Sulfonation Reaction for the Synthesis of Anionic Surfactants for Enhanced Oil Recovery (EOR) Application

by

Mohammad Jeffrey Bin Ibrahim

Dissertation submitted in partial fulfilment of

the requirements for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

May 2013

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CERTIFICATION OF APPROVAL

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Approved by,

____
(AP Dr Isa M Tan)

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
May 2013

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

MOHAMMAD JEFFREY BIN IBRAHIM

ABSTRACT

Enhance oil recovery (EOR) is performed in the tertiary stage in oil production. One of the preferred methods for EOR application is chemical flooding using surfactants. The two main principles of EOR are to reduce the mobility ratio and increase the capillary number. Anionic surfactants is widely used in detergents product because of it capability to reduce the surface tension between oil and water. The amount of surfactants adsorption can be minimized as the result of repulsion between anionic surfactants and sandstone. Anionic surfactants are produced by attaching SO_3 to fatty alcohols increase the performance of the surfactants. Sodium bisulfite is reacted together with methalyl chloride and fatty alcohols to produce anionic surfactants sulfonate. The kinetics of the sulfonation reaction process and the factors that can optimize the yield of sulfonate products are now being investigated and reported.

ACKNOWLEDGEMENT

The writer of this report is a Chemical Engineering student from Universiti Teknologi PETRONAS (UTP). This final year report title is ‘Sulfonation Reaction for the Synthesis of Anionic Surfactants for EOR Application’. First of all, the authors like to express my gratitude to Allah the Almighty God because of His will; the author managed to complete first part of final year project on January 2013.

The author also would to express his sincere gratitude to Associate Professor Dr Isa M Tan, supervisor for author Final Year Project for his dedication, support and enthusiasm guiding author to complete his work on time.

Not forgetting, the graduate assistance Muhammad Sagir and Muhammad Mushtaq for serving as mentors to help the author in research development. The successful completion of this project would not have been possible without their guide and supports.

The gratitude also extends to all Universiti Teknologi PETRONAS stuffs especially the laboratory technician/assistance for their commitment and supports.

Lastly, the author would like to thank everyone who involve directly or indirectly throughout this research.

Thank you.

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CHAPTER 1

INTRODUCTION

1. INTRODUCTION

1.1 Background of study

Sulfonation reaction involved the attachment of sulfur trioxide (SO_3) into an organic compound. There are several techniques usually used for sulfonation reaction purpose. Sulfonation can be done by reacting the organic compound with Chlorosulfonic Acid, Oleum or/and using pure sulfur trioxide in falling film reactors. However, the present method face a lot of problems including high operating cost, high maintenance cost, high corrosion rate, low yield of reaction and not environmental friendly. Sulfonation using Sodium Bisulfite, $NaHSO_3$ is not widely known but is used in this study.

Surfactants contain hydrophobic part and hydrophilic part which are useful for lowering interfacial tension between oil and water. Typically, surfactants enhance the removal of grease and oil from clothes, dish washes or any other application. Currently, a lot of researchers are doing research to utilize surfactants for the chemical EOR application.

Anionic surfactants sulfonate is one of the potential candidates to be used for the chemical EOR application. The qualities of the surfactants give significant impact toward the amount of recovery. Preparation of surfactants is a complex procedure, as the surfactants need to be tailored accordingly to match the reservoir properties. For instance, for reservoir that has high negatively charged rocks having an anionic surfactants sulfonate is highly desirable.

This paper will study the factors affecting the reaction synthesis of the sulfonation process. Preparation of Alkoxylated Alcohol sulfonate was adopted from Paul D. Berger experiment [1]. The sulfonation yield will be analysed, important data will be taken and formulation can be achieved once all the parameters to optimize the yield of sulfonate product has been identified.

1.2 Problem Statements

Sulfonation is a process of attaching sulfur trioxide (SO_3) into organic compound structure. However the effectiveness of sulfonation process depends on several factors. The product yield is affected by temperature. However, uncontrolled temperature may lead to the formation of by-products or black solutions were formed. Next, the conversion is also affected by the concentration of SO_3 reagent /donator used for sulfonation. Incompatible concentration may lead to the formation of unsulfonated compound. Ineffective yield will lead to the formation of low quality sulfonate surfactants product which can decrease the performance of surfactants during EOR. The factors that affect the effectiveness using sodium bisulfite sulfonation reaction with non-ionic surfactants are unknown.

1.3 Objectives and Scope of Study

The core objective for this thesis is to investigate the reaction kinetics of the sulfonation process using sodium bisulfite ($NaHSO_3$) with non-ionic surfactants. The effect of rate of the reaction will be determined throughout experiment. The effects of reactant mole ratio, catalyst and temperature of reaction will be investigated.

Preparations of anionic surfactants sulfonate were adopted from Berger's [1] and O'lenick [9] literature. As the non-ionic surfactants is prepare first. Sulfonation process begin after this. The synthesis parameter such as reaction temperature, addition of catalyst and mole ratio of the reactants will be manipulated to determine the concentration of anionic surfactants sulfonate produced in step 2 reaction. All data will be recorded and analysed.

1.4 Feasibility of the Project within Scope and Time Frame

This project is feasible within the identified time allocated. Therefore, this project was divided into two parts. The first part for January 2013 semester, the author will be focusing on the project proposal, project title selection and the literature review based on the project topic which is the ‘Sulfonation Reaction for the Synthesis of Anionic Surfactants for EOR Application’. The problem statements and objectives will be determined. The scope of study will be limitation on the area of project interest. Meanwhile, the second part for this project in May 2013 semester will be focusing on the experimental data collection and analysis.

All the experiments will be carried out in UTP. The equipment’s and apparatus required can be found at blocks 3, 4, 5, 15 and J. The chemical reagents will be supplied by UTP for project purpose. Experiment procedure will be conducted.

To make sure this project achieves its targets within the limitation, the project will be executed tally as per plan during all stage of the project.

CHAPTER 2

LITERATURE REVIEW

2. LITERATURE REVIEW

2.1 Principle of Enhanced Oil Recovery (EOR).

Oil production is achieved over three phases. It begins with the discovery of thr new oilfield, where the primary phase of the production flow powered by reservoir pressure. Upon well maturity, the pressure inside the reservoir depleted and production declined. Therefore, the secondary oil production begins with the injection of water or gas into the reservoir in order to supply energy for the production to continue. As the method is no longer economical as the cost of water or gas injection become too narrow and surpass the production income the secondary phase stop. This EOR phase marks the commencement of tertiary phase of oil production [6].

Commonly EOR is used to recover 40% to 60% of oil reserve (Isa, 2013)

The main principle of EOR is based on two principles: decreasing the mobility ratio and increasing the capillary number [2] .Mobility ratio (M) is denoted as;

$$M = \text{ʎ}ing / \text{ʎ}ed = (k/\mu)ing / (k/\mu)ed \;\ldots\ldots\ldots\ldots\ldots\ldots\; (1)$$

Where, k is effective permeability, µ is viscosity of the fluids, ing denotes displacing and ed is displaced. In this case, the ‘*displacing fluid’* is water/surfactants and the ‘*displaced fluid’* is oil. It is desire for $M<1$ for EOR to become more effective. If $M>1$, displacing fluid will flow past most of the displaced fluid, therefore the efficiency of displacing the oil from rock pore declines and more water will be produced instead of hydrocarbons. For maximum displacement and easier oil sweeping by displacing fluid the M value should be lesser than 1.

A sample of graph of displaced oil versus mobility ratio is taken from Farouq [4] using Buckley-Leverett (BL) theory as in figure 2.0

Volume of Fluid Enter – Volume of Fluid Leaving = Change in Fluid Volume ………..(2)

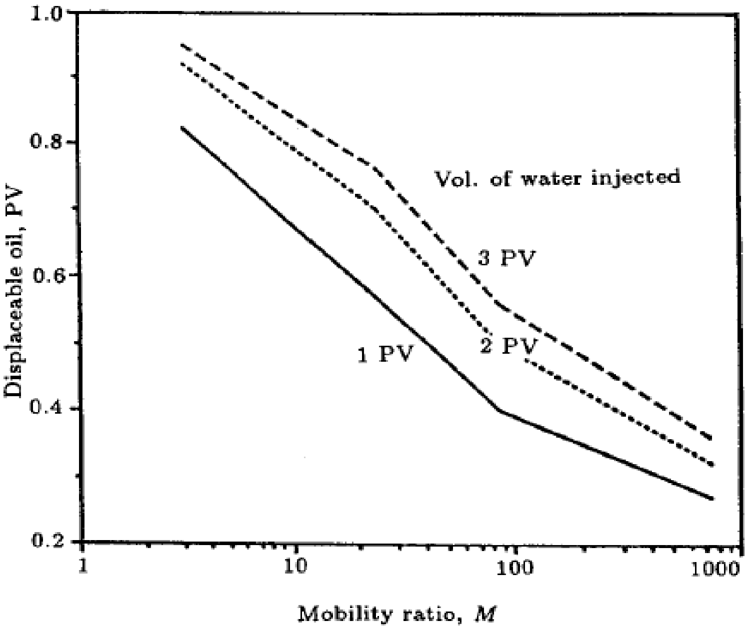


Figure 2.0. Effect of mobility ratio on water flood recovery. S.M Farouq on the principle of EOR

From figure 2.0, the oil displaced increases as the mobility ratio decreased. The M value can be made smaller by lowering the viscosity of oil and/or increasing the viscosity of the displacing fluid, decreasing the permeability of oil while increasing the permeability of displacing fluid.

Another principle in EOR implementation is to increase the capillary number, N_c. the capillary number formulas shown below:

$$Nc = \frac{\upsilon\mu}{\sigma} = \frac{k\Delta\rho}{\sigma L} \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{(3)}$$

Where, ν is the Darcy velocity of the displacing fluid, μ is the viscosity of displaced fluid, σ is the interfacial tension between displaced fluid and displacing fluid, k is the effective permeability of displacing fluid, $\frac{\Delta\rho}{L}$ is the pressure gradient. To increase the capillary number, the viscosity of oil or displaced fluid can be reduce, increase the pressure gradient and decrease the interfacial tension between displaced fluid and displacing fluid.

Generally, EOR is divided into three categories which are Gas Injection, Thermal Recovery and Chemical Flooding. Today there were four main categories used widely in EOR application as shown in Table 1.

Table 2.1. Typical EOR techniques.

Gas Injection	**Thermal Recovery**
• CO_2 gas • N_2 gas	• In-situ combustion • Cyclic steam combustion • Steam flooding / Hot Water flooding
Chemical Flooding	**Other**
• Micellar-Polymer • Alkaline-Surfactants • Alkaline-Surfactants-Polymer	• Carbonated water flood • Microbial • Electromagnetic heating

2.2 Surfactants Sulfonate

Surfactants are used to remove oil by reducing the interfacial tension (IFT) between oil and water. Surfactants is an organic compound called ‘*amphiphilic*’ where it consist of ‘*hydrophobic’* group “*head*” and polar ‘*hydrophilic’* group is the “*tail*”. In other word, they are soluble in organic solvent and water [3]. Surfactants are classified according to the ionic nature of the head group. Classes of ionic surfactants are the anionic, cationic, non-ionic and amphoteric/zwitterionic surfactants (Ottewill, 1984) as described in Sheng [3]. Among these ionic classes type of surfactants, the anionic surfactants are the most preferable to be used in chemical EOR. It exhibits the nature of having repulsion with the negative charge of sandstone and limestone rock which reduces the losses of chemical due to adsorption which can reduced the recovery factor.

The production of sulfonate ionic surfactants has been widely produced and many papers have been published. Taken from the Hunstman technical bulletin [4], high quality of sulfonate ionic surfactants can give high tolerant to high salinity brine, high temperature condition and capable to make ultra-low IFT (oil-aqueous) using alkylaryl sulfonates to produce their surfactants [4].

According to Rusell D. et al [5], an aqueous fluid containing a water soluble alkylpolyalkoxyalkyl sulfonate or alkylarylpolyalkoxyalkyl sulfonate and a water-insoluble polyethoxylated aliphatic alcohol or polyethoxylated alkylphenol nonionic surfactant proved to work very efficient in high salinity and high temperature reservoir conditions.

Another invention by Paul D. Berger [1] claimed to produce 2-Alkyl alkoxylated alcohol sulfonate capable to resist high temperature and electrolyte by reacting alkoxylated alcohol or alkyphenol, first with methalyl chloride then sulfonated with a bisulfite salt to form alkylphenol ether sulfonate.

2.3 Sulfonation Reaction

Sulfonation in general refers to the addition of the sulfur trioxide, SO_3 into organic compounds to produce sulphate compound. In more technical terms, sulfonation according to Ortega J.A.T [15] is defined as an electrophilic chemical reaction where sulfonic group is incorporated into a molecule with the capability to donate electrons.

According to CHEMITHON [7] article, a pure SO_3 will behave aggressively with the organic compound as electrophilic reagent. The reaction occurs instantaneously and it produces a high temperature known as exothermic reaction during reaction. Lack of control of the temperature reaction will lead to the formation of by-product. Having an effective cooling system is advisable and recommended. Sulfonated products will have a high viscosity with low heat transfer coefficient. Manipulating the ratio of reactant especially the SO_3 employed to improve the yield of sulfonated product [7].

At present, researcher has developed some of the sulfonate reagents or donors to reduce the SO_3 reactivity during sulfonation process for safety reason. Among the SO_3 reagents or donors are the Sodium Bisulfite, Sulfamic Acid, and Chlorosulfonic Acid.

Referring to one of the Berger literatures [9], several catalysts such as H_2SO_4, methane sulfonic acid, sulfosuccinic acid and other strong acid capable to catalysed the reaction, reducing the reaction temperature and improve the yields of end product.

Charles J.N. and Ned F.S.[14], preparing the sulfonated product by reaction of bisulfite with olefins having 2 to 40 carbons atoms. The experiment was done at the present of catalyst, water and alcohols as a solvent during sulfonation reaction. The reaction is preferable to be done at temperature within 100^oC to about 120^oC and surfactants added from 0.1 to 5% by weight compare olefins to sodium bisulfite. The catalyst was seen to increase the product concentration by 80% olefin conversion using aluminium nitrate as catalyst.

Referring to Ellis et al [13], the investigation of the bisulfite reaction with olefins by producing alkyl sulfonated from reaction of bisulfite ions to olefins double bonds. According to the experiment result, preparing of alkyl sulfonate salts using is preferable to be done about 1:1 to 1:1.5 ratio of olefin to bisulfite. In addition, the preferable reaction temperature is from 80^oC to about 90^oC.

According to Hirasaki [11] the alcohols based surfactants sulfonate is believed by for having the capability to decrease the equilibration time and micro-emulsion activity. An experiment was performed which give high solubilisation without any gel formations were seen with a sharp and crystal clear different interfaces between the micro emulsion and the excess amount of oil-water which is very good to be apply in chemical injection for EOR application. Therefore the TDA-6 ethoxylate is used throughout this project as anionic surfactants.

Sulfonation process for this research will be achieved by improving the method extracted from Paul. D.B [1] research paper. The reagent or sulfur trioxide donors used throughout this experiment is Sodium Bisulfite. The concentration of the sulfonated formation can be known by using two phase titration method.

2.4 Two Phase Titration

Most widely used for surfactants analysis is the two-phase titration of ionic surfactants with surfactants of opposite charge according to Cullum the author of Introduction to Surfactant Analysis [12].

Typical titration can be performed using sodium hydroxide, NaOH in the presence of phenolphthalein. Two phase titration is preferred as it has less sensitivity to interference with foreign (non-surfactants) species according to Zelenez [8]. According to him, at initial the anionic surfactant is presence in aqueous solution. The dimidium bromide reacts with anionic surfactants to form a salt which is insoluble in water, but is soluble in chloroform. Two layers were formed at this stage where the top layer is gold colour where the disulfine blue of mixed indicator dissolve in aqueous phase, and the bottom layer present as a pink colour solution. As Hyamine 1622 is added, the dimidium bromide begins to transfer into aqueous phase from chloroform. The pink solution becomes progressively slower pale until it turns completely into grey colour solution indicating the equivalence point of reaction. Blue colour solution can be form on bottom layer if more Hyamine 1622 is added to the solution.

