PEER REVIEW

LEMBAR
HASIL PENILAIAN SEJAWAT SEBIDANG ATAU PEER REVIEW
KARYA ILMIAH : JURNAL ILMIAH

Judul Jurnal Ilmiah (Artikel)	: Molecular Modelling as a Downstream Effort in the Discovery of Novel Anionic Sulphate Surfactants
Penulis Jurnal Ilmiah*	: **Ponco Iswanto**, Eva Vaulina YD
Jumlah Penulis	: 2 Orang
Status Penulis	: Penulis ke-1
Identitas Jurnal Ilmiah	:
a. Nama Jurnal	: IOP Conference Series : Material Science and Engineeering
b. Nomor ISSN	: 17578981,1757899X
c. Edisi	: 959(2020)011001
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f. Alamat web	: https://www.scimagohr.com/journalsearch.php?q=19700200831&tip=sid
g. Terindeks di	: Scimago

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5. Indikasi plagiasi : tidak ada indikasi plagiasi
6. Kesesuaian bidang ilmu : sangat sesuai, kimia fisik

Purwokerto,
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Mengetahui,
Dekan FMIPA

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ARTIKEL

Preface

IOP Conf. Series: Materials Science and Engineering **959** (2020) 011001 doi:10.1088/1757-899X/959/1/011001

Speech by the chairman of the committee

Ladies and gentlemen, welcome to the 15th Joint Conference on Chemistry (JCC) 2020.

1. The honorable, Rector of Universitas Kristen Satya Wacana.
2. The honorable, Dean of Faculty of Science and Mathematics, Universitas Kristen Satya Wacana.
3. The honorable, head of Department/Study Program, members of Chemistry Consortium (Univ. Diponegoro, Univ. Negeri Semarang, Univ. Sebelas Maret Surakarta, and Univ. Jend. Soedirman Purwokerto).
4. The honorable, Keynote Speakers.
5. The honorable, invited presenters, presenters, and all the conference participants.

First of all, we thank God for this extraordinary opportunity, so that we can hold the 15th JCC 2020, during pandemic COVID-19. At first, we were still confused and doubtful about the implementation of this conference. It also happened to be the first time we become the organizers of this prestigious Conference. But once again thanks to God's blessing and support from our colleagues, leaders, and support from the extraordinary Consortium, so that we can move forward with certainty.

At this moment, the challenge of a very bad situation due to the COVID-19 pandemic has spread to almost all countries, including Indonesia, so that we must face it together. Every component of this country must start moving according to its duties and portions. Likewise, with this consortium of five universities, the annual agenda in the form of an international conference must continue on time. Even though COVID-19 has not subsided yet, the 6 months that have just passed have educated us to be able to walk with Corona, which we don't know yet, when it will completely disappear. Although the plan has changed drastically due to the current condition, the 15th JCC will be held online and only for one day.

We invite four Keynote Speakers: Prof. Hadi Noor from Universitas Teknologi Malaysia, Prof Hidetoshi Sato from Kwansei gakuin University, Japan, Prof. Ming -Kang Tsai from National Taiwan Normal University, Taiwan, and Dr. Tatas HP Brotosudarmo, Dipl. Chem., Ph.D from Indonesia, which also the previous Chief of HKI period 2018. Several invited speakers from members of the consortium also attend this 15th JCC. We also want to report that there are 60 papers that come from various places, for ex. Taiwan, Japan, Vietnam, Malaysia.

The 15th JCC activity would not have been possible without the help of many parties, therefore allow me as the chairman of the committee to say many thanks to all parties that we cannot mention one by one. Especially for my internal committee members, I would like to express my highest appreciation for the hard work and extraordinary cooperation for the implementation of the 15th JCC. We also thank all the 15th JCC participants who have joined online. Finally, we apologize if in the implementation there is something that is not pleasing to the hearts of all the participants. Thank you and have a good conference.

Chair of the Organizing Committee: Dra. Hartati Soetjipto, M.Sc.

