

Quantitative Relationship Analysis Of Anionic Surfactan Structures Of Sulfate Group Based On Large Ab Initio Calculations

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Abstract	<p>a:3:{i:0;s:1576:"Detergent has a unique ability to remove impurities, both water-soluble and non-soluble. It is because of the detergent, especially surfactant molecules (surface active agent) that serves to decrease interfacial tension so as to release the dirt on the surface of the material. Common types of surfactants used in detergents are anionic type in the form of sodium lauryl sulfate (C₁₂H₂₅SO₄Na). Sodium lauryl sulfate (C₁₂H₂₅SO₄Na) is an anionic surfactant that is used in industrial products such as floor cleaning products, car washing soap, and some household goods such as soap, toothpaste, and shampoo. The development of sulfate anionic surfactant is still performed to obtain a qualified surfactant. One of the parameter to determine the quality of the anionic surfactant is a critical micelle concentration (CMC). But the determination of CMC experimentally is difficult. Therefore, there needs to be a mathematical model to predict the CMC. The aim of this research is to prepare the mathematical equation to calculate the value of the CMC sulfate anionic surfactant class. This research was conducted with the depiction of any anionic sulfate groups to three-dimensional model of the compound, followed by optimizing the structure of the model class sulfate anionic surfactant with Large Ab Initio calculation method. Furthermore, descriptors were analyzed statistically with Multiple Linear Regression method (MLR). The results of statistical calculations show that to calculate the theoretical value of the CMC anionic sulfate groups this QSPR equation can be used :";i:1;s:79:"Log CMC = -170.181 - 0.383LogP + 0.027RD - 0 .008Avdw + 0 .804qC1 - 521. 846qC2";i:2;s:59:"n = 10 r2 = 0.996 SE = 0.6777 F = 75.257 PRESS = 0.01217112";}</p>
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