This end point will be noted, and the yield percentage of anionic surfactant sulfonate can be determined using equation as written in section 4.3.2.

CHAPTER 3

RESEARCH METHODOLOGY

3. RESEARCH METHODOLOGY

3.1 Research Methods

This research will be focussing mainly on the study of kinetic synthesis of anionic surfactant sulfonation process. To meet the research objectives, the methodologies are divided into three stages which are;

1. Defining and Planning Stage
    a. Research definition and literature review
    b. Research problem statement identification
    c. Research objectives defined
    d. Defining research scope of study
    e. Determine research activities
    f. Chemical and hardware listing and preparation

2. Research Initiation Stage
    a. Extract procedure from literature review
    b. Preparation of base experiment
    c. Observe the important synthesis parameters
    d. Perform sample testing and recording data

3. Analyse and Conclusion Stage
    a. Result analysing for the base sulfonate product

b. Perform other experiment by manipulating the parameter conditions.
c. Record all data and comparing the results
d. Documentation

3.2 Project Activities

3.2.1 Details Project Activities

Table 3.2. Research activities

Phase	Activities Description
Pre Experiment	Literature review on related topics
	Identify research problem statement and objective
	Extract literature research procedure
Experiment	Preparation of chemicals 1. Anionic surfactants 2. Mixed indicator 3. Solution for two phase titration
	Preparation of instruments: three necked round bottom flask, burette, beakers, retort stand, sucker, hot plate & stirrer, oil, Nitrogen tank, boiling chips (refer to Appendix 1)
	Preparation of MSDS (refer appendix)
	Experiment setup and follow the standard of procedure (SOP). Take note the parameter condition
	Take sample to run yield test using titration
Post Experiment	Perform calculation and analyse data
	Documentation on findings

3.2.2 Chemical Reagents

1. TDA-6 Ethoxylate or Fatty Acids
2. Methyl Chloride (3-Chloro-Methyl Propene)

3. Sodium Bisulphate
4. Ethanol
5. Potassium Hydroxide
6. Nitrogen Gas
7. Mixed Indicator Stock Solution (Blue)
8. 2.5 M Sulfuric Acid
9. Aluminium Nitrate
10. Chloroform
11. 0.004 M Hyamine 1622

3.3 Preparation of Chemicals

3.3.1 Anionic Surfactants

Standard non-ionic surfactant is prepared using William Synthesis according to O'Lenick's [9]. Alcohols or surfactants being used is Novel TDA-6 which is then reacted with Potassium Hydroxide and Methalyl Chloride. Full procedure will be discussed in chapter 4.

3.3.2 Mixed Indicator Solution

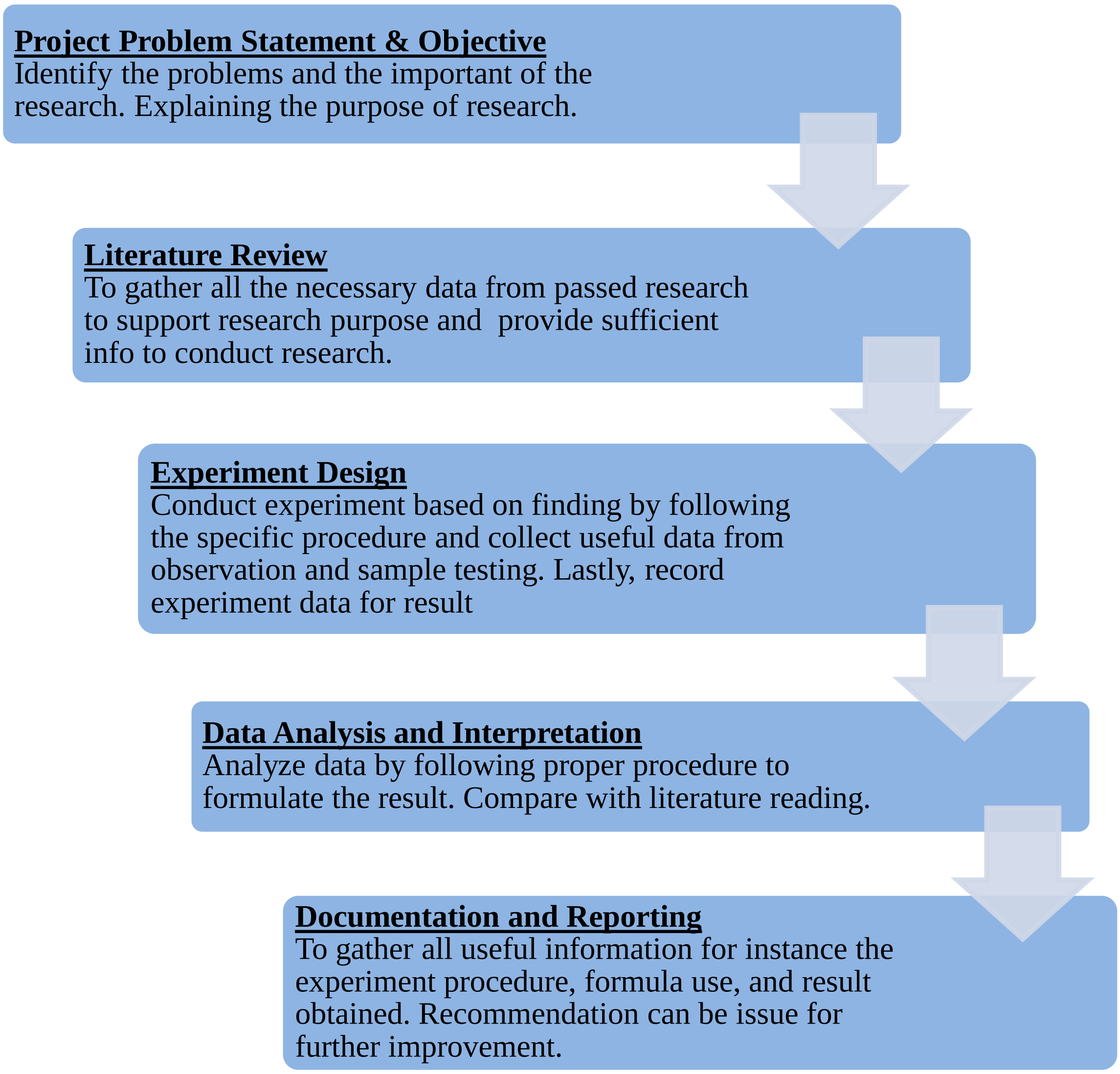
Mixed indicator solution is prepared by mixing 20 mL of dimidium bromide, 200 mL distilled water and 20 mL of 2.5 M Sulfuric Acid into 1 L of volumetric flask. Filled distilled water until mark position.

3.3.3 Two phase titration

Preparation for the titration process of the anionic surfactants sulfonate followed the procedure mentioned by Zelenev in his book [8]. The procedure of titration process begins by taking 0.5 g to 0.7 g of sample into flask. 25 mL of water, 5 mL of mixed indicator solution and 5 mL of Chloroform is mixed together with the sample. Drop of 0.004 M Hyamine 1622 is added until reach the end point of the titration is reached where the aqueous layer which is pink become progressively grey.

3.4 Research Key Milestone

To meet the research objectives, the following process flow chart has been designed to make sure the project can be finish on time.



Project Problem Statement & Objective
Identify the problems and the important of the research. Explaining the purpose of research.

Literature Review
To gather all the necessary data from passed research to support research purpose and provide sufficient info to conduct research.

Experiment Design
Conduct experiment based on finding by following the specific procedure and collect useful data from observation and sample testing. Lastly, record experiment data for result

Data Analysis and Interpretation
Analyze data by following proper procedure to formulate the result. Compare with literature reading.

Documentation and Reporting
To gather all useful information for instance the experiment procedure, formula use, and result obtained. Recommendation can be issue for further improvement.

Figure 3.4. Research milestone

3.4 Timeline for FYP II (Gantt chart)

Table 3.4 FYP II Gantt's chart table.

No	Detail \ Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1	Project Work	🟦	🟦	🟦	🟦	🟦	🟦	🟦	Midsem Break							
2	Submission of Progress Report									🟦						
3	Project Work Continues									🟦	🟦	🟦				
4	PRE- SEDX												🟦			
5	Submission of Draft Report													🟦		
6	Submission of Dissertation (Soft Bounded)														🟦	
7	Submission of Technical Paper														🟦	
8	Oral Presentation															🟦
9	Submission of Full Report (Hard Bound) W15															

Important Date:

[8] Submission of Progress Report – 8th July 2013

[4] Pre-SEDX Presentation –31st July 2013

[5] Submission of Draft 1 report – 5th August 2013

[6, 7] Submission of Dissertation Report (Soft Bound) and Technical Report- 15th August 2013

[8] Oral Presentation – 26-30th August 2013

[9] Full Report (Hard Bound)- 30th September 2013

CHAPTER 4

RESULTS AND DISCUSSION

4.0 RESULT AND DISCUSSION

4.1 Data Gathering & Analysis

4.1.1 Experiments Variables

Before the experiment begin, to meet the research objectives all the variable parameters need to be determined. This research was done in a room condition with pressure of 1 atm. Each sample was prepared by small scale batch using only 250 ml three necked round bottom flask. All the experiment parameters are as in table 4.

Table 4. Experiment variables and parameters

Variables	Parameters
Manipulated	Reactants Mole Ratio, Temperature, Catalyst
Fixed	Non-ionic Surfactants Concentration, Pressure
Respond	Yield Per cent of the Product

4.1.2 Preparation of Anionic Surfactants Sulfonate

The experiment is divided into two parts; preparation of the anionic surfactants and sulfonation of anionic surfactants.

The experiment procedure;

1. Preparation of the non-ionic surfactants

Figure 4.1. Non-ionic Surfactants Novel TDA-6 Ethoxylate Based

a) Preparation of solution following Olenick's [9] following the Williamson synthesis method where 0.05mol of alcohol (Novel TDA-6 Ethoxylate, mw: 467 g/mol), 0.05 mol KOH and 0.05 mol methalyl chloride (3-Chloro, 2-methyl-1-propane, mw: 90.6 g/mol) are mixed together at temperature 90-100 degree for 7 to 8 hours.
b) Nitrogen gas is used to purge out H_2O vapour formation during the reaction.
c) The solution is cooled down to room temperature. White precipitate (KCl) is formed.
d) Centrifuge is use to remove solids from the solution.
e) Final solution is shown in figure 4.1.

2. Sulfonation of non-ionic surfactants

Figure 4.2. Before and after two phase titration

a) Sulfonation of non-ionic surfactant was prepared using procedure written in Berger literature [10] by mixing 25 g of ethanol, 25 g of water, 0.005 mol surfactants and 0.005mol of Sodium Bisulfite.
b) The solution is then reflux at the boiling point temperature.
c) Approximately 0.5 to 0.7g of samples is taken gradually to estimate the yield of product by two phase titration as described in section 3.3.3.
d) Note the amount of Hyamine 1622 use and perform yield calculation.
e) Repeat steps from "a" to "d" until 24 hours of reaction time.

4.1.3 Experiment flow chart

The experimental flow chart was designed as below based on the procedure described in part 4.1.2.

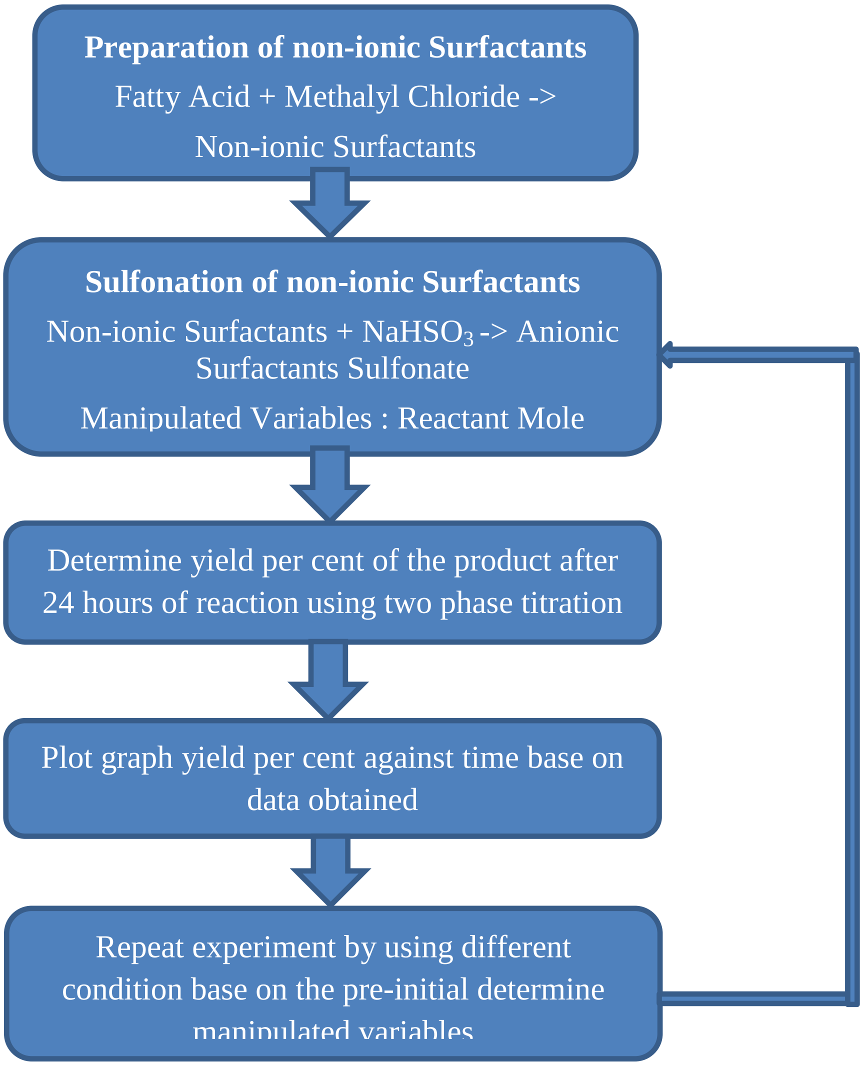


Figure 4.3. Overall experiment design

4.2 Experiment Results

4.2.1 Non-ionic Surfactants Reaction (Step 1)

The non-ionic surfactants for this research purpose was prepared by reacting the fatty acids or commercially known as Novel TDA-6 Ethoxylate with Potassium Choride, KCl and Methalyl Chloride. The reaction mechanisms for step one and two are shown in part 4.3.1. The FTIR result for the first step is shown in table 5.

Table 4.2. FTIR result for Step 1 Reaction, based on FTIR Appendix 3

Functional Group	**Molecular Motion**	**Wave Numbers, cm^{-1}**
Alkanes	=CH Stretch	3077.27
Alkanes	C=C Stretch	1637.80
Alcohols	O-H Stretch	3467.38
Ethers	C-O-C Stretch (diaryl)	1112.01

The functional group alkenes or the double bonds are present at the wavenumber of 3077.27 cm-^{1} for =CH stretch and 1637.80 cm^{-1} for C=C stretch. This indicates the presence of double bonds that can be used to attach SO_3 group during sulfonation process. Other than that, alcohols with the functional group of O-H stretch also presence at the wavenumber of 3418.96 cm^{-1}. Lastly, ethers group were seen with C-O-C stretch at 1112.01 cm^{-1}.

4.2.2 Sulfonation Reaction of non-ionic Surfactants (Step 2 Reaction)

Step 1 solution sample is shown in figure 3. The reaction proceeds to step 2 reaction or known as sulfonation reaction of non-ionic surfactants using sodium bisulfite, $NaHSO_3$ as sulfur trioxide, SO_3 donors. The reaction for step 2 is similar for all experiment, only the condition will be manipulated.