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Table of contents

Volume 959

2020

Previous issue

15th Joint Conference on Chemistry (JCC 2020) 9 September 2020, Salatiga, Indonesia

Accepted papers received: 13 October 2020
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Open all abstracts

Preface

Analytical Chemistry

Glucose-water interactions at increasing concentrations and temperatures as revealed by Near-Infrared Spectroscopy

F S Rondonuwu, A Setiawan, J Muninggar and F F Karwur

+ Open abstract View article PDF

Computational Chemistry

OPEN ACCESS 012004

Ab initio computational study: Adsorption of CO molecule on various base metal oxide surfaces

I Kurnia, P Siahaan and A Suseno

+ Open abstract View article PDF

Chemistry Education

OPEN ACCESS 012005

Self-assessment of chemistry laboratory basic skills using performance scoring rubrics at the chemistry teacher training

I B N Sudria, I W Redhana, I W Suja and I N Suardana

+ Open abstract View article PDF

OPEN ACCESS 012006

The effectiveness of online learning by EdPuzzle in polymer materials on students' problem-solving skills

Giyanto, L Heliawaty and B Rubini

+ Open abstract View article PDF

Enviromental

OPEN ACCESS 012007

Chemically induced demulsification of water in crude oil emulsion from East Kalimantan oil fields

A P Gustianthy, D Febriantini, B Purnomo, S U Muzayanha and R Noverdi

+ Open abstract View article PDF

OPEN ACCESS 012008

The addition effect of *Pseudomonas aeruginosa* on biodegradation of methyl orange dye by brown-rot fungus *Fomitopsis pinicola*

A S Purnomo, D M Rahayu, R Nawfa and S R Putra

+ Open abstract View article PDF

OPEN ACCESS 012009

Polyelectrolyte Complex (PEC) film based on chitosan as potential edible films and their antibacterial activity test

N Ismillayli, I G A S Andayani, R Honiar, B Mariana, R K Sanjaya and D Hermanto

+ Open abstract View article PDF

OPEN ACCESS 012010

Response surface methodology optimization of Congo Red dye adsorption onto MnFe-LDH adsorbent

L V Tan, N T H Tham and D T Sy

+ Open abstract View article PDF

OPEN ACCESS 012011

Identification and simulation model of mixed solutions of diethanolamine (DEA) and methyl diethanolamine (MDEA) for removal of acid gases

D Febriantini, S Pebriani, Usman, B Purnomo, A K Rianto, A S Nugraha and N Khoirunnisa

+ Open abstract View article PDF

Energy

OPEN ACCESS 012012

Study of final temperature and heating rate variation to pyrolysis of Acacia (*Acacia mangium W.*) wood waste

Pranoto, K D Nugrahaningtyas and R N O Putri

+ Open abstract View article PDF

Material

OPEN ACCESS 012013

Carbon and zinc oxide synthesized by gelatin template as potential material for fight viruses covid-19: Future potential material

M Ulfa, D Prasetoko and M Fajar

+ Open abstract View article PDF

OPEN ACCESS 012014

Synthesis and characterizations of C-3-Nitrophenylcalix[4]resorcinarene as a potential chemosensor for La(III) ions

K T A Priyangga, Y S Kurniawan and L Yuliati

+ Open abstract View article PDF

OPEN ACCESS 012015

Synthesis and characterization of silver nanoparticles supported on highly ordered Biphenylene-Bridged Periodic Mesoporous Organosilica

A M Khikmah, Y K Krisnandi and I Abdullah

+ Open abstract View article PDF

OPEN ACCESS 012016

Synthesis of nanocomposites cellulose-Fe3O4/ZnO as novel green catalyst for biodiesel production from coconut oil

S N A R Azahra and Helmiyati

+ Open abstract View article PDF

OPEN ACCESS 012017

Adsorption capability for Congo Red on exfoliated graphene-decorated $CoFe_2O_4$ nanocomposite: Kinetic, isotherm, thermodynamic and recyclability studies

L V Tan, N T Hong-Tham and P V Thinh

+ Open abstract View article PDF

OPEN ACCESS 012018

Silver nanoparticles (AgNPs) as photocatalyst in the photodegradation of rhemazol brilliant blue

I E Suprihatin, G A D Lestari, R Mardhani and V Edoway

+ Open abstract View article PDF

OPEN ACCESS 012019

Synthesis of Carbon Nanotubes (CNT) by Chemical Vapor Deposition (CVD) using a biogas-based carbon precursor: A review

