

ABSTRAK

Surfaktan anionik sulfat merupakan jenis surfaktan yang banyak digunakan sebagai agen pembersih. Penemuan dan pengembangan molekul surfaktan anionik sulfat perlu dilakukan karena memiliki dampak yang sangat besar, baik dibidang sains maupun ekonomi. Analisis Hubungan Kuantitatif Struktur-Sifat Fisik (HKSS) nilai Konsentrasi Misel Kritis (KMK) terhadap surfaktan anionik golongan sulfat telah dilakukan. Penelitian ini dilakukan dengan tujuan mendapatkan model persamaan matematika terbaik untuk menghitung konsentrasi misel kritis teoritis surfaktan anionik golongan sulfat. Penelitian dilakukan dengan menggunakan model tiga dimensi dari senyawa surfaktan anionik golongan sulfat dan perhitungan dilakukan menggunakan metode *ab initio* 6-31G**. Senyawa $C_{16}SO_4Na$ memiliki nilai tertinggi di beberapa deskriptor seperti log P sebesar 7,4; indeks refraktivitas sebesar $86,72 \text{ \AA}^3$; berat molekul sebesar 344,5 sma; polarisabilitas sebesar $1124,6 \text{ \AA}^3$; luas permukaan Van der Waals sebesar $701,64 \text{ \AA}^2$ dan volume Van der Waals sebesar $1124,6 \text{ \AA}^3$. Deskriptor momen dwi kutub tertinggi dimiliki oleh sebyawa $C_{10}SO_4Na$ sebesar 11,218 debye. Deskriptor muatan bersih atom C polar tertinggi sebesar 0,20925 dimiliki oleh senyawa $C_{12}C(C_2)SO_4Na$, sedangkan muatan bersih atom C non polar tertinggi dimiliki oleh $C_6C(C_6)SO_4Na$ sebesar -0,33193. Hasil perhitungan statistik diperoleh persamaan regresi linier dengan parameter statistik sebagai berikut : $n = 12$; $r = 0,984$; $r^2 = 0,968$; $SE = 0,1788$; $F_{hitung}/F_{tabel} = 8,389609$ dan $PRESS = 0,293388944$.

Kata kunci : KMK, *ab initio*, 6-31G**, surfaktan anionik sulfat, HKSS

ABSTRACT

Sulfate anionic surfactant is one the type of surfactant that is widely used as a cleaning agent. The discovery and development of sulfate anionic surfactant molecules need to be studied because it has a very large impact, both in the field of science an economics. It has been studied about The Quantitative Structure-Property Relationships (QSPR) of the Concentration Micelle Critic theoretical sulfate anionic surfactant. The research was to obtain the best equation model and to calculate the Concentration Micelle Critic theoretical sulfate anionic surfactant. The research was done by using molecullar modelling of 12 sulfate anionic surfactants in three dimensional compound and the calculation was performed by ab initio 6-31G** method. The geometrical results of sulfate anionic surfactant produce descriptor data. The $C_{16}SO_4Na$ compound has the highest value in some descriptors such as log P value of 7.4; refraction index value of 86.72 Å³; molecular weight value of 344.5 amu; polarization value of 1124,6 Å³; the Van der Waals surface area value of 701.64 Å² and the Van der Waals volume value of 1124.6 Å³. The highest dipole moment descriptor is owned by $C_{10}SO_4Na$ compound of 11.218 debye. The highest net charge descriptor of polar C atoms is 0.20925 owned by $C_{12}C(C_2)SO_4Na$ compound, while the highest net charge of non-polar C atoms is $C_6C(C_6)SO_4Na$ compound of -0.33193. The results of statistical calculation was obtain by linear regression equations with the following statistical parameters: $n = 12$; $r = 0.984$; $r^2 = 0.968$; $SE = 0.1788$; $F_{count}/F_{table} = 8.389609$ and $PRESS = 0.293388944$.

Keyword : CMC, ab initio, 6-31G**, sulfate anionic surfactant, QSPR