The FTIR result for this reaction is shown in figure table 6 where the success of step 2 is monitored by the development of the sulfonate peaks.

Table 4.3. FTIR result for Step 2 reaction, based on FTIR result Appendix 4

Functional Group	**Molecular Motion**	**Wane Numbers, cm^{-1}**
Sulfonates	S=O Stretch	1352.07
Sulfonates	S-O Stretch	950.96

4.2.3 Sulfonation of Non-ionic Surfactants (Mole Ratio Effect)

The first experiments for step 2 reactions were done by controlling the amount of reactant mole ratio particularly the mole of $NaHSO_3$ added. The mole of non-ionic surfactants will be constant, whereas the mole for $NaHSO_3$ will be different from 1.0, 1.2, 1.3, 1.6 and 2.0.

The reaction was done at the boiling point temperature which is 82.5 degree Celsius. The determination of the sulfonate product yield progress is performed by the two phase titration which will be discussed on discussion part.

Below show the result of product yield after 24 hours of reaction at constant temperature and pressure. The experiment result for part 4.2.3 to investigate the effect of mole ratio is shown in figure 4.4.

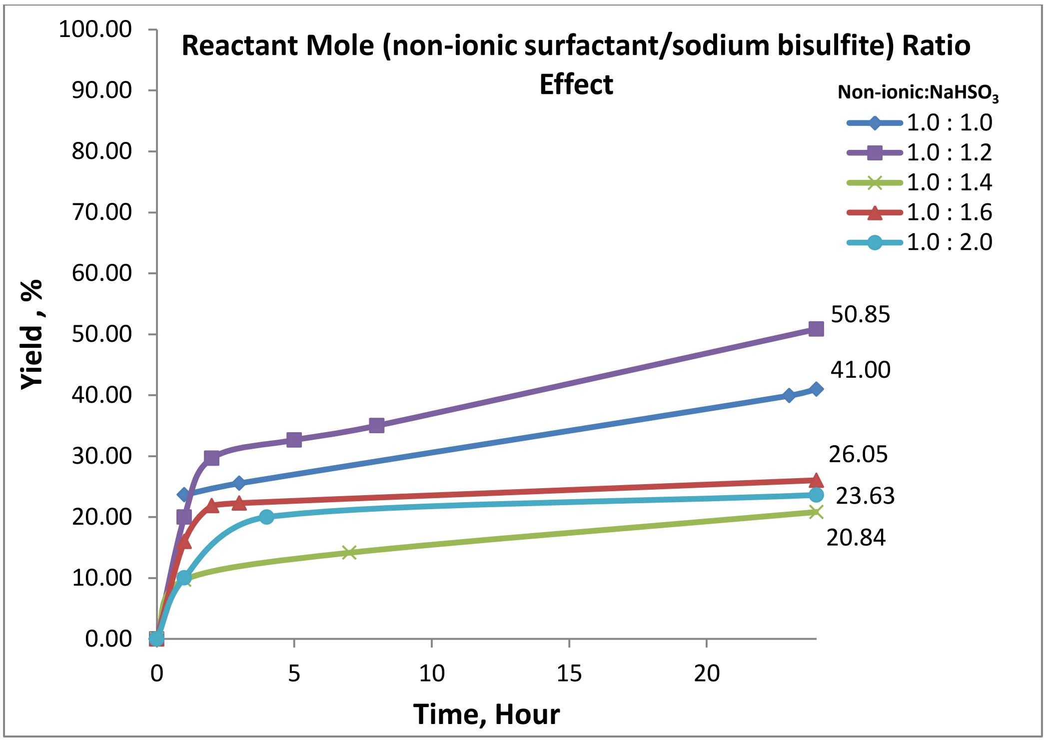


Figure 4.4. Reactants mole ratio effect results

Based on the graph shown in figure 4.4, the highest yield recorded after 24 hours reaction is 50.85 per cent at the condition of 1.0:1.2 between the Non-ionic Surfactants to $NaHSO_3$. Meanwhile, the least yield recorded at 1.0:1.4 with only 20.84 per cent yield.

4.2.4 Sulfonation of Non-ionic Surfactants (Catalyst Effects)

The second experiment for step 2 reaction was accomplished done by the addition of the Aluminium Nitrate, $Al(NO3)_3$ to investigate the effect of catalyst on the sulfonation reaction. Based on the last experiment, the experiment was setup in the similar way the employing the 1.0:1.2 ratios of non-ionic surfactants to $NaHSO_3$ configuration. The temperature is setup at boiling point temperature. Addition of 3 wt% $Al(NO_3)_3$ is added to as a catalyst to determine the effect of catalyst on the sulfonation reaction.

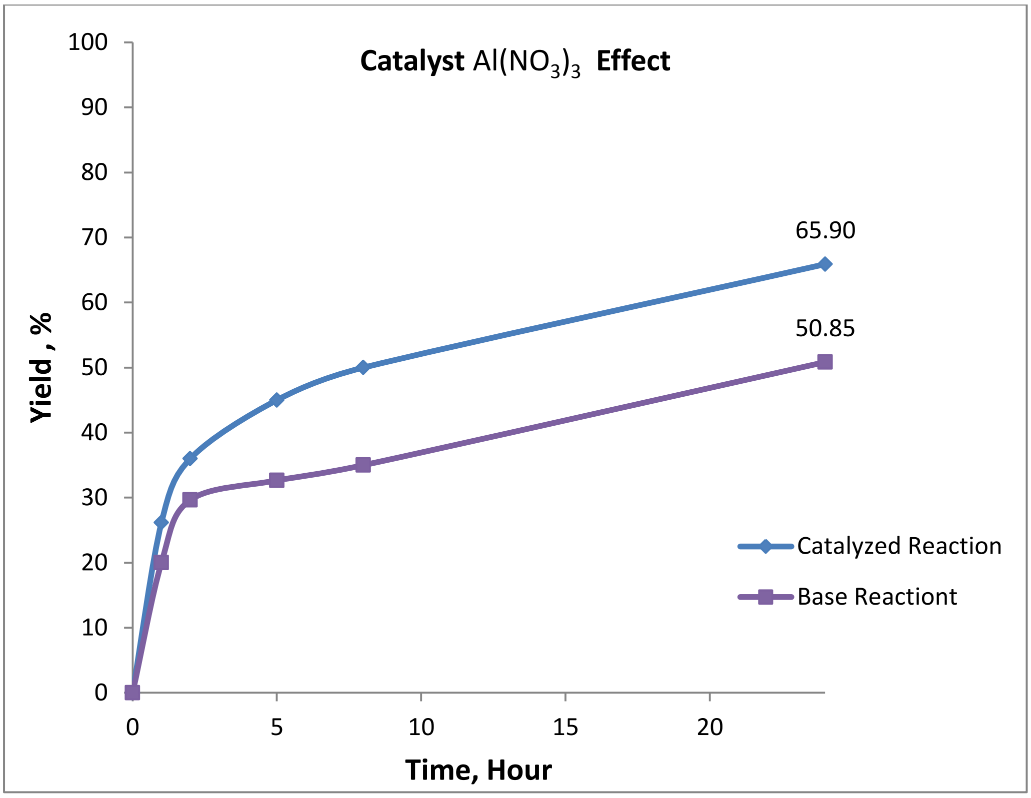


Figure 4.5. Catalyst effect results

Based on the graph shown in figure 4.5, the highest yield recorded after 24 hours reaction is 65.90 per cent at the condition after catalyst $Al(NO_3)_3$ is added. Meanwhile, the lesser yield recorded at only 50.85 per cent yield without catalyst. This show almost 30% of increment when compare with base experiment as shown in figure 4.5.

4.2.5 Sulfonation of Non-ionic Surfactants (Temperature Effects)

The third experiments for step 2 reaction were setup using the previous two experiments that obtained the highest yield. At 1.0:1.2 ratio of the non-ionic surfactants to $NaHSO_3$ in the presence of catalyst the last experiment is setup to investigate the reaction effects at different reaction temperatures from room temperature reaction, 40 degree Celsius, 60 degree Celsius and boiling point temperatures. The experiment result for part 4.2.5 to investigate the effect of mole ratio is shown in figure 4.6.

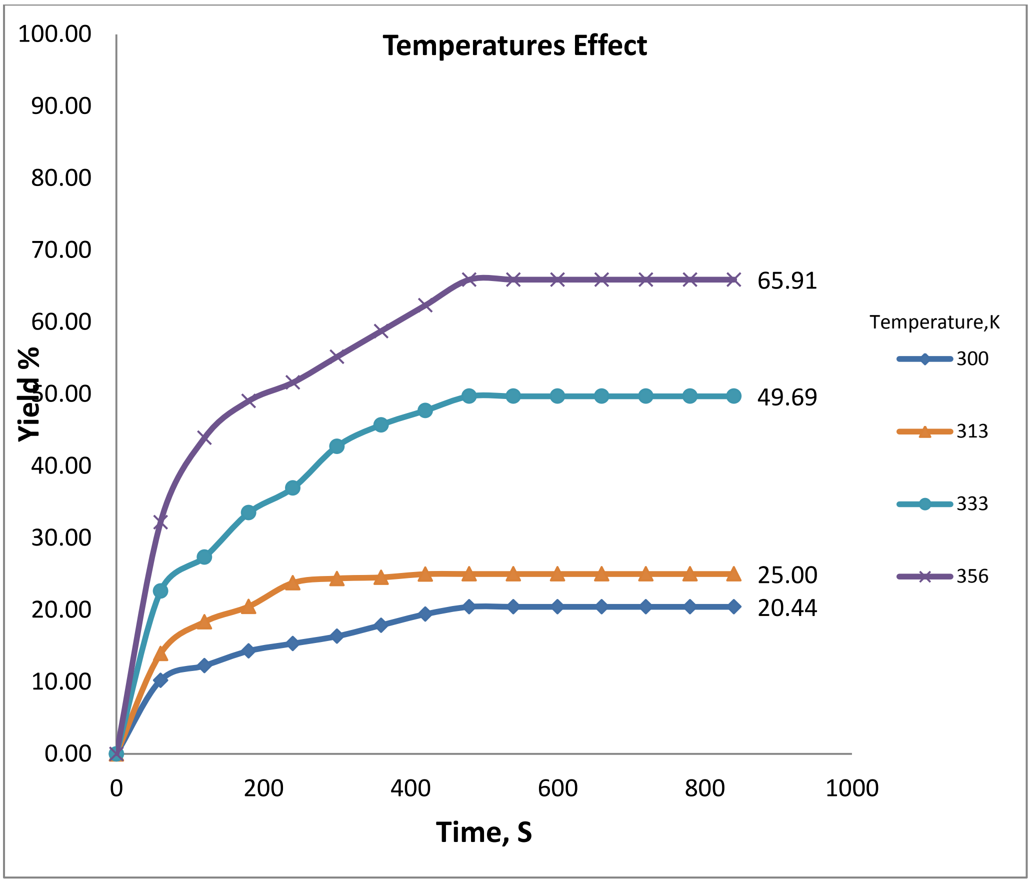


Figure 4.6. Temperature effect results using 1:1.2 $\frac{ionic\ surfactant}{NaHSO3}$ and 3 wt % $Al(NO_3)_3$

Based on figure 4.6, the result for yield against time at different temperatures showed that the highest products yield was in the boiling point temperature condition or 82.5 degree Celsius (356 K) with the yield of 65.91 % in contrast to the least yield obtained at the room temperature condition a value of 20.44 % yield.

4.3 Experiment Discussions

4.3.1 Overall Reaction Mechanism

The preparation of non-ionic surfactant was performed using Williamson synthesis reaction [6]. The double bonds are expected to be formed after the step 1 reaction. This reaction is useful to increase the stability of surfactants to alkali and at the same time the attachment to chain can be achieved for property improvement to avoid loses during EOR application [1] can be achieved. The mechanism of these reactions shown below:

Step 1 Reaction:

TDA-6 Ethoxylate		**Potassium Hydroxide**		**Surfactants Salts**
$R\text{-}O\text{-}(CH_2CH_2O)_x\text{-}OH$	+	KOH	$\xrightarrow{N_2}$	$R\text{-}O\text{-}(CH_2CH_2O)_x\text{-}OK + H_2O$

Surfactants Salts		**Methalyl Chloride**		**Non-ionic Surfactants**
$R\text{-}O\text{-}(CH_2CH_2O)_x\text{-}OK$	+	$CH_2{=}C\,(CH_3)\,CH_2\text{-}Cl$	$\xrightarrow{N_2}$	$R\text{-}O\text{-}(CH_2CH_2O)_x\text{-}O\,CH_2\,C(CH_3){=}CH_2 + KCl$

Step 2 Reaction

Non-ionic Surfactants		**Sodium Bisulfite**		**Anionic Surfactants Sulfonate**
$R\text{-}O\text{-}(CH_2CH_2O)_x\text{-}O\,CH_2C(CH_3){=}CH_2$	+	$NaHSO_3$	$\xrightarrow[\text{Ethanol/ H2O}]{\text{Reflux}}$	$R\text{-}O\text{-}(CH_2CH_2O)_x\text{-}O\,CH_2\text{-}C\,(CH_3)\,CH_2(SO_3)\,^{-}Na$

During step 1 reaction, water was immediately removed during the oxidation stop using Nitrogen gas purge to avoid the formation of black solution which can cause desulfonation. Desulfonation will hinder further reaction of sulfonation reaction in step 2 which can be reduced the yield of the final product. Reaction is performed at 1 atm and temperature 82.5 degree Celsius. Two phase of solid (white) and liquid were formed at the end of reactions a result of precipitation between K^+ with Cl^- to produce KCl salts. This salts is removed using centrifuge (see appendix 2) before step 2 reaction can begin. Based on FTIR result as shown in table 4.2, the unsaturated compound alkenes were seen at the wavenumber of 3077.27 $cm\text{-}^1$ for =CH stretch and 1637.80 cm^{-1} for C=C stretch. This is provides the evidence of the presence of double bonds formed at the end of step 1 reaction. The double bond is exhibited for further reaction during step 2 reaction in order to attach sulfur trioxide.

The reaction for step 2 begins by refluxing the end product from reaction step 1 with ethanol and water as solvents. The SO_3 molecules are expected to be attached at the double bond on the methalyl chloride chain when $NaHSO_3$ is added into step 1 reaction product as free electrons is presence for further reaction. Based on FTIR result as shown in table 4.3 the sulfonate groups were seen at the wavenumbers of 1352.07 cm-1 for S=O stretch and 950.96 for S-O stretch. Therefore, it is true that the sulfur trioxide group will be attached at the double bonds produced during step 1 reaction. The tendency for sulfonated product to yield in higher concentration depends on certain factors condition which will be discussed later.

4.3.2 Estimation of Anionic Surfactants Sulfonate Concentration

The extent of the reaction for sulfonation process was estimated using two phase titration as recommended by Zelenez [8] by titrating 0.004M Hyamine 1622 into a solution consisting of anionic surfactants sulfonate, mixed indicator, chloroform and solvents. Two layers of liquids with different colours were seen before the titration begins (refer appendix 1). The end point was determined when the pink solution (bottom part) changed completely into grey colour solution. The result for product yield was calculated using following expression.

$$Yield\ Percentage, \% = \frac{V\ x\ MW\ x\ N}{W\ x\ 1000}\ x\ 100 \text{ ………….(4)}$$

Where,

V = Volume of 0.004 M 1622 Hyamine used

N = Normality of the 1622 Hyamine

W = Weight of the sulfonated sample (0.5 to 0.7 grams)

MW = Molecular weight of the sulfonate sample

Based on the observation, the reaction between Hyamine 1622 between the solutions is faster at the beginning and the last reaction before the bottom solution turns completely grey. The condition of solution volume should be consistent throughout the experiments to make sure the estimation of end product concentration can be determined accurately.