D D Saputri, A M Jan'ah and T E Saraswati

+ Open abstract View article PDF

OPEN ACCESS 012020

Sol-gel synthesis and photocatalytic activity of biomimetic calcium manganese oxide catalysts

W Setyarini, Nurhayati, N Dewi, R Anggraini, S S Siregar, E Amiruddin and A Awaluddin

+ Open abstract View article PDF

OPEN ACCESS 012021

Synthesis of indium sulfide photoanode, its characterization and application for degradation of methylene blue and methyl orange

Gunawan, A Haris and W Septina

+ Open abstract View article PDF

Natural Chemistry

OPEN ACCESS 012022

The potency of *Hibiscus tiliaceus* leaves as antioxidant and anticancer agents via induction of apoptosis against MCF-7 cells

Y Andriani, M Sababathy, H Amir, PR Sarjono, DF Syamsumir, S Sugiwati and MNI Kassim

+ Open abstract View article PDF

OPEN ACCESS 012023

The effect of leaching agent on molecularly imprinted membrane urea transport process based on polyeugenoxy acetic acid

M C Djunaidi, T Wahyuni, R A Lusiana, D S Widodo and Pardoyo

+ Open abstract View article PDF

OPEN ACCESS 012024

Formulation of the Lemongrass (*Cymbopogon citratus*) essential oil-based eco-friendly diffuse solution

T T K Ngan, T T Hien, P H Danh, L T H Nhan and L X Tien

+ Open abstract View article PDF

OPEN ACCESS 012025

Application of coconut oil from Ben Tre Province (Vietnam) as the main detergent for body wash products

T T K Ngan, T T Hien, N T C Quyen, P N Q Anh, L T H Nhan, M H Cang, D D Nhat, N D Phuc and L G Bach

+ Open abstract View article PDF

OPEN ACCESS 012026

Development and evaluation of shampoo products based on coconut oil source from Ben Tre Province (Vietnam)

T T K Ngan, T T Hien, L T H Nhan, M H Cang, P H Danh, N D Phuc and L G Bach

+ Open abstract View article PDF

OPEN ACCESS 012027

Study on the formula to produce shampoo derived from Lemongrass (*Cymbopogon citratus* (D.C.) Stapf.) essential oil

T T Hien, P T Nhut, L G Bach, N P T Nhan and L T H Nhan

+ Open abstract View article PDF

OPEN ACCESS 012028

The effect of chemical refining process on the physicochemical and fatty acid composition of water melon seed oil (*Citrulus lanatus* L.)

H Soetjipto, C P Septiyarini and S Hartini

+ Open abstract View article PDF

OPEN ACCESS 012029

Optimization infusion condition on flavonoid and antioxidant activity of herb beverages using response surface methodology

Y Martono and J Muninggar

+ Open abstract View article PDF

OPEN ACCESS 012030

Hydrolysis of sorghum starch to glucose using organic acid catalyst from rosella flower extract (*Hibiscus sabdariffa* L.)

Riniati, S H Abdulloh, R H Fauziyah and Istiqomaturohmah

+ Open abstract View article PDF

OPEN ACCESS 012031

Interaction of mutant PBP2a and bioactive compounds from Streptomyces with anti-MRSA activities

A Laksono, A Asnani and P Iswanto

+ Open abstract View article PDF

OPEN ACCESS 012032

The agronomic performance and artemisinin content of colchicine-induced polyploid genotypes *Artemisia cina*

M M Herawati, E Pudjihartati, T D Kurnia and A W Setiawan

+ Open abstract View article PDF

Organic Synthesis

OPEN ACCESS 012033

Synthesis of poly pyridine-2-ylmethyl 2-(eugenoxy) acetate (PMEOA) as a metal mixture carrier

M C Djunaidi, H Cahyono, Ismiyarto, D Siswanta and Jumina

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Molecular modelling as a downstream effort in the discovery of novel anionic sulphate surfactants

IOP Conf. Series: Materials Science and Engineering **959** (2020) 012002 doi:10.1088/1757-899X/959/1/012002

Molecular modelling as a downstream effort in the discovery of novel anionic sulphate surfactants

