, electrostatic potential maps were also used to visualize the polarization and assess the reactivity level of each molecule. Alkyl benzene sulfate(ABS) showed less activity and better stability. Alkyl group based detergent analogues showed better activity and less stability compared to the Alkyl benzene sulfate(ABS) due to their geometrical aspects. Depending on the degree of branching detergency performance and biodegradability were also discussed.

Richard Kyung
CRG-NJ

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