4.3.3 Reactant Mole Ratio Effect Experiment

To determine the effect of mole ratio towards the formation of the end product, reaction was done using a fixed temperature and the same anionic surfactants concentration. Five sets of experiment were done at mole ratios of 1:1, 1:1.2, 1:1.4, 1:1.6 and 1:2.0 of anionic surfactants over sodium bisulfite. Based on Ellis et al[13], it preferable to react at the condition when mole ratio about 1:1.0 to 1:1.5 as to avoid large amount of excess bisulfite in minimizing residual inorganic material in the end product. The statement can be supported using this experiment result as shown in figure 4.4, when the amount per cent weight ratio of sodium bisulfite to anionic surfactants is twice the amount, the recorded yield of sulfonated product only 23.63% after 24 hours of reaction. Whereas, the highest yield was recorded using 1.0:1.2 mole ratio with the 50.85% yield. The comparison of reactants ratio effects is shown in table 4.4.

Table 4.4. The best reactants mole ratio shown in highlighted row.

Reactant Mole Ratio (Non-ionic Surfactants:$NaHSO_3$)	**Yield, %**
1.0:1.0	41.00
1.0:1.2	**50.85**
1.0:1.4	20.84
1.0:1.6	26.05
1.0:2.0	20.84

4.3.4 Catalyst Effect Experiment

To determine the effect of catalyst toward the formation of the end product after 24 hours, according to Norton [14] the highest olefin conversion when reacting Dodecene-1 and $NaHSO_3$ has achieved in the presence of $Al(NO_3)_3$ where 80 per cent conversion were recorded.

Reaction only happened during the successful collisions between reactants molecules. The minimum amount of energy require for reaction to happen known as the activation energy for the reaction to proceed. Catalyst is known to provide an alternative path for the reaction by lowering the amount of activation energy. The addition of 3 wt % of $Al(NO_3)_3$ had improved the conversion per cent by almost 30 per cent. Table 4.5 shows the summary effect of catalyst on end product yield per cent.

Table 4.5. Summary effect of catalyst

Reaction	**Yield, %**
No Catalyst	50.85
With Catalyst 3 wt % of $Al(NO_3)_3$	65.90

4.3.5 Temperature Effect Experiment

To determine the effect of temperature towards the formation of the end product with time the experiment was performed at standard room temperature, 40°C, 60°C, and 82.5°C temperature. Based on the results the sulfonation reaction is shown to be temperature dependent. The higher the temperature, the higher the conversion yields of sulfonated product. Which is true when related to molecular level where the molecules tend to move faster as the energy gained from heating, will be higher the chances for successful collisions to happen.

This theory can be related to Arrhenius Equation. According to the equation the higher the temperature is the higher the reaction rate. The energy required for reaction can be expressed in –Ea / RT as written in the equation below.

$$k(T) = Ae^{\frac{-Ea}{RT}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(5)$$

Where,

A = Pre-exponential factor

k = Chemical reaction constant

Ea = Activation energy

R = Gas constant

T = Temperature (kelvin)

The chemical reaction constant, k value is different for different temperature. This relationship leads support to the original Arrhenius Equation given below:

$$In\ \frac{k2}{k1} = -\frac{Ea}{R}\left(\frac{1}{T2} - \frac{1}{T1}\right) \ \ldots\ldots\ldots\ldots\ldots\ldots..(6)$$

The value of k for each temperature is determine by plotting graph of natural log against time as shown in figure 4.7 to figure 4.10. The slope value is equal to the reaction constant, k.

The reaction for step 2 reactions is a first order reaction based on figure 4.10 graph of natural log concentration against time which was plotted based on experiment result using 1.0:1.2 mole ratios of anionic surfactants to $NaHSO_3$ with present of catalyst and reacted at the boiling point reaction temperature.

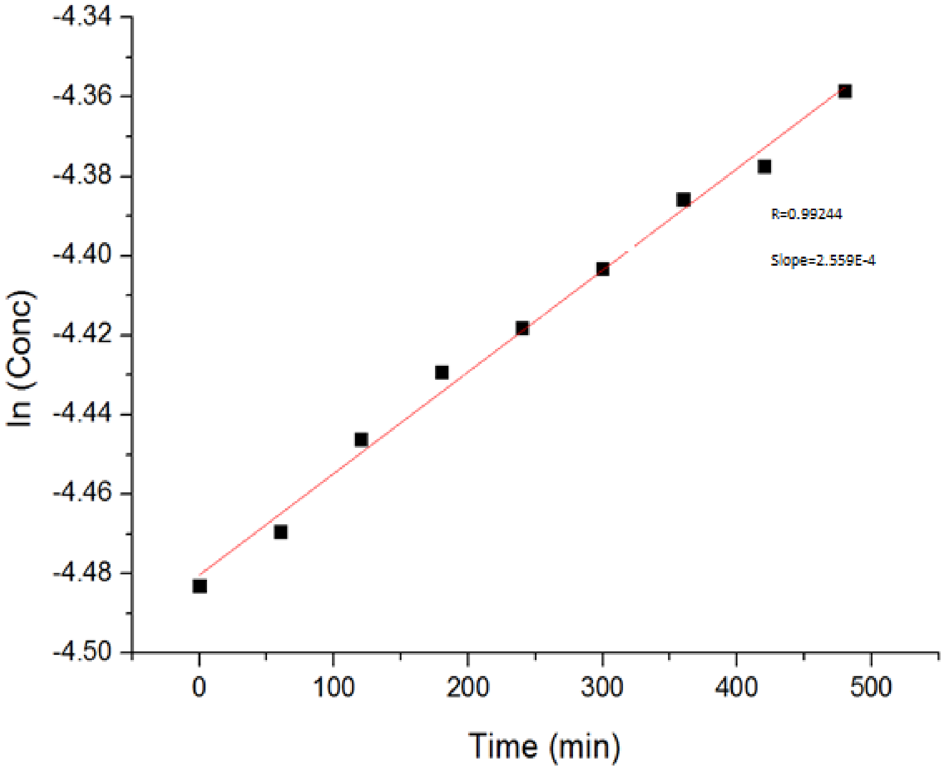


Figure 4.7. Concentration against time at 27 degree Celsius.

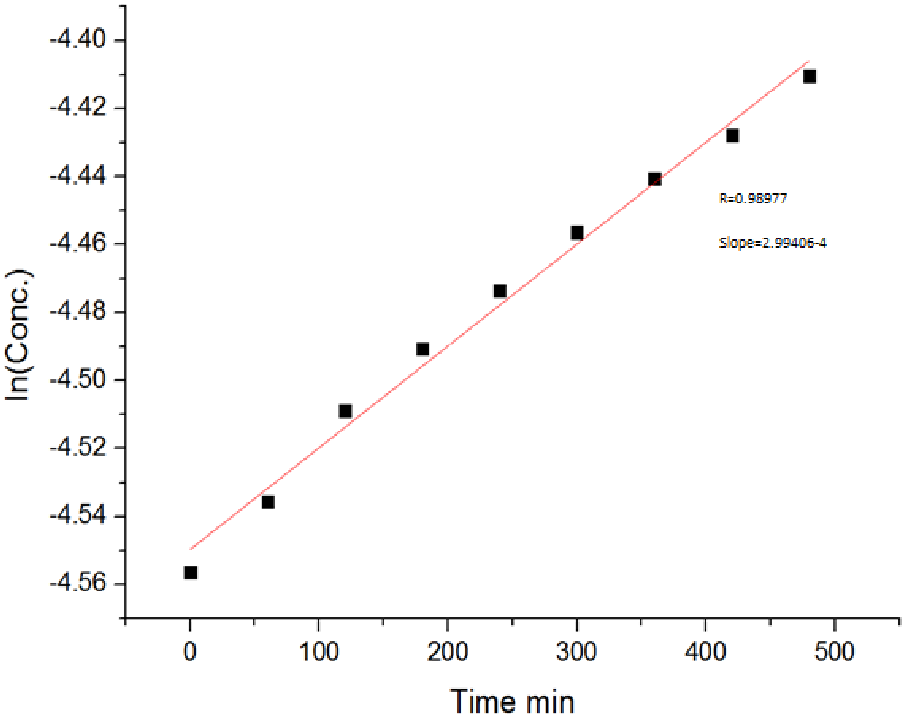


Figure 4.8. Concentration against time at 40 degree Celsius.

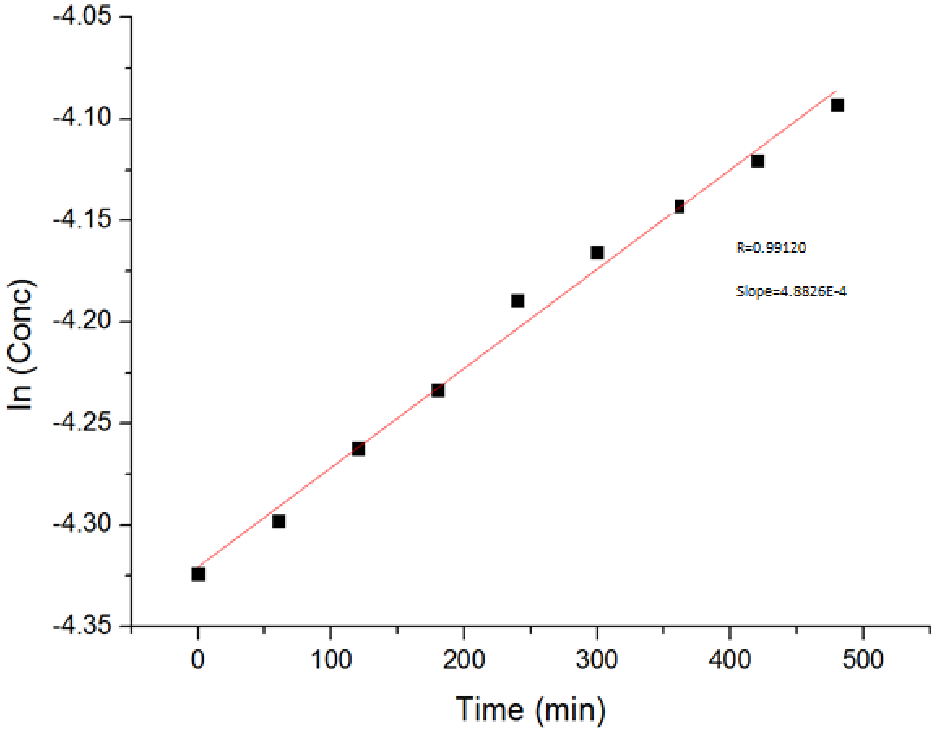


Figure 4.9. Concentration against time at 60 degree Celsius.

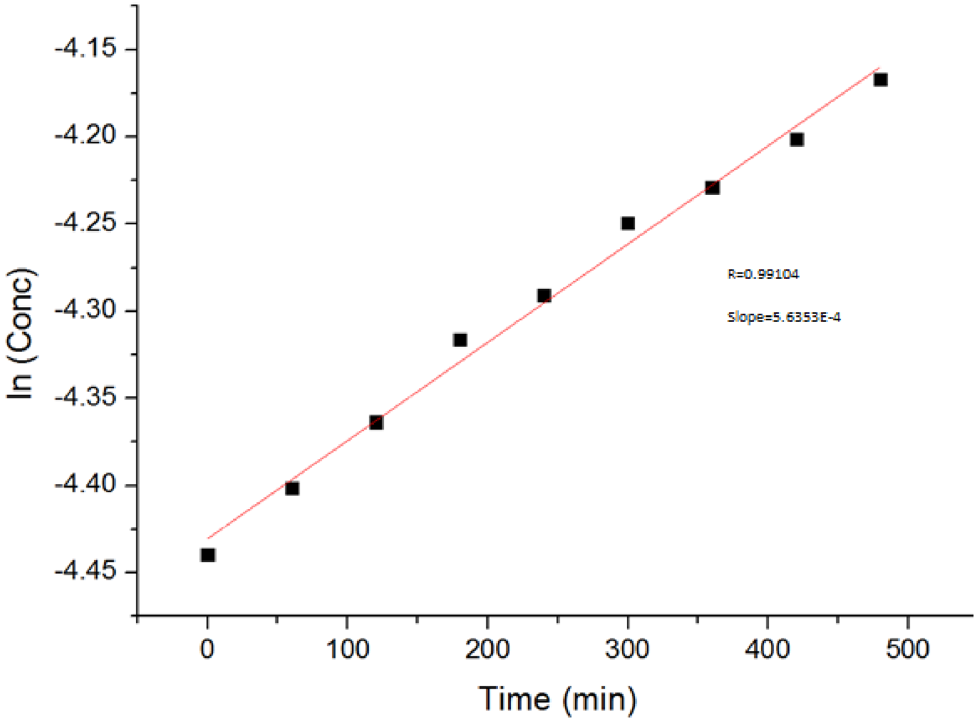


Figure 4.10. Concentration against time at 82.5 degree Celsius.

From the value of slope, the value of k for each temperature can be determined shown in table 9.

Table 4.6. k value for each temperature

Temperature, K	**Yield, %**	**Rate Constant,k min^{-1}**
300	20.44	2.55E-04
313	25.00	2.99E-04
333	49.69	4.88E-04
356	65.91	5.66E-04

From these k values, the calculated value for activation energy, Ea is 12,642.46 J $mol^{-1}k^{-1}$ when calculated using equation 6. From this value, it is smaller the activation energy for hydrolysis process of sucrose which usually about 29.2 kJ mol^{-1} k^{-1} to 35.2kJ mol^{-1} k^{-1}.

On the other hand, the value of rate constant increases with time which prove the theory of the Arrhenius, the higher the temperature, more energy will be absorbed by molecules; more frequent the collision for reaction. Hence, the bigger the rate of successful collision for the reaction to take place.

The rate order for step 2 reaction is not consider as second order of reaction because we unable to get straight line when the graph of 1/concentration against time was plotted shown in figure 4.11.

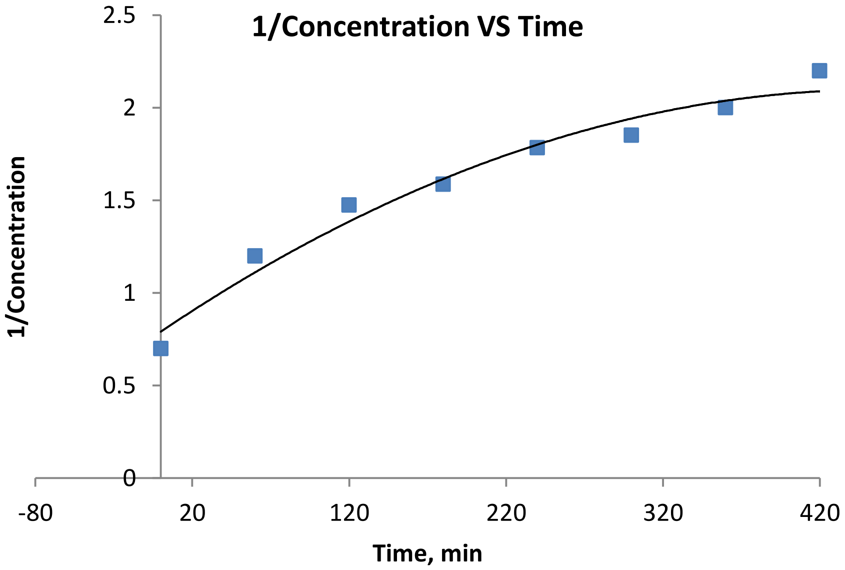


Figure 4.11. 1/concentration against time at 82.5 degree Celsius.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.0 CONCLUSION AND RECOMMENDATION

5.1 Conclusion

To recall all the objectives stated on Chapter 1, there are three objectives defined for this project. First, to study the effects of reactants mole ratio in the sulfonation reaction of the non-ionic surfactants. Secondly, to study the effect of catalyst in the sulfonation reaction of the non-ionic surfactants. Lastly, to study the effect of the reaction temperature in the sulfonation reaction of the non-ionic surfactants. Several results was obtained and discussed in Chapter 4.