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Abstract. Sulphate anionic surfactant is a type of surfactant that is widely used as a cleaning agent. The discovery and development of anionic sulphate surfactant molecule is necessary because it has a huge impact, both in science and economics. Molecular modelling to produce new anionic sulphate surfactant molecules has been carried out. The mathematical equation of the Quantitative Structure-Property Relationship (QSPR) based on Ab Initio has been obtained. Molecules that were candidates for structural modelling and modification were those that have the smallest critical micelle concentration (CMC). The smallest experimental data was $C_{16}H_{33}SO_4Na$ with a CMC value = 0.000579 M. The result of this study was $C_{17}H_{35}SO_4Na$ molecules with a theoretical CMC value of 0.000515 M.

1. Introduction

The population in the world is increasing every year, indirectly it will encourage the use of cleaning materials, namely detergents used for washing clothes, household utensils, transportation and industrial fields for the past 40 years [1]. Detergent contains ingredients that have surface active agent (surfactants). Detergents that are sold freely in the market usually contain 20-40% surfactants, while the rest are chemicals called additives or detergent builders which function to increase the clean power of detergents. Generally, after the use of surfactants, the waste is simply disposed of into the environment. The surfactant content contained in detergents is generally a type of anionic surfactant. Anionic surfactants are a type of surfactant that is non-degradable, so their high use causes environmental pollution [2]. One of the parameters used to determine the performance of the surfactant is the Critical Micelle Concentration (CMC). CMC is the concentration of saturated surfactant in an emulsion or it can also be interpreted as the concentration of surfactant when there is a physical change of two phases that do not mix with each other [3].

There are two ways, classic and modern, to obtain new molecules. The classical method is done in the laboratory using laboratory materials and equipment. The weakness of the classical method is causing environmental pollution, while the modern method is done by using computer technology and software in it. The modern method is known as the computational chemistry approach. The advantage of the computational chemistry approach is that it is environmentally friendly [4].

The computation method used is the ab initio method with a large basis set (6-31G**). The ab initio method was chosen because the results of the calculations obtained have a high degree of accuracy in providing information about the physical properties of a molecule [5]. The computational chemistry approach taken to design new molecules is the analysis Quantitative Structure-Property

Relationship (QSPR). In producing a novel molecular design, it cannot be separated from the experimental data that has been done by previous researchers. Experimental data in the form of physicochemical properties are used to create mathematical equations [6]. Mathematical equations are used to predict the physicochemical properties of new molecules. The aim of this research was to obtain the best QSPR mathematical equation which can be used to find the theoretical CMC value for the needs of the new sulphate group anionic surfactant compound.

2. Methods

2.1. Material and equipment

The tools and materials needed in this research were: One computer with a Core i5 Processor, 2 GB RAM; Hyperchem 8.0 Software; 3-dimensional structural model for anionic sulphate surfactant molecules; Experimental data of CMC value of 26 anionic surfactant molecules, see table 1.

Table 1. The experimental data on the critical micelle concentration (CMC) value of the 26 molecules of anionic sulphate surfactant. Atom H is not included in the structure [7].

Number	Name of Molecule	Log CMC Experiment	Number	Name of Molecule	Log CMC Experiment
1	$C_{16}SO_4Na$	–3.237	14	$C_7C(C_6)SO_4Na$	–2.013
2	$C_{14}SO_4Na$	–2.658	15	$C_9C(C_4)SO_4Na$	–2.171
3	$C_{12}C(C_2)SO_4Na$	–2.658	16	$C_8C(C_8)SO_4Na$	–2.629
4	$C_{10}C(C_4)SO_4Na$	–2.469	17	$C_7C(C_7)SO_4Na$	–2.177
5	$C_{11}SO_4Na$	–1.783	18	$C_{15}SO_4Na$	–2.921
6	C_9SO_4Na	–1.209	19	$C_7C(C_7)CSO_4Na$	–2.523
7	$C_6C(C_6)SO_4Na$	–1.714	20	$C_{10}C(C_5)SO_4Na$	–2.269
8	$C_{10}SO_4Na$	–1.481	21	$C_{12}C(C)SO_4Na$	–1.081
9	$C_8C(C)SO_4Na$	–1.328	22	$C_{13}SO_4Na$	–2.367
10	$C_5C(C_5)SO_4Na$	–1.081	23	$C_9C(C_9)SO_4Na$	–3.027
11	C_8SO_4Na	–0.854	24	$C_{10}EO_2SO_4Na$	–1.925
12	$C_{12}SO_4Na$	–2.066	25	$C_{12}C(C_3)SO_4Na$	–2.764
13	$C_{11}C(C)SO_4Na$	–2.187	26	$C_{12}EOSO_4Na$	–2.396

