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COMPUTATIONAL INVESTIGATION OF STRUCTURAL, ELECTRONIC AND THERMODYNAMIC PROPERTIES OF NONYLPHENOL ETHOXYLATE SURFACTANTS

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Abstract: Nonylphenol ethoxylates (NPEs) are group of non-ionic surfactants commonly known as Tergitol NP surfactants. The hydrophilic-lipophilic-balance (HLB value) is used as the key parameter by surfactant formulators to study the properties of non-ionic surfactants. Even though the HLB values of two surfactants are equal or close enough to each other, the expected properties cannot be obtained by replacing one surfactant with another one. This issue leads to a necessity to carry out many trial and error tests to identify the equivalent surfactants in industrial applications. The strong hydrogen bonding with water, Gibbs free energy change of solvation (ΔG_{solv}), molecular dipole moment and maximum absorption wavelength (λ_{max}) have been developed as key performance indicators of a better surfactant in this research work. Computed results predict that NPEs are well stabilized in the aqueous medium with the extension of ethoxylate chain length, illustrating a linear relationship of ΔG_{solv} with respect to the number of ethylene oxide units. This evidence has been further supported by the decrease in hydrogen bond length, between the NPEs and water molecules with the extension of the ethoxylate chain of the surfactant. Among ortho- , meta-, and para-substituted NPEs, due to the presence of higher dipole moments of meta-substituted NPEs indicated that they form more efficient secondary interactions in aqueous medium. Moreover meta-substituted NPEs demonstrate relatively higher thermodynamic stability (than ortho- and para- substituted NPEs) due to the presence the highest HOMO-LUMO gap.
Keywords: Nonylphenol ethoxylates, NP surfactants, thermodynamic properties.

INTRODUCTION

A surfactant (surface active agent) is a chemical agent capable of reducing the surface tension of a liquid in which it is dissolved. The distinct properties of the surfactants in the aqueous medium can be described with the presence of a hydrophilic group and a hydrophobic chain in the molecule [1,2]. Nonylphenolethoxylate surfactants (NPEs) are odorless, pale yellow liquids or waxes which commercially abbreviated as Tergitol NP surfactants [3]. A molecule of Nonylphenolethoxylates contains one lipophilic, nonyl-hydrocarbon chain and one hydrophilic, ethoxylate chain (Figure 1). Most of physical properties such as melting point,

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