Based on the project findings, it can be concluded that the preferable reactant mole ratio can be used is 1:1.2 the ratio of anionic surfactants to sodium bisulfite. This gives a good result compared to the other ratios. The yield per cent of final product recorded was 50.85% shown in figure 4.4. The sulfonation reaction is reactant concentration dependent as it appeared to be a first order reaction base on plotted graph of concentration against time shown in figure 4.10.

On the basis to study the effect of catalyst toward the sulfonation reaction, it can be concluded that the presence of $Al(NO_3)_3$ as catalyst increase the concentration of end product by 30%. Based on figure 4.5 in Chapter 4, the recorded yield per cent is 65.91% when using the mole ratio of 1:1.2 and reacted at the boiling point temperature which is at 82.5 ^oC.

Results on the effect of temperature against time showed in figure 4.6 shows that the higher the reaction temperature, the greater the concentration of end product yields. The more heat is applied during reaction of step 2, the more frequents the molecules collided and resulting more the successful collision reaction. The activation energy, Ea calculated is 12,642.46 J $mol^{-1}k^{-1}$ when using the alternative version of Arrhenius equation. Furthermore, the value of rate constant increases with time shown in table 4.6. This shows that the sulfonation reaction also temperature dependent.

From all the result, the author believed the research objectives are achieved when the sulfonation reaction of non-ionic surfactants can produce high yield sulfonated product which is 65.91% using 1:1.2 mole of non-ionic surfactants to sodium bisulfite at present of catalyst and reacted at the boiling point temperature which is 82.5^oC.

5.2 Recommendation

From this research, the author recommends several future works as follows:

1. The compatibility of reactants mole ratio is different which each other as the higher the number of carbons used as surfactants source the more compact and the geometry of the molecules structures hindered double bonds which make it harder for a successful reaction to happen. Thus the reactants mole ratio should be study in order to produce high yield of sulfonated product when using different type of ionic surfactants.
2. The effect of the amount and type of catalyst should be studied in order to minimize the amount usage of expensive catalyst for bigger production of sulfonated anionic surfactants product.
3. The effect of pressure toward reaction should be studied as it can improve the yield of sulfonated product.
4. The effect of pH value during the reactions should be investigated as it can affect the yield of sulfonated anionic surfactants.

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APPENDIX

1. Experiment Setup.

Three necked round bottom flask is heated, Nitrogen gas is allow to purge out the formation of water.

2. Two phase separation using centrifuge

- Top layer: Non-ionic Surfactants (Liquid)
- Bottom layer: Potassium Chloride (Solids)

3. FTIR result based on Step 1 reaction

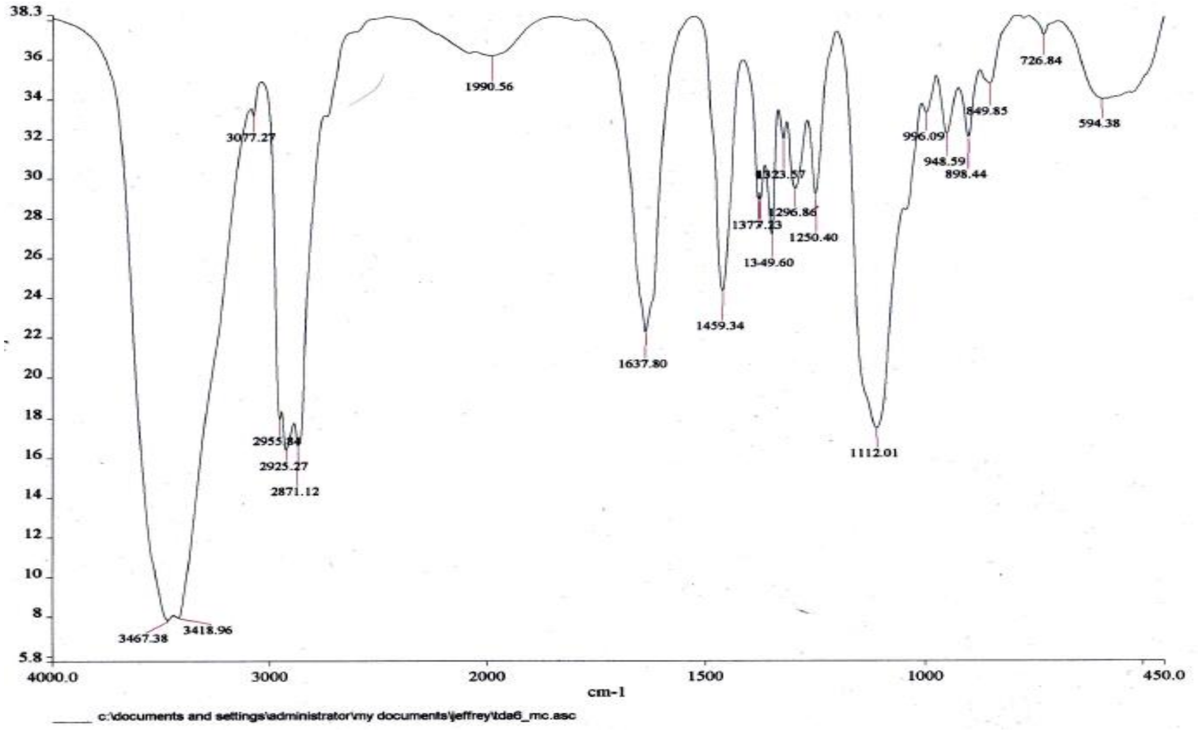
Step 1 reaction:

TDA-6 Ethoxylate + **Potassium Hydroxide** → **Surfactants Salts**

$R\text{-}O\text{-}(CH_2CH_2O)_x\text{-}OH + KOH \xrightarrow{N_2} R\text{-}O\text{-}(CH_2CH_2O)_x\text{-}OK + H_2O$

Surfactants Salts + **Methalyl Chloride** → **Non-ionic Surfactants**

$R\text{-}O\text{-}(CH_2CH_2O)_x\text{-}OK + CH_2{=}C\ (CH_3)\ CH_2\text{-}Cl \xrightarrow{N_2} R\text{-}O\text{-}(CH_2CH_2O)_x\text{-}O\ CH_2C(CH_3){=}CH_2 + KCl$

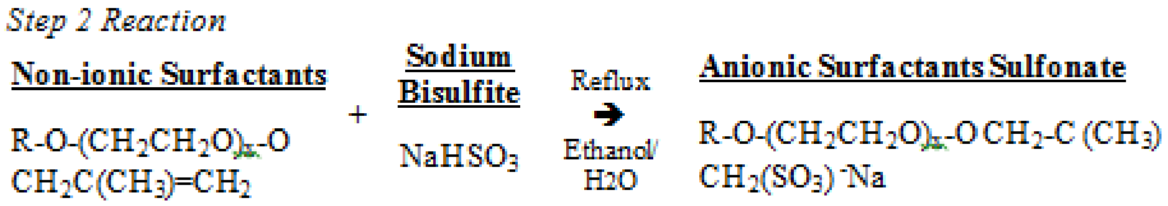


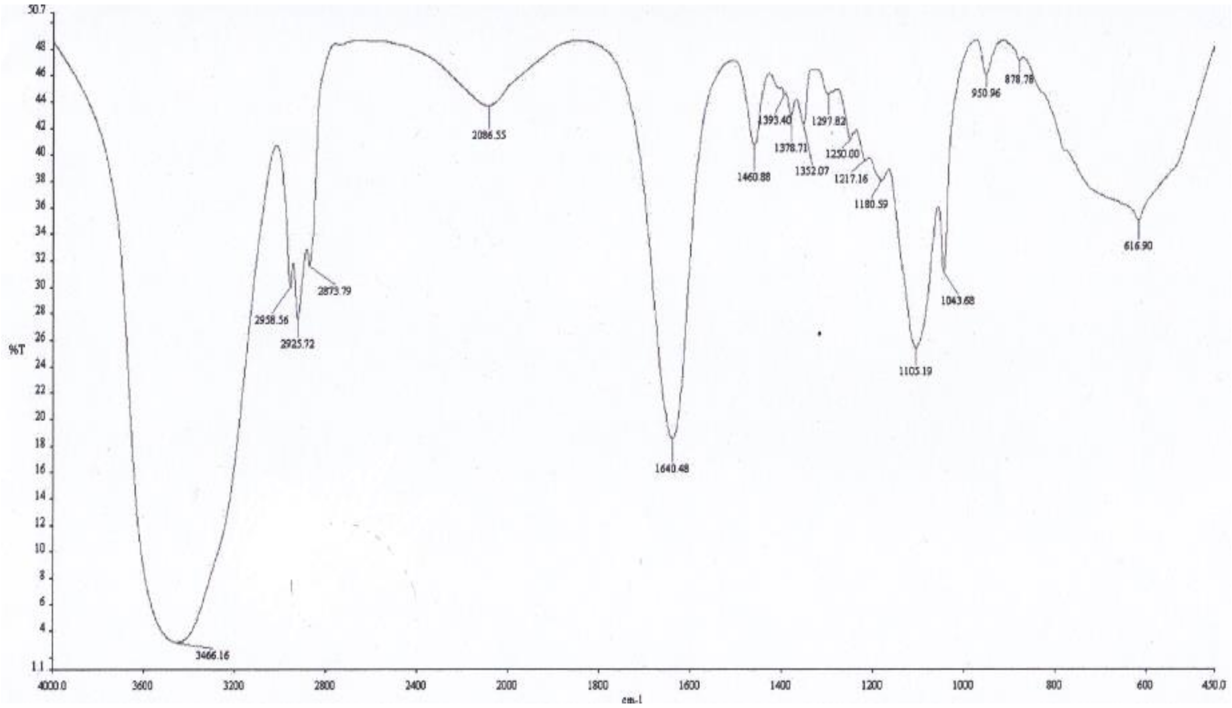
FTIR result for experiment step 1reaction is summarized base on Appendix 5

Functional Group	Molecular Motion	Wane Numbers, cm^{-1}
Alkanes	=CH Stretch	3077.27
Alkanes	C=C Stretch	1637.80
Alcohols	O-H Stretch	3467.38

Ethers	C-O-C Stretch (diaryl)	1112.01

4. FTIR result based on Step 2 reaction





FTIR result for experiment step 2reaction is summarized base on Appendix 5

Functional Group	**Molecular Motion**	**Wane Numbers, cm^{-1}**
Sulfonates	S=O Stretch	1352.07
Sulfonates	S-O Stretch	950.96

5. IR Absorptions for Representatives Functional Groups

Functional Group	Molecular Motion	Wavenumber (cm^{-1})
alkanes	C-H stretch	2950-2800
	CH_2 bend	~1465
	CH_3 bend	~1375
	CH_2 bend (4 or more)	~720
alkenes	=CH stretch	3100-3010
	C=C stretch (isolated)	1690-1630
	C=C stretch (conjugated)	1640-1610
	C-H in-plane bend	1430-1290
	C-H bend (monosubstituted)	~990 & ~910
	C-H bend (disubstituted - E)	~970
	C-H bend (disubstituted - 1,1)	~890
	C-H bend (disubstituted - Z)	~700
	C-H bend (trisubstituted)	~815
alkynes	acetylenic C-H stretch	~3300
	C,C triple bond stretch	~2150
	acetylenic C-H bend	650-600
aromatics	C-H stretch	3020-3000
	C=C stretch	~1600 & ~1475
	C-H bend (mono)	770-730 & 715-685
	C-H bend (ortho)	770-735
	C-H bend (meta)	~880 & ~780 & ~690
	C-H bend (para)	850-800
alcohols	O-H stretch	~3650 or 3400-3300

	C-O stretch	1260-1000
ethers	C-O-C stretch (dialkyl)	1300-1000
	C-O-C stretch (diaryl)	~1250 & ~1120
aldehydes	C-H aldehyde stretch	~2850 & ~2750
	C=O stretch	~1725
ketones	C=O stretch	~1715
	C-C stretch	1300-1100
carboxylic acids	O-H stretch	3400-2400
	C=O stretch	1730-1700
	C-O stretch	1320-1210
	O-H bend	1440-1400
esters	C=O stretch	1750-1735
	C-C(O)-C stretch (acetates)	1260-1230
	C-C(O)-C stretch (all others)	1210-1160
acid chlorides	C=O stretch	1810-1775
	C-Cl stretch	730-550
anhydrides	C=O stretch	1830-1800&1775-1740
	C-O stretch	1300-900
amines	N-H stretch (1 per N-H bond)	3500-3300
	N-H bend	1640-1500
	C-N Stretch (alkyl)	1200-1025
	C-N Stretch (aryl)	1360-1250
	N-H bend (oop)	~800
amides	N-H stretch	3500-3180
	C=O stretch	1680-1630
	N-H bend	1640-1550
	N-H bend (1^{o})	1570-1515
alkyl halides	C-F stretch	1400-1000
	C-Cl stretch	785-540

	C-Br stretch	650-510
	C-I stretch	600-485
nitriles	C,N triple bond stretch	~2250
isocyanates	-N=C=O stretch	~2270
isothiocyanates	-N=C=S stretch	~2125
imines	R_2C=N-R stretch	1690-1640
nitro groups	-NO_2 (aliphatic)	1600-1530&1390-1300
	-NO_2 (aromatic)	1550-1490&1355-1315
mercaptans	S-H stretch	~2550
sulfoxides	S=O stretch	~1050
sulfones	S=O stretch	~1300 & ~1150
sulfonates	S=O stretch	~1350 & ~11750
	S-O stretch	1000-750
phosphines	P-H stretch	2320-2270
	PH bend	1090-810
phosphine oxides	P=O	1210-1140

6. Chemicals MSDS

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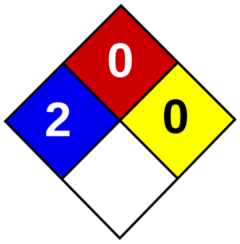
Science Lab.com
Chemicals & Laboratory Equipment



Health	2
Fire	0
Reactivity	0
Personal Protection	E

Material Safety Data Sheet

Aluminum nitrate nonahydrate MSDS

Section 1: Chemical Product and Company Identification

Product Name: Aluminum nitrate nonahydrate

Catalog Codes: SLA1981

CAS#: 7784-27-2

RTECS: BD1050000

TSCA: TSCA 8(b) inventory: Aluminum nitrate nonahydrate

CI#: Not available.

Synonym:

Chemical Name: aluminum nitrate nonahydrate

Chemical Formula: Al(NO3)3.9H2O

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Aluminum nitrate nonahydrate	7784-27-2	100

Toxicological Data on Ingredients: Aluminum nitrate nonahydrate: ORAL (LD50): Acute: 3632 mg/kg [Rat]. 3980 mg/kg [Mouse]. 4280 mg/kg [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (permeator). Prolonged exposure may result in skin burns and ulcerations. Over-exposure by inhalation may cause respiratory irritation.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to lungs, mucous membranes. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:

Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention if symptoms appear.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: Not applicable.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container.

Large Spill:
Oxidizing material. Stop leak if without risk. Avoid contact with a combustible material (wood, paper, oil, clothing...). Keep substance damp using water spray. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Keep away from combustible material.. Do not ingest. Do not breathe dust. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes.

Storage:
Keep container tightly closed. Keep container in a cool, well-ventilated area. Separate from acids, alkalies, reducing agents and combustibles. See NFPA 43A, Code for the Storage of Liquid and Solid Oxidizers.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 2 Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.

Odor: Not available.

Taste: Not available.

Molecular Weight: 375.13 g/mole

Color: Not available.

pH (1% soln/water): Not available.

Boiling Point: Decomposition temperature: 135°C (275°F)

Melting Point: 73°C (163.4°F)

Critical Temperature: Not available.

Specific Gravity: 1.058 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water.

Solubility:

Easily soluble in cold water. Soluble in hot water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Eye contact. Inhalation. Ingestion.