2.2. Molecular modelling

Molecular modelling begins with depictions on the Hyperchem 8.0 Program canvas. This study also used the molecular structure data of anionic surfactants along with the CMC values obtained from the experimental results. The chemical structure of the anionic sulphate surfactant molecule used in this study was made a two-dimensional (2D) model using the Hyperchem 8.0 device. The model is then equipped with a hydrogen atom on each atom, and is formed into a three-dimensional (3D) structure using the Build menu (Add H and Model Build). The picture of the anionic sulphate surfactant molecule is then saved in .HIN format [8]. The surfactant molecules described were optimized to form the most stable structure.

2.3. CMC calculation

In order to calculate CMC the sulphate anionic surfactant molecule was calculated based on equation (1). The mathematical equations to predict [9] resulting from Ab Initio's Quantitative Structure-Properties Relationship were:

$$\lg CMC = -5.665 + 0.042(BM) - 0.095(Pol) - 0.012(Vvdw) - 0.027(MD) + 1.418(QC1) - 14.562(QC2) \quad (1)$$

The lg CMC is the logarithmic of the CMC, after which it is constant. BM and Pol were molecular weight and polarizability. Then Vvdw and MD were van der Waals volumes and dipole moments. Then QC1 and QC2 were the net charges of atoms C1 (C polar) and C2 (C non polar), see equation (1).

3. Result and discussion

3.1. Molecular modelling of surfactant sulphate group

Anionic surfactants are surfactants whose alkyl portion is attached to an anion. Its hydrophilic nature comes from the ionic head which is usually a sulphate group or a sulfonate group [4]. One of the important properties that can indicate the quality of the surfactant is the value of CMC. CMC is an important property of a surfactant which indicates the critical concentration limit of the surfactant in a solution. Surfactants have good quality if the CMC value is getting smaller.

This study used the sulphate group anionic surfactant in a linear chain. Molecular modelling of sulphate group surfactants was carried out on the Hyperchem 8.0 canvas on the build menu. The modelling of the structure of the sulphate group anionic surfactant on the Hyperchem 8.0 canvas is shown in figure 1. One molecule of the sulphate anionic surfactant was a molecule of Sodium Lauryl Sulphate, $C_{17}H_{35}SO_4Na$.

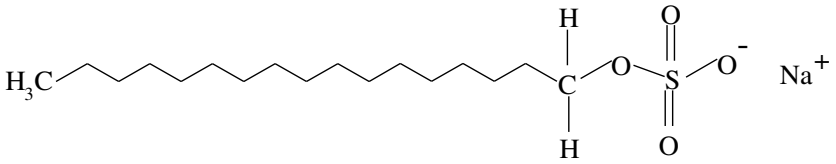

Figure 1. Molecular modelling of anionic surfactants for the sulphate group, Sodium Lauryl Sulphate, $C_{17}H_{35}SO_4Na$.

3.2. Geometry optimization and CMC calculation

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$$\begin{aligned}
\lg CMC &= -5.665 + 0.042(BM) - 0.095(Pol) - 0.012(Vvdw) - 0.027(MD) \\
&\quad + 1.418(QC1) - 14.562(QC2) \\
&= -5.665 + 0.042.\,(358.51) - 0.095.\,(34.18) - 0.012(1180.60) - 0.027(9.485) \\
&\quad + 1.418(0.10534) - 14.562(-0.332393) \\
&= -5.665 + 15.05742 - 3.2471 - 14.1672 - 0.256095 + 0.14937212 + 4.84031 \\
&= -3.288 \\
CMC &= 10^{-3.288}\ M = 0.000515\ M
\end{aligned}$$

The theoretical CMC value or the calculation result of the $C_{17}H_{35}SO_4Na$ molecule obtained was 0.000515 M and this was actually lower than the $C_{16}H_{33}SO_4Na$ molecule which was 0.000579 M.