Toxicity to Animals: Acute oral toxicity (LD50): 3632 mg/kg [Rat].

Chronic Effects on Humans: Causes damage to the following organs: lungs, mucous membranes.

Other Toxic Effects on Humans:
Hazardous in case of skin contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (permeator).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: CLASS 5.1: Oxidizing material.

Identification: : Aluminum Nitrate UNNA: UN1438 PG: III

Special Provisions for Transport: Marine Pollutant

Section 15: Other Regulatory Information

Federal and State Regulations: TSCA 8(b) inventory: Aluminum nitrate nonahydrate

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada):
CLASS C: Oxidizing material. CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R8- Contact with combustible material may cause fire. R36/38- Irritating to eyes and skin.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 0

Reactivity: 0

Personal Protection: E

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 0

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/11/2005 11:15 AM

Last Updated: 05/21/2013 12:00 PM

Material Safety Data Sheet
Ethanol, Absolute

ACC# 89308

Section 1 - Chemical Product and Company Identification

MSDS Name: Ethanol, Absolute
Catalog Numbers: NC9602322
Synonyms: Ethyl Alcohol; Ethyl Alcohol Anhydrous; Ethyl Hydrate; Ethyl Hydroxide; Fermentation Alcohol; Grain Alcohol; Methylcarbinol; Molasses Alcohol; Spirits of Wine.
Company Identification:

Fisher Scientific
1 Reagent Lane
Fair Lawn, NJ 07410

For information, call: 201-796-7100
Emergency Number: 201-796-7100
For CHEMTREC assistance, call: 800-424-9300
For International CHEMTREC assistance, call: 703-527-3887

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
64-17-5	Ethanol	ca.100	200-578-6

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: colorless clear liquid. Flash Point: 16.6 deg C.
Warning! Causes severe eye irritation. **Flammable liquid and vapor.** Causes respiratory tract irritation. This substance has caused adverse reproductive and fetal effects in humans. May cause central nervous system depression. May cause liver, kidney and heart damage. Causes moderate skin irritation.
Target Organs: Kidneys, heart, central nervous system, liver.

Potential Health Effects
Eye: Causes severe eye irritation. May cause painful sensitization to light. May cause chemical conjunctivitis and corneal damage.
Skin: Causes moderate skin irritation. May cause cyanosis of the extremities.
Ingestion: May cause gastrointestinal irritation with nausea, vomiting and diarrhea. May cause systemic toxicity with acidosis. May cause central nervous system depression, characterized by excitement, followed by headache, dizziness, drowsiness, and nausea. Advanced stages may cause collapse, unconsciousness, coma and possible death due to respiratory failure.
Inhalation: Inhalation of high concentrations may cause central nervous system effects characterized by nausea, headache, dizziness, unconsciousness and coma. Causes respiratory tract irritation. May cause narcotic effects in high concentration. Vapors may cause dizziness or suffocation.
Chronic: May cause reproductive and fetal effects. Laboratory experiments have resulted in mutagenic effects. Animal studies have reported the development of tumors. Prolonged exposure may cause liver, kidney, and heart damage.

Section 4 - First Aid Measures

Eyes: Get medical aid. Gently lift eyelids and flush continuously with wate r.
Skin: Get medical aid. Wash clothing before reuse. Flush skin with plenty of soap and water.
Ingestion: Do not induce vomiting. If victim is conscious and alert, give 2-4 cupfuls of milk or water. Never give anything by mouth to an unconscious person. Get medical aid.
Inhalation: Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid. Do NOT use mouth-to-mouth resuscitation.
Notes to Physician: Treat symptomatically and supportively. Persons with skin or eye disorders or liver, kidney, chronic respiratory diseases, or central and peripheral nervous sytem diseases may be at increased risk from exposure to this substance.
Antidote: None reported.

Section 5 - Fire Fighting Measures

General Information: Containers can build up pressure if exposed to heat and/or fire. As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Vapors may form an explosive mixture with air. Vapors can travel to a source of ignition and flash back. Will burn if involved in a fire. Flammable Liquid. Can release vapors that form explosive mixtures at temperatures above the flashpoint. Use water spray to keep fire-exposed containers cool. Containers may explode in the heat of a fire.
Extinguishing Media: For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam. For large fires, use water spray, fog, or alcohol-resistant foam. Use water spray to cool fire-exposed containers. Water may be ineffective. Do NOT use straight streams of water.
Flash Point: 16.6 deg C (61.88 deg F)
Autoignition Temperature: 363 deg C (685.40 deg F)
Explosion Limits, Lower:3.3 vol %
Upper: 19.0 vol %
NFPA Rating: (estimated) Health: 2; Flammability: 3; Instability: 0

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks: Absorb spill with inert material (e.g. vermiculite, sand or earth), then place in suitable container. Remove all sources of ignition. Use a spark-proof tool. Provide ventilation. A vapor suppressing foam may be used to reduce vapors.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Use only in a well-ventilated area. Ground and bond containers when transferring material. Use spark-proof tools and explosion proof equipment. Avoid contact with eyes, skin, and clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep container tightly closed. Keep away from heat, sparks and flame. Avoid ingestion and inhalation. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames.
Storage: Keep away from heat, sparks, and flame. Keep away from sources of ignition. Store in a tightly closed container. Keep from contact with oxidizing materials. Store in a cool, dry, well-ventilated area away from incompatible substances. Flammables-area. Do not store near perchlorates, peroxides, chromic acid or nitric acid.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Use explosion-proof ventilation equipment. Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use adequate general or local exhaust ventilation to keep airborne concentrations below the permissible exposure limits.
Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
Ethanol	1000 ppm TWA	1000 ppm TWA; 1900 mg/m3 TWA 3300 ppm IDLH	1000 ppm TWA; 1900 mg/m3 TWA

OSHA Vacated PELs: Ethanol: 1000 ppm TWA; 1900 mg/m3 TWA
Personal Protective Equipment
Eyes: Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin: Wear appropriate protective gloves to prevent skin exposure.
Clothing: Wear appropriate protective clothing to prevent skin exposure.
Respirators: A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever workplace conditions warrant a respirator's use.

Section 9 - Physical and Chemical Properties

Physical State: Clear liquid
Appearance: colorless
Odor: Mild, rather pleasant, like wine or whis
pH: Not available.
Vapor Pressure: 59.3 mm Hg @ 20 deg C
Vapor Density: 1.59
Evaporation Rate: Not available.
Viscosity: 1.200 cP @ 20 deg C
Boiling Point: 78 deg C
Freezing/Melting Point:-114.1 deg C
Decomposition Temperature: Not available.
Solubility: Miscible.
Specific Gravity/Density:0.790 @ 20°C
Molecular Formula:C_2H_5OH
Molecular Weight:46.0414

Section 10 - Stability and Reactivity

Chemical Stability: Stable under normal temperatures and pressures.
Conditions to Avoid: Incompatible materials, ignition sources, excess heat, oxidizers.
Incompatibilities with Other Materials: Strong oxidizing agents, acids, alkali metals, ammonia, hydrazine, peroxides, sodium, acid anhydrides, calcium hypochlorite, chromyl chloride, nitrosyl perchlorate, bromine pentafluoride, perchloric acid, silver nitrate, mercuric nitrate, potassium-tert-butoxide, magnesium perchlorate, acid chlorides, platinum, uranium hexafluoride, silver oxide, iodine heptafluoride, acetyl bromide, disulfuryl difluoride, tetrachlorosilane + water, acetyl chloride, permanganic acid, ruthenium (VIII) oxide, uranyl perchlorate, potassium dioxide.
Hazardous Decomposition Products: Carbon monoxide, irritating and toxic fumes and gases, carbon dioxide.
Hazardous Polymerization: Will not occur.

Section 11 - Toxicological Information

RTECS#:
CAS# 64-17-5: KQ6300000
LD50/LC50:
CAS# 64-17-5:
Draize test, rabbit, eye: 500 mg Severe;
Draize test, rabbit, eye: 500 mg/24H Mild;
Draize test, rabbit, skin: 20 mg/24H Moderate;
Inhalation, mouse: LC50 = 39 gm/m3/4H;
Inhalation, rat: LC50 = 20000 ppm/10H;
Oral, mouse: LD50 = 3450 mg/kg;
Oral, rabbit: LD50 = 6300 mg/kg;
Oral, rat: LD50 = 7060 mg/kg;
Oral, rat: LD50 = 9000 mg/kg;
Carcinogenicity:
CAS# 64-17-5: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: Ethanol has been shown to produce fetotoxicity in the embryo or fetus of laboratory animals. Prenatal exposure to ethanol is associated with a distinct pattern of congenital malformations that have collecetively been termed the "fetal alcohol syndrome".
Teratogenicity: Oral, Human - woman: TDLo = 41 gm/kg (female 41 week(s) after conception) Effects on Newborn - Apgar score (human only) and Effects on Newborn - other neonatal measures or effects and Effects on Newborn - drug dependence.
Reproductive Effects: Intrauterine, Human - woman: TDLo = 200 mg/kg (female 5 day(s) pre-mating) Fertility - female fertility index (e.g. # females pregnant per # sperm positive females; # females pregnant per # females mated).
Neurotoxicity: No information available.
Mutagenicity: DNA Inhibition: Human, Lymphocyte = 220 mmol/L.; Cytogenetic Analysis: Human, Lymphocyte = 1160 gm/L.; Cytogenetic Analysis: Human, Fibroblast = 12000 ppm.; Cytogenetic Analysis: Human, Leukocyte = 1 pph/72H (Continuous).; Sister Chromatid Exchange: Human, Lymphocyte = 500 ppm/72H (Continuous).
Other Studies: Standard Draize Test(Skin, rabbit) = 20 mg/24H (Moderate) Standard Draize Test: Administration into the eye (rabbit) = 500 mg (Severe).

Section 12 - Ecological Information

Ecotoxicity: Fish: Rainbow trout: LC50 = 12900-15300 mg/L; 96 Hr; Flow-through @ 24-24.3°CFish: Rainbow trout: LC50 = 11200 mg/L; 24 Hr; Fingerling (Unspecified)Bacteria: Phytobacterium phosphoreum: EC50 = 34900 mg/L; 5-30 min; Microtox test When spilled on land it is apt to volatilize, biodegrade, and leach into the ground water, but no data on the rates of these processes could be found. Its fate in ground water is unknown. When released into water it will volatilize and probably biodegrade. It would not be expected to adsorb to sediment or bioconcentrate in fish.
Environmental: When released to the atmosphere it will photodegrade in hours (polluted urban atmosphere) to an estimated range of 4 to 6 days in less polluted areas. Rainout should be significant.
Physical: No information available.
Other: No information available.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to

ensure complete and accurate classification.
RCRA P-Series: None listed.
RCRA U-Series: None listed.

Section 14 - Transport Information

	US DOT	Canada TDG
Shipping Name:	Not reviewed.	No information available.
Hazard Class:		
UN Number:		
Packing Group:		

Section 15 - Regulatory Information

US FEDERAL

TSCA
CAS# 64-17-5 is listed on the TSCA inventory.
Health & Safety Reporting List
None of the chemicals are on the Health & Safety Reporting List.
Chemical Test Rules
None of the chemicals in this product are under a Chemical Test Rule.
Section 12b
None of the chemicals are listed under TSCA Section 12b.
TSCA Significant New Use Rule
None of the chemicals in this material have a SNUR under TSCA.
CERCLA Hazardous Substances and corresponding RQs
None of the chemicals in this material have an RQ.
SARA Section 302 Extremely Hazardous Substances
None of the chemicals in this product have a TPQ.
SARA Codes
CAS # 64-17-5: acute, chronic, flammable.
Section 313 No chemicals are reportable under Section 313.
Clean Air Act:
This material does not contain any hazardous air pollutants.
This material does not contain any Class 1 Ozone depletors.
This material does not contain any Class 2 Ozone depletors.
Clean Water Act:
None of the chemicals in this product are listed as Hazardous Substances under the CWA.
None of the chemicals in this product are listed as Priority Pollutants under the CWA.
None of the chemicals in this product are listed as Toxic Pollutants under the CWA.
OSHA:
None of the chemicals in this product are considered highly hazardous by OSHA.
STATE
CAS# 64-17-5 can be found on the following state right to know lists: California, New Jersey, Pennsylvania, Minnesota, Massachusetts.

California Prop 65
WARNING: This product contains Ethanol, a chemical known to the state of California to cause developmental reproductive toxicity.
California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives
Hazard Symbols:
F

Risk Phrases:

R 11 Highly flammable.

Safety Phrases:

S 16 Keep away from sources of ignition - No smoking.
S 33 Take precautionary measures against static discharges.
S 7 Keep container tightly closed.
S 9 Keep container in a well-ventilated place.

WGK (Water Danger/Protection)

CAS# 64-17-5: 0

Canada - DSL/NDSL

CAS# 64-17-5 is listed on Canada's DSL List.

Canada - WHMIS

This product has a WHMIS classification of B2, D2A.

Canadian Ingredient Disclosure List

CAS# 64-17-5 is listed on the Canadian Ingredient Disclosure List.

Section 16 - Additional Information

MSDS Creation Date: 7/27/1999
Revision #4 Date: 3/18/2003

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall Fisher be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if Fisher has been advised of the possibility of such damages.

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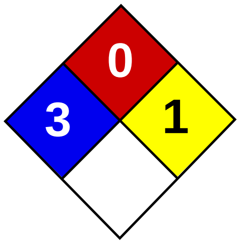


Health	3
Fire	0
Reactivity	2
Personal Protection	J

Material Safety Data Sheet
Potassium hydroxide MSDS

Section 1: Chemical Product and Company Identification

Product Name: Potassium hydroxide

Catalog Codes: SLP4096, SLP3085, SLP4900, SLP2071

CAS#: 1310-58-3

RTECS: TT2100000

TSCA: TSCA 8(b) inventory: Potassium hydroxide

CI#: Not available.

Synonym:

Chemical Name: Potassium Hydroxide

Chemical Formula: KOH

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Potassium hydroxide	1310-58-3	100

Toxicological Data on Ingredients: Potassium hydroxide: ORAL (LD50): Acute: 273 mg/kg [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (corrosive, irritant), of eye contact (irritant, corrosive), of ingestion, of inhalation. The amount of tissue damage depends on length of contact. Eye contact can result in corneal damage or blindness. Skin contact can produce inflammation and blistering. Inhalation of dust will produce irritation to gastro-intestinal or respiratory tract, characterized by burning, sneezing and coughing. Severe over-exposure can produce lung damage, choking, unconsciousness or death. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to upper respiratory tract, skin, eyes. Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure of the eyes to a low level of dust can produce eye irritation. Repeated skin exposure can produce local skin destruction, or dermatitis. Repeated inhalation of dust can produce varying degree of respiratory irritation or lung damage.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention immediately.

Skin Contact:
In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Cover the irritated skin with an emollient. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention immediately.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention immediately.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: metals, acids

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards:
Violent reaction or ignition under appropriate conditions with acids, alcohols, p-bis(1,3-dibromoethyl) benzene, cyclopentadiene, germanium, hyponitrous acid, maleic anhydride, nitroalkanes, 2-nitrophenol, potassium peroxodisulfate, sugars, 2,2,3,3-tetrafluoropropanol, thorium dicarbide. Molten ortho -nitrophenol reacts violently with potassium hydroxide. When potassium hydroxide and tetrachloroethane are heated, a spontaneously flammable gas, chloroacetylene, is formed. When phosphorus is boiled in a solution of potassium hydroxide, phosphine gas is evolved which is spontaneously flammable. 1,2-Dichloroethylene and Potassium hydroxide reaction produces chloroacetylene which is spontaneously flammable in air. Potassium Persulfate and a little Potassium hydroxide and water will ignite. When wet, attacks metals such as aluminum, tin, lead, and zinc, producing flammable hydrogen gas.