4. Conclusion

The results of the study concluded that the mathematical equations resulting from the quantitative structure-properties relationship of Ab Initio could be used to predict sulphate anionic surfactants. The theoretical CMC value was $C_{17}H_{35}SO_4Na$ of 0.000515 M.

Acknowledgment

We, *Soedirman Group for Computational Chemistry*, Physical Chemistry Laboratory, Department of Chemistry, Faculty of Mathematics and Natural Sciences, Unsoed, would like to express our gratitude for the financial support. This support is provided through Competency Improvement Research Grant, LPPM Unsoed, with a Contract Number: T/584/UN23.18/PT.01.03/2020.

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Molecular modelling as a downstream effort in the discovery of novel anionic sulphate surfactants

Molecular modelling as a downstream effort in the discovery of novel anionic sulphate surfactants

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Abstract. Sulphate anionic surfactant is a type of surfactant that is widely used as a cleaning agent. The discovery and development of anionic sulphate surfactant molecule is necessary because it has a huge impact, both in science and economics. Molecular modelling to produce new anionic sulphate surfactant molecules has been carried out. The mathematical equation of the Quantitative Structure-Property Relationship (QSPR) based on Ab Initio has been obtained. Molecules that were candidates for structural modelling and modification were those that have the smallest critical micelle concentration (CMC). The smallest experimental data was $C_{16}H_{33}SO_4Na$ with a CMC value = 0.000579 M. The result of this study was $C_{17}H_{35}SO_4Na$ molecules with a theoretical CMC value of 0.000515 M.

1. Introduction

The population in the world is increasing every year, indirectly it will encourage the use of cleaning materials, namely detergents used for washing clothes, household utensils, transportation and industrial fields for the past 40 years [1]. Detergent contains ingredients that have surface active agent (surfactants). Detergents that are sold freely in the market usually contain 20-40% surfactants, while the rest are chemicals called additives or detergent builders which function to increase the clean power of detergents. Generally, after the use of surfactants, the waste is simply disposed of into the environment. The surfactant content contained in detergents is generally a type of anionic surfactant. Anionic surfactants are a type of surfactant that is non-degradable, so their high use causes environmental pollution [2]. One of the parameters used to determine the performance of the surfactant is the Critical Micelle Concentration (CMC). CMC is the concentration of saturated surfactant in an emulsion or it can also be interpreted as the concentration of surfactant when there is a physical change of two phases that do not mix with each other [3].

There are two ways, classic and modern, to obtain new molecules. The classical method is done in the laboratory using laboratory materials and equipment. The weakness of the classical method is causing environmental pollution, while the modern method is done by using computer technology and software in it. The modern method is known as the computational chemistry approach. The advantage of the computational chemistry approach is that it is environmentally friendly [4].

The computation method used is the ab initio method with a large basis set (6-31G**). The ab initio method was chosen because the results of the calculations obtained have a high degree of accuracy in providing information about the physical properties of a molecule [5]. The computational chemistry approach taken to design new molecules is the analysis Quantitative Structure-Property

Relationship (QSPR). In producing a novel molecular design, it cannot be separated from the experimental data that has been done by previous researchers. Experimental data in the form of physicochemical properties are used to create mathematical equations [6]. Mathematical equations are used to predict the physicochemical properties of new molecules. The aim of this research was to obtain the best QSPR mathematical equation which can be used to find the theoretical CMC value for the needs of the new sulphate group anionic surfactant compound.

2. Methods

2.1. Material and equipment

The tools and materials needed in this research were: One computer with a Core i5 Processor, 2 GB RAM; Hyperchem 8.0 Software; 3-dimensional structural model for anionic sulphate surfactant molecules; Experimental data of CMC value of 26 anionic surfactant molecules, see table 1.

Table 1. The experimental data on the critical micelle concentration (CMC) value of the 26 molecules of anionic sulphate surfactant. Atom H is not included in the structure [7].