Special Remarks on Explosion Hazards:

Potentially explosive reaction with bromoform + crown ethers, chlorine dioxide, nitrobenzene, nitromethane, nitrogen trichloride, peroxidized tetrahydrofuran, 2,4,6-trinitrotoluene. Reaction with ammonium hexachloroplatiate(2-) + heat forms heat sensitive explosive product. Potassium hydroxide will cause explosive decomposition of maleic anhydride. Detonation will occur when potassiuim hydroxide is mixed with n-methyl-nitroso urea and methylene chloride. Nitrogen trichloride explodes on contact with potassium hydroxide.

Section 6: Accidental Release Measures

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. If necessary: Neutralize the residue with a dilute solution of acetic acid.

Large Spill:
Corrosive solid. Stop leak if without risk. Do not get water inside container. Do not touch spilled material. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Neutralize the residue with a dilute solution of acetic acid. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep container dry. Do not ingest. Do not breathe dust. Never add water to this product. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as organic materials, metals, acids, moisture.

Storage: Keep container tightly closed. Keep container in a cool, well-ventilated area. Do not store above 23°C (73.4°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Synthetic apron. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor and dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
CEIL: 2 (mg/m3) from OSHA (PEL) [United States] CEIL: 2 (mg/m3) from ACGIH (TLV) [United States] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid. (Solid pellets.)

Odor: Odorless.

Taste: Not available.

Molecular Weight: 56.11 g/mole

Color: White.

pH (1% soln/water): 13 [Basic.]

Boiling Point: Decomposition temperature: 1384°C (2523.2°F)

Melting Point: 380°C (716°F)

Critical Temperature: Not available.

Specific Gravity: 2.044 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water.

Solubility:
Easily soluble in cold water, hot water. Insoluble in diethyl ether.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Incompatible materials, dust generation, exposure to moist air or water.

Incompatibility with various substances:
Highly reactive with acids. Reactive with organic materials, metals, moisture.

Corrosivity:
Extremely corrosive in presence of aluminum, brass, and zinc. Slightly corrosive in presence of copper, of stainless steel(304). Non-corrosive in presence of stainless steel(316).

Special Remarks on Reactivity:
Hygroscopic (absorbs moisture from air). When dissolved in water or alcohol or when the solution is treated with acid, much heat is generated. Reacts violently with acids, halogens, halogenated hydrocarbons, maleic anhydride, organic anhydrides, isocyanates, alkylene oxides, epichlorhydrin, aldehydes, alcohols, gylcols, phenols, cresols, caprolactum solution. Also incompatible with nitro compounds (nitrobenzene, nitromethane, nitrogen trichloride), organic materials, acid anhydrides, acid chlorides, magnesium, peroxidized tetrahydrofuran, chlorine dioxide, maleic dicarbide, sugars. When wet attacks metals such as aluminum, tin, lead, and zinc.

Special Remarks on Corrosivity:
When wet, attacks metals such as aluminum, tin, lead, and zinc, producing flammable hydrogen gas. Severe corrosive effect on brass and bronze.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Inhalation. Ingestion.

Toxicity to Animals: Acute oral toxicity (LD50): 273 mg/kg [Rat].

Chronic Effects on Humans:

MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. May cause damage to the following organs: upper respiratory tract, skin, eyes.

Other Toxic Effects on Humans:
Extremely hazardous in case of inhalation (lung corrosive). Very hazardous in case of skin contact (corrosive, irritant), of eye contact (corrosive), of ingestion, .

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: May affect genetic material based on animal data.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes severe skin irritation and burns. Eyes: Causes severe eye irritation and burns. May cause irreversible eye injury. Inhalation: Causes severe irritation and burns of the respiratory tract and mucous membranes. Irritation may lead to chemical pneumonitis Ingestion: Harmful if swallowed. May cause severe and permanent damage to the digestive tract. Causes severe irritation and burns of the gastrointestinal (digestive) tract with abdominal pain, vomiting and possible death. May cause perforation of the digestive tract. Chronic Potential Health Effects: Chronic contact with dilute solutions of potassium hydroxide can cause dermatitis. Inhalation can produce chronic productive cough, and shortness of breath.

Section 12: Ecological Information

Ecotoxicity: Ecotoxicity in water (LC50): 80 mg/l 24 hours [Mosquito Fish].

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: Class 8: Corrosive material

Identification: : Potassium hydroxide, solid UNNA: 1813 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
New York release reporting list: Potassium hydroxide Pennsylvania RTK: Potassium hydroxide Florida: Potassium hydroxide Minnesota: Potassium hydroxide Massachusetts RTK: Potassium hydroxide New Jersey: Potassium hydroxide California Director's List of Hazardous Substances: Potassium hydroxide TSCA 8(b) inventory: Potassium hydroxide CERCLA: Hazardous substances.: Potassium hydroxide: 1000 lbs. (453.6 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS D-1B: Material causing immediate and serious toxic effects (TOXIC). CLASS E: Corrosive solid.

DSCL (EEC):

HMIS (U.S.A.):

Health Hazard: 3

Fire Hazard: 0

Reactivity: 2

Personal Protection: j

National Fire Protection Association (U.S.A.):

Health: 3

Flammability: 0

Reactivity: 1

Specific hazard:

Protective Equipment:
Gloves. Synthetic apron. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 08:23 PM

Last Updated: 05/21/2013 12:00 PM

Material Safety Data Sheet
3-Chloro-2-methylpropene, 90%

ACC# 01633

Section 1 - Chemical Product and Company Identification

MSDS Name: 3-Chloro-2-methylpropene, 90%
Catalog Numbers: AC148420000, AC148420010, AC148420500, AC148422500
Synonyms: Methallyl chloride.
Company Identification:

Acros Organics N.V.
One Reagent Lane
Fair Lawn, NJ 07410

For information in North America, call: 800-ACROS-01
For emergencies in the US, call CHEMTREC: 800-424-9300

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
563-47-3	3-Chloro-2-methylpropene	90	209-251-2

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: clear, colorless liquid. Flash Point: -12 deg C.
Danger! Extremely flammable liquid and vapor. Vapor may cause flash fire. May cause allergic skin reaction. May cause eye, skin, and respiratory tract irritation. May be harmful if swallowed or inhaled. Cancer suspect agent. Dangerous for the environment.
Target Organs: Blood.

Potential Health Effects

Eye: May cause eye irritation.
Skin: May cause skin irritation.
Ingestion: May cause irritation of the digestive tract. The toxicological properties of this substance have not been fully investigated. May be harmful if swallowed.
Inhalation: May cause respiratory tract irritation. May be harmful if inhaled. Vapors may cause dizziness or suffocation.
Chronic: No information found.

Section 4 - First Aid Measures

Eyes: Flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid immediately.
Skin: Get medical aid. Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Remove contaminated clothing and shoes.
Ingestion: Never give anything by mouth to an unconscious person. Get medical aid immediately. Do NOT induce vomiting. If conscious and alert, rinse mouth and drink 2-4 cupfuls of milk or water.

Inhalation: Get medical aid immediately. Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.
Notes to Physician: Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

General Information: As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Vapors may form an explosive mixture with air. Vapors can travel to a source of ignition and flash back. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. Use water spray to keep fire-exposed containers cool. Extremely flammable liquid and vapor. Containers may explode in the heat of a fire. Will be easily ignited by heat, sparks or flame.
Extinguishing Media: For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam. For large fires, use water spray, fog, or alcohol-resistant foam. Use water spray to cool fire-exposed containers. Water may be ineffective. Use agent most appropriate to extinguish fire. Do NOT use straight streams of water.
Flash Point: -12 deg C (10.40 deg F)
Autoignition Temperature: 540 deg C (1,004.00 deg F)
Explosion Limits, Lower:2.30 vol %
Upper: 8.10 vol %
NFPA Rating: (estimated) Health: 2; Flammability: 3; Instability: 1

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks: Absorb spill with inert material (e.g. vermiculite, sand or earth), then place in suitable container. Avoid runoff into storm sewers and ditches which lead to waterways. Clean up spills immediately, observing precautions in the Protective Equipment section. Remove all sources of ignition. Use a spark-proof tool. Provide ventilation. A vapor suppressing foam may be used to reduce vapors.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Use with adequate ventilation. Ground and bond containers when transferring material. Avoid contact with eyes, skin, and clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep container tightly closed. Keep away from heat, sparks and flame. Avoid ingestion and inhalation. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames. Pure vapor will be uninhibited and may polymerize in vents or other confined spaces.
Storage: Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances. Refrigerator/flammables.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use adequate general or local explosion-proof ventilation to keep airborne levels to acceptable levels.
Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
3-Chloro-2-			

methylpropene	none listed	none listed	none listed

OSHA Vacated PELs: 3-Chloro-2-methylpropene: No OSHA Vacated PELs are listed for this chemical.
Personal Protective Equipment
Eyes: Wear chemical splash goggles. Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin: Wear appropriate protective gloves to prevent skin exposure.
Clothing: Wear appropriate protective clothing to prevent skin exposure.
Respirators: A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever workplace conditions warrant respirator use. Wear a NIOSH/MSHA or European Standard EN 149 approved full-facepiece airline respirator in the positive pressure mode with emergency escape provisions.

Section 9 - Physical and Chemical Properties

Physical State: Liquid
Appearance: clear, colorless
Odor: sharp odor - penetrating odor
pH: Not available.
Vapor Pressure: 133 mbar @ 19 C
Vapor Density: 3.12
Evaporation Rate: Not available.
Viscosity: 0.42 mPas 20 deg C
Boiling Point: 71 - 72 deg C @ 760 mm Hg
Freezing/Melting Point:-80 deg C
Decomposition Temperature: Not available.
Solubility: 0.05 wt% (20 c)
Specific Gravity/Density:.9280g/cm3
Molecular Formula:C_4H_7Cl
Molecular Weight:90.55

Section 10 - Stability and Reactivity

Chemical Stability: Stable under normal temperatures and pressures.
Conditions to Avoid: Incompatible materials, ignition sources, excess heat, strong oxidants.
Incompatibilities with Other Materials: Strong oxidizing agents, strong bases.
Hazardous Decomposition Products: Hydrogen chloride, carbon monoxide, carbon monoxide, carbon dioxide.
Hazardous Polymerization: May occur.

Section 11 - Toxicological Information

RTECS#:
CAS# 563-47-3: UC8050000
LD50/LC50:
CAS# 563-47-3:
Inhalation, mouse: LC50 = 7000 mg/m3/2H;
Inhalation, rat: LC50 = 34 gm/m3/30M;
Oral, mouse: LD50 = 1370 mg/kg;
Oral, rat: LD50 = 848 mg/kg;
Oral, rat: LD50 = 580 mg/kg;

.

Carcinogenicity:
CAS# 563-47-3:

- **ACGIH:** Not listed.
- **California:** carcinogen, initial date 7/1/89
- **NTP:** Suspect carcinogen
- **IARC:** Not listed.

Epidemiology: No information found
Teratogenicity: No information found
Reproductive Effects: No information found
Mutagenicity: No information found
Neurotoxicity: No information found
Other Studies:

Section 12 - Ecological Information

Ecotoxicity: Fish: Goldfish: LC50 = 14 mg/L; 24 Hr.; Modified ASTMD1345Bacteria: Phytobacterium phosphoreum: EC50 = 154 mg/L; 5, 15, 30 minutes; Microtox test No data available.
Environmental: An estimated BCF value of 10 was calculated for using a measured water solubility of 1400 mg/l at 25 deg C(1) and a recommended regression-derived equation. According to a classification scheme, this BCF value suggests that bioconcentration in aquatic organisms is low.
Physical: Vapor-phase 3-chloro-2-methyl-1-propene is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals and ozone; the half-lives for these reactions in air are estimated to be about 10 and 27 hours, respectively.
Other: In an aerobic aqueous screening test, 3-chloro-2-methyl-1-propene at 30 mg/l was incubated with a sludge inoculum; 89-107% of the theoretical BOD was measured at 4 weeks. 3-chloro-2-methyl-1-propene, seeded with a wastewater effluent, reached 42% of the theoretical BOD in 5 days.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.
RCRA P-Series: None listed.
RCRA U-Series: None listed.

Section 14 - Transport Information

	US DOT	Canada TDG
Shipping Name:	METHYL ALLYL CHLORIDE	METHYLALLYL CHLORIDE
Hazard Class:	3	3
UN Number:	UN2554	UN2554
Packing Group:	II	II
Additional Info:		FLASHPOINT -12 C

Section 15 - Regulatory Information

US FEDERAL

TSCA

CAS# 563-47-3 is listed on the TSCA inventory.

Health & Safety Reporting List

None of the chemicals are on the Health & Safety Reporting List.

Chemical Test Rules

None of the chemicals in this product are under a Chemical Test Rule.

Section 12b

None of the chemicals are listed under TSCA Section 12b.

TSCA Significant New Use Rule

None of the chemicals in this material have a SNUR under TSCA.

CERCLA Hazardous Substances and corresponding RQs

None of the chemicals in this material have an RQ.

SARA Section 302 Extremely Hazardous Substances

None of the chemicals in this product have a TPQ.

Section 313

This material contains 3-Chloro-2-methylpropene (CAS# 563-47-3, 90%),which is subject to the reporting requirements of Section 313 of SARA Title III and 40

Clean Air Act:

This material does not contain any hazardous air pollutants.
This material does not contain any Class 1 Ozone depletors.
This material does not contain any Class 2 Ozone depletors.

Clean Water Act:

None of the chemicals in this product are listed as Hazardous Substances under the CWA.
None of the chemicals in this product are listed as Priority Pollutants under the CWA.
None of the chemicals in this product are listed as Toxic Pollutants under the CWA.

OSHA:

None of the chemicals in this product are considered highly hazardous by OSHA.

STATE

CAS# 563-47-3 can be found on the following state right to know lists: New Jersey, Pennsylvania, Minnesota, Massachusetts.

California Prop 65

The following statement(s) is(are) made in order to comply with the California Safe Drinking Water Act:

WARNING: This product contains 3-Chloro-2-methylpropene, a chemical known to the state of California to cause cancer.
California No Significant Risk Level: CAS# 563-47-3: 5 æg/day NSRL

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols:

F+ N

Risk Phrases:

R 12 Extremely flammable.
R 20/22 Harmful by inhalation and if swallowed.
R 43 May cause sensitization by skin contact.
R 51/53 Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Safety Phrases:

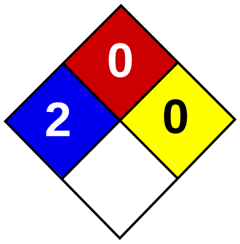
S 16 Keep away from sources of ignition - No smoking.
S 26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
S 36/37/39 Wear suitable protective clothing, gloves and eye/face protection.

S 37 Wear suitable gloves.
S 45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).
S 9 Keep container in a well-ventilated place.
S 28A After contact with skin, wash immediately with plenty of water .
S 61 Avoid release to the environment. Refer to special instructions /safety data sheets.

WGK (Water Danger/Protection)
CAS# 563-47-3: 2
Canada - DSL/NDSL
CAS# 563-47-3 is listed on Canada's NDSL List.
Canada - WHMIS
This product has a WHMIS classification of B2.
This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.
Canadian Ingredient Disclosure List

Section 16 - Additional Information

MSDS Creation Date: 7/21/1999
Revision #5 Date: 11/20/2008



Health	2
Fire	0
Reactivity	0
Personal Protection	E

Material Safety Data Sheet

Sodium bisulfite MSDS

Section 1: Chemical Product and Company Identification

Product Name: Sodium bisulfite

Catalog Codes: SLS3526, SLS1309

CAS#: 7631-90-5

RTECS: VZ2000000

TSCA: TSCA 8(b) inventory: Sodium bisulfite

CI#: Not available.