Number	Name of Molecule	Log CMC Experiment	Number	Name of Molecule	Log CMC Experiment
1	$C_{16}SO_4Na$	–3.237	14	$C_7C(C_6)SO_4Na$	–2.013
2	$C_{14}SO_4Na$	–2.658	15	$C_9C(C_4)SO_4Na$	–2.171
3	$C_{12}C(C_2)SO_4Na$	–2.658	16	$C_8C(C_8)SO_4Na$	–2.629
4	$C_{10}C(C_4)SO_4Na$	–2.469	17	$C_7C(C_7)SO_4Na$	–2.177
5	$C_{11}SO_4Na$	–1.783	18	$C_{15}SO_4Na$	–2.921
6	C_9SO_4Na	–1.209	19	$C_7C(C_7)CSO_4Na$	–2.523
7	$C_6C(C_6)SO_4Na$	–1.714	20	$C_{10}C(C_5)SO_4Na$	–2.269
8	$C_{10}SO_4Na$	–1.481	21	$C_{12}C(C)SO_4Na$	–1.081
9	$C_8C(C)SO_4Na$	–1.328	22	$C_{13}SO_4Na$	–2.367
10	$C_5C(C_5)SO_4Na$	–1.081	23	$C_9C(C_9)SO_4Na$	–3.027
11	C_8SO_4Na	–0.854	24	$C_{10}EO_2SO_4Na$	–1.925
12	$C_{12}SO_4Na$	–2.066	25	$C_{12}C(C_3)SO_4Na$	–2.764
13	$C_{11}C(C)SO_4Na$	–2.187	26	$C_{12}EOSO_4Na$	–2.396

2.2. Molecular modelling

Molecular modelling begins with depictions on the Hyperchem 8.0 Program canvas. This study also used the molecular structure data of anionic surfactants along with the CMC values obtained from the experimental results. The chemical structure of the anionic sulphate surfactant molecule used in this study was made a two-dimensional (2D) model using the Hyperchem 8.0 device. The model is then equipped with a hydrogen atom on each atom, and is formed into a three-dimensional (3D) structure using the Build menu (Add H and Model Build). The picture of the anionic sulphate surfactant molecule is then saved in .HIN format [8]. The surfactant molecules described were optimized to form the most stable structure.

2.3. CMC calculation

In order to calculate CMC the sulphate anionic surfactant molecule was calculated based on equation (1). The mathematical equations to predict [9] resulting from Ab Initio's Quantitative Structure-Properties Relationship were:

$$\lg CMC = -5.665 + 0.042(BM) - 0.095(Pol) - 0.012(Vvdw) - 0.027(MD) + 1.418(QC1) - 14.562(QC2) \quad (1)$$

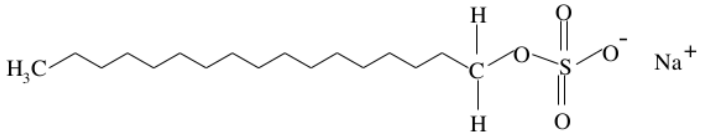
The lg CMC is the logarithmic of the CMC, after which it is constant. BM and Pol were molecular weight and polarizability. Then Vvdw and MD were van der Waals volumes and dipole moments. Then QC1 and QC2 were the net charges of atoms C1 (C polar) and C2 (C non polar), see equation (1).

3. Result and discussion

3.1. Molecular modelling of surfactant sulphate group

Anionic surfactants are surfactants whose alkyl portion is attached to an anion. Its hydrophilic nature comes from the ionic head which is usually a sulphate group or a sulfonate group [4]. One of the important properties that can indicate the quality of the surfactant is the value of CMC. CMC is an important property of a surfactant which indicates the critical concentration limit of the surfactant in a solution. Surfactants have good quality if the CMC value is getting smaller.

This study used the sulphate group anionic surfactant in a linear chain. Molecular modelling of sulphate group surfactants was carried out on the Hyperchem 8.0 canvas on the build menu. The modelling of the structure of the sulphate group anionic surfactant on the Hyperchem 8.0 canvas is shown in figure 1. One molecule of the sulphate anionic surfactant was a molecule of Sodium Lauryl Sulphate, $C_{17}H_{35}SO_4Na$.



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