Synonym: Sulfurous acid, monosodium salt; Sulfurous acid, monosodium salt; Sodium sulhydrate; Sodium hydrogen sulfite; Sodium acid sulfite; Monosodium sulfite; Hydrogen sulfite sodium

Chemical Name: Sodium Bisulfite

Chemical Formula: NaHSO3

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Sodium bisulfite	7631-90-5	100

Toxicological Data on Ingredients: Sodium bisulfite: ORAL (LD50): Acute: 2000 mg/kg [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects: Hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation.

Potential Chronic Health Effects:
Slightly hazardous in case of inhalation (lung irritant). CARCINOGENIC EFFECTS: 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to lungs, skin. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:

Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation: Not available.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: Not applicable.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

Large Spill:
Use a shovel to put the material into a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Do not ingest. Do not breathe dust. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, alkalis.

Storage: Keep container tightly closed. Keep container in a cool, well-ventilated area.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 5 (mg/m3) from OSHA (PEL) [United States] Inhalation TWA: 5 (mg/m3) from ACGIH (TLV) [United States] Inhalation TWA: 5 (mg/m3) [United States] Inhalation TWA: 5 (mg/m3) [United Kingdom (UK)] Inhalation TWA: 5 (mg/m3) [Canada] InhalationConsult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.

Odor: Sulfurous. (Slight.)

Taste: Disagreeable.

Molecular Weight: 104.07 g/mole

Color: White. Off-white.

pH (1% soln/water): Not available.

Boiling Point: Not available.

Melting Point: Decomposes.

Critical Temperature: Not available.

Specific Gravity: 1.48 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water.

Solubility:

Easily soluble in hot water. Soluble in cold water. Soluble in 3.5 parts cold water. Soluble in 2 parts boiling water. Soluble in 70 parts alcohol Insoluble in liquid chloride, ammonia.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Incompatible materials

Incompatibility with various substances: Reactive with oxidizing agents, acids.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Slowly oxidized to sulfate on exposure to air.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Inhalation. Ingestion.

Toxicity to Animals: Acute oral toxicity (LD50): 2000 mg/kg [Rat].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast. May cause damage to the following organs: lungs, skin.

Other Toxic Effects on Humans: Hazardous in case of skin contact (irritant), of ingestion, of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May affect genetic material (mutagenic). May cause cancer based on animal test data. No human data found.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes skin irritation. Eyes: Causes eye irritation. Inhalation: Can cause respiratory tract irritation with cough, wheezing, and shortness of breath. It can produce anaphylaxis or other hypersensivity reactions in some sensitized individuals. Ingestion: May be harmful if swallowed. It may cause nausea, vomiting, diarrhea, abdominal pain, gastric hemorrhage. Extremely large amounts may affect behavior/central nervous system and may produce central nervous system stimulation, irritation, seizures and may also cause, cyanosis, respiratory depression, apnea, circulatory disturbances, hypotension and cardiovascular collapse. May cause asthmatic reaction in sensitized individuals. Chronic Potential Health Effects: Inhalation: Prolonged or repeated inhalation may cause bronchitis to develop with cough, phlegm, and/or shortness of breath. It can cause an asthma-like allergy or other hypersensivity reactions such as anaphylaxis, angioedema, bronchoconstriction, flushing, diaphoresis, urtiacaria, tachycardia, and hypotension in sensitized individuals. Futures exposures may cause shortness of breath, wheezing, cough, and/or chest tightness. Skin: Prolonged or repeated skin contact can cause dermatitis. Ingestion: Prolonged or repeated ingestion may affect the liver, and blood

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: Not a DOT controlled material (United States).

Identification: Not applicable.

Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey.: Sodium bisulfite Illinois toxic substances disclosure to employee act: Sodium bisulfite Illinois chemical safety act: Sodium bisulfite New York release reporting list: Sodium bisulfite Pennsylvania RTK: Sodium bisulfite Minnesota: Sodium bisulfite Massachusetts RTK: Sodium bisulfite Massachusetts spill list: Sodium bisulfite New Jersey: Sodium bisulfite New Jersey spill list: Sodium bisulfite Louisiana spill reporting: Sodium bisulfite California Director's List of Hazardous Substances: Sodium bisulfite TSCA 8(b) inventory: Sodium bisulfite TSCA 8(a) PAIR: Sodium bisulfite TSCA 8(d) H and S data reporting: Sodium bisulfite: Effective date: 1/26/94; Sunset date: 6/30/98 CERCLA: Hazardous substances.: Sodium bisulfite: 5000 lbs. (2268 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada): CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R22- Harmful if swallowed. R31- Contact with acids liberates toxic gas. S25- Avoid contact with eyes. S46- If swallowed, seek medical advice immediately and show this container or label.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 0

Reactivity: 0

Personal Protection: E

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 0

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/11/2005 12:32 PM

Last Updated: 05/21/2013 12:00 PM

Material Safety Data Sheet

SECTION 1 IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

Trade name	NOVEL® TDA-6 Ethoxylate	
Synonyms	Ethoxylated Alcohol, Trideceth-6	
Use	Industrial use, Surfactant	
Company	Sasol North America Inc.	
Address	900 Threadneedle, Ste 100, Houston, TX 77079	
Telephone	CHEMTREC North America Transportation Emergency (24-hr)	(800) 424-9300
	CHEMTREC World Wide	(703) 527-3887
	Other Emergencies (24-hr)	(337) 494-5142
	MSDS and Product Information (8:00am-4:30pm CST)	(337) 494-5080
	Health and Safety Information (7:30am-4:00pm CST)	(281) 588-3492
E-mail address	info@us.sasol.com	

SECTION 2 HAZARDS IDENTIFICATION

Emergency Overview

Appearance	Clear to slightly hazy liquid
Odour	mild
Precautions	**WARNING!** CAUSES EYE AND SKIN IRRITATION. Avoid contact with skin, eyes and clothing. Wash thoroughly after handling.
Environmental precautions	Do not flush into surface water or sanitary sewer system. Readily biodegradable.

Potential Health Effects

Eyes	Irritating to eyes. May cause corneal inflammation.
Skin	Causes skin irritation.
Inhalation	Irritating to respiratory system.
Ingestion	Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhoea.
Additional advice	This product may contain residual levels of alcohols which, even under normal handling conditions, may smell and irritate the eyes, nose, and throats of some individuals.

(See Section 11 for Toxicological Information)

SECTION 3 COMPOSITION/INFORMATION ON INGREDIENTS

Components	CAS-No.	Weight percent
Isotridecanol, ethoxylated	9043-30-5	100

See Section 8 for Exposure Guidelines and Section 15 for Regulatory Classifications.

SECTION 4 FIRST AID MEASURES

Eye contact Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

Skin contact Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. When symptoms persist or in all cases of doubt seek medical advice. Wash contaminated clothing before re-use.

Inhalation Remove to fresh air. If breathing is irregular or stopped, administer artificial respiration. Call a physician immediately.

Ingestion If swallowed, call a poison control centre or doctor immediately. Do not induce vomiting without medical advice. Never give anything by mouth to an unconscious person.

SECTION 5 FIREFIGHTING MEASURES

FLAMMABLE PROPERTIES

Flash point	165 °C 330 °F
Autoignition temperature	approximately 355 °C 671 °F
Flammable limits in air % by volume	**Lower explosion limit:** no data available **Upper explosion limit:** no data available
Fire/explosion	NFPA Class IIIB combustible liquid.
Suitable extinguishing media	Water spray, Foam, Dry chemical, Carbon dioxide (CO2)
Protective equipment and precautions for firefighters	Wear self contained breathing apparatus for fire fighting if necessary.

Further information	Keep containers and surroundings cool with water spray. Do not use a solid water stream as it may scatter and spread fire. Collect contaminated fire extinguishing water separately. This must not be discharged into drains.

SECTION 6 ACCIDENTAL RELEASE MEASURES

Methods and materials for containment and cleaning up	Evacuate personnel to safe areas. Remove all sources of ignition. Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Do not flush into surface water or sanitary sewer system.

SECTION 7 HANDLING AND STORAGE

Safe handling advice	Take precautionary measures against static discharges.
Storage/Transport pressure	Ambient
Load/Unload temperature	15 - 38 C
Storage and handling materials	Suitable: Carbon steel coated with baked phenolic. Any moisture may cause rusting of carbon steel. If product is moisture free, uncoated carbon steel tanks.
Further information on storage conditions	When stored in the liquid form, ethoxylates should be padded with a dry inert gas, such as nitrogen, to prevent oxygen or air from entering the tank. Prolonged storage in the presence of air or oxygen may cause product degradation. Oxidation is not expected when stored under a nitrogen atmosphere. Inert gas blanket and breathing system needed to maintain color stability. Use dry inert gas having at least -40°C (-40°F) dew point.

SECTION 8 EXPOSURE CONTROLS/PERSONAL PROTECTION

ENGINEERING MEASURES

Ensure adequate ventilation, especially in confined areas. Trace amounts of ethylene oxide may be present in the product and could accumulate in vapor spaces of storage or transport vessels.

PERSONAL PROTECTIVE EQUIPMENT

Eyes	Wear as appropriate: Goggles, Face-shield
Skin	Full protective clothing, chemical boots, and chemical gloves. High standards of skin care and personal hygiene should be exercised at all times.
Inhalation	Use respirator when performing operations involving potential exposure to vapour of the product. Use NIOSH approved respiratory protection.

EXPOSURE GUIDELINES

Components	Exposure limit(s)
	There are no exposure limits established for this product. Trace amounts of ethylene oxide may be present in this product. The ethylene oxide in this product is not expected to result in significant exposures or present a health hazard.

PEL=	Permissible Exposure Limits	TWA=	Time Weighted Average (8 hr.)
TLV=	Threshold Limit Value	STEL=	Short Term Exposure Limit (15 min.)
EL=	Excursion Limit	WEEL=	Workplace Environmental Exposure Level

SECTION 9 PHYSICAL AND CHEMICAL PROPERTIES

Appearance	liquid
Colour	Clear to slightly hazy
Odour	mild
Form	liquid
Boiling point/boiling range	approximately > 253 °C > 487 °F
Vapour pressure	< 1 mm Hg @ 20 °C
Vapour density	16.21
Water solubility	partly miscible
Viscosity	25.87 cSt @ 40 °C
Viscosity, dynamic	approximately 25 mPa.s @ 50 °C

Melting point/range	-9 °C 16 °F
Density	0.979 g/cm3 @ 20 °C 8.15 lb/gal @ 71.6 °C
pH	6 - 8

SECTION 10 STABILITY AND REACTIVITY

Conditions to avoid	Reacts slowly with air or oxygen. Storage under heated conditions in the presence of air or oxygen increases reaction rate. For example, after storing at 95°F/35°C for 30 days in the presence of air, there is measureable oxidation of the ethoxylate. Lower temperatures will allow for longer storage time and higher temperatures will shorten the storage time if stored under an air or oxygen atmosphere.
Hazardous decomposition products	When storing this product in air or oxygen, decomposition may occur, generating vapors which could be irritating. Ensure adequate ventilation, especially in confined areas. Oxidation is not expected when stored under a nitrogen atmosphere.
Materials to avoid	Can react with strong oxidizers, inorganic acids, and halogens.
Hazardous polymerisation	None.

SECTION 11 TOXICOLOGICAL INFORMATION

Additional Remarks	Information given is based on data obtained from similar substances.
Eyes	Primary irritation (rabbit): 32 - 50.8 (Maximum score is 110.)
Skin	Primary irritation (rabbit): 4 hours 4.1 - 7.1 (Maximum score is 8.0.)
Inhalation	LC50 value expected to exceed the saturated vapor concentration in air.
Ingestion	Acute oral toxicity LD50 (rat): > 2,000 mg/kg

CARCINOGENICITY

No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

SECTION 12 ECOLOGICAL INFORMATION

Aquatic toxicity

Toxicity to fish	LC50 (Danio rerio (zebra fish)) 96 hours: 5.8 mg/l;OECD Test Guideline 203; Test substance: C13-6 Ethoxylate;

Toxicity to aquatic invertebrates	EC50 (Daphnia magna (Water flea)) 48 hours: 2.5 mg/l; OECD Test Guideline 202; Test substance: C13-6 Ethoxylate;
Toxicity to algae	ErC50 (Desmodesmus subspicatus (green algae)) 72 hours: 8.2 mg/l; OECD Test Guideline 201; Test substance: C13-6 Ethoxylate;
Biodegradation	Readily biodegradable. OECD Test Guideline 301B (28 d): > 60 % Test substance C13-6 Ethoxylate

SECTION 13 DISPOSAL CONSIDERATIONS

Waste Code	Any unused product or empty containers may be disposed of as non-hazardous in accordance with state and federal requirements. Re-evaluation of the product may be required by the user at the time of disposal, since the product uses, transformations, mixtures, contamination, and spillage may change the classification. If the resulting material is determined to be hazardous, please dispose in accordance with state and federal (40 CFR 262) hazardous waste regulations.
Disposal methods	Dispose of only in accordance with local, state, and federal regulations.
Empty containers.	Empty containers retain product residue (liquid and/or vapor) and can be dangerous. DO NOT PRESSURIZE, CUT, WELD, BRAZE, SOLDER, DRILL, GRIND, OR EXPOSE SUCH CONTAINERS TO HEAT, FLAME, SPARKS, STATIC ELECTRICITY, OR OTHER SOURCES OF IGNITION; THEY MAY EXPLODE AND CAUSE INJURY OR DEATH. Empty drums should be completely drained, triple-rinsed, properly bunged and promptly returned to a drum reconditioner, or properly disposed.

SECTION 14 TRANSPORT INFORMATION

DOT	UN 3082, Environmentally hazardous substance, liquid, n.o.s.(Alcohol C12-16 poly (1-6) ethoxylate), 9, III , Marine pollutant This product is regulated as a hazardous material according to the Department of Transportation only in bulk quantities (greater than 119 gallons per package).
IATA	not regulated
IMDG	not regulated

SECTION 15 REGULATORY INFORMATION

U.S. FEDERAL REGULATIONS

OSHA Hazards

Eye irritation, Skin irritation

TSCA Inventory Listing

Components	CAS-No.
Poly(oxy-1,2-ethanediyl), a-isotridecyl-w-hydroxy-	9043-30-5

SARA 302 Status

Components	CAS-No.	Weight percent

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 311/312 Classification

"Immediate (acute) health hazard"

SARA 313 Chemical

Components	CAS-No.	Weight percent

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US. EPA CERCLA Hazardous Substances (40 CFR 302)

Components	Reportable Quantity	Weight percent
none		

INTERNATIONAL REGULATIONS

WHMIS Classification

Class D, Division 2, Subdivision B: Toxic material.

European Union

This surfactant complies with the biodegradability criteria as laid down in Regulation (EC) No.648/2004 on detergents. Data to support this assertion are held at the disposal of the competent authorities of the Member States and will be made available to them, at their direct request or at the request of a detergent manufacturer.

Xn: Harmful
R22: Harmful if swallowed.
R41: Risk of serious damage to eyes.

Australian Inventory of Chemical Substances (AICS) Listing

Listed

Japanese Minister of International Trade and Industry (MITI) Inventory Listing
Listed

Canadian Domestic Substance List (DSL) Inventory Listing
Listed

Canadian Non-Domestic Substance Listing (NDSL)
Not listed

European Inventory of Existing Commercial Chemical Substances (EINECS) Listing
Listed

Philippines Inventory List (PICCS)
Listed

Korean Inventory List
Listed

China Inventory List
Listed

Please note: The names and CAS numbers which are used for this product in the stated inventories may deviate from the information which is listed in Section 3.

STATE REGULATIONS

California Prop. 65

Components	CAS-No.
Ethylene Oxide	75-21-8

Sasol North America Inc. ethoxylates may contain detectable quantities of ethylene oxide which is a chemical on the California Proposition 65 list. The level is typically below 1.0 ppm, although it may vary. The manufacturing process is controlled to reduce the residual ethylene oxide content.

SECTION 16 OTHER INFORMATION

HAZARD RATINGS

	Health	Flammability	Physical Hazard/ Instability
HMIS®	2	1	0
NFPA	1	1	0