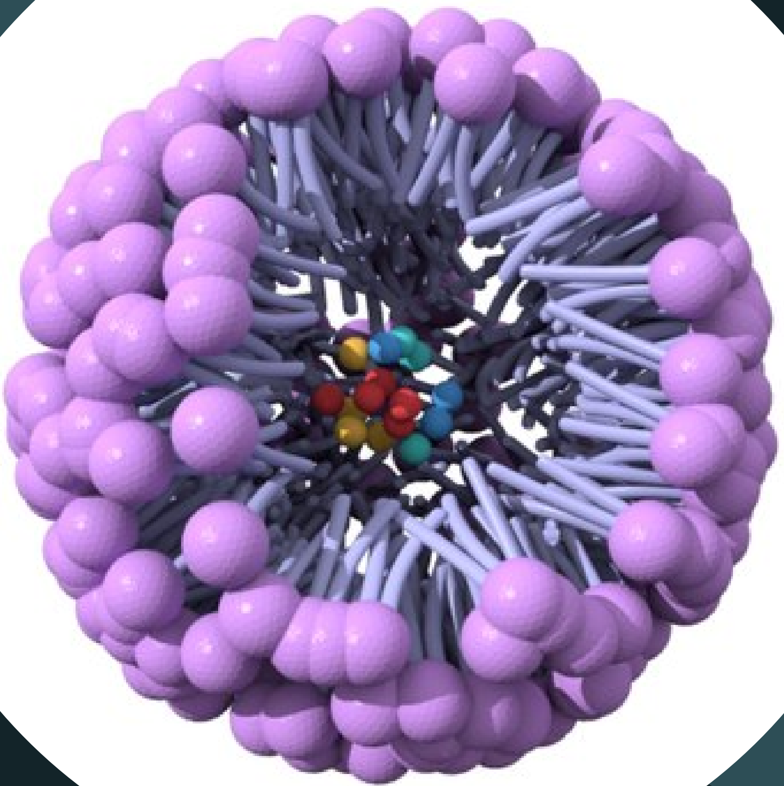
SURFACTANTS



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2022-2023

Course Outline

- **Definition, Surfactant Types and Structures**
- **The Influence of Atomic Bonds and Molecular Attractive Forces on Interfaces**
- **Surface Activity including Surface Tension/Pressure/Transport and Micelle Formation**
- **Surface Tension Measuring Methods**
- **Surfactant Types in details**
    - **Anionic surfactant**
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    - **Amphoteric surfactant**
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- **Surfactants Mechanism of Action**
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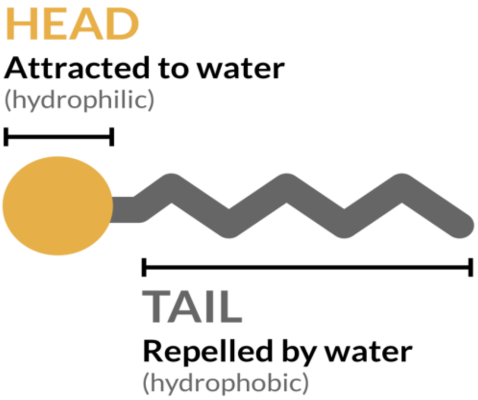
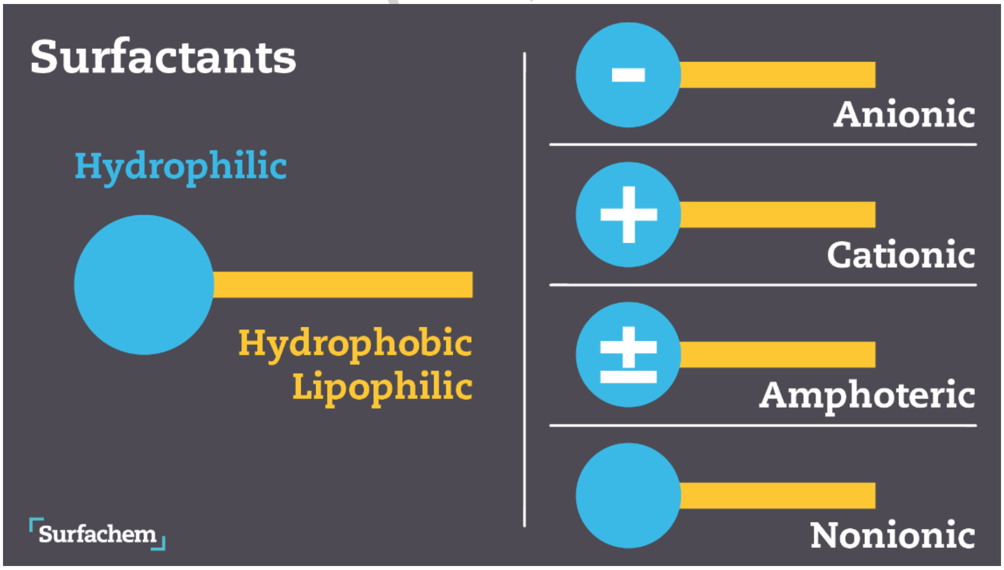
What are surfactants?

Surfactants are a class of chemical compounds that are commonly used in many industrial and consumer products due to their ability to reduce the surface tension between two liquids or between a liquid and a solid. The term "surfactant" is short for "surface-active agent".

Surfactants have both hydrophilic (water-loving) and hydrophobic (water-repelling) properties in the same molecule. This allows them to interact with and affect the behaviour of both polar and non-polar substances. In water-based systems, surfactants can be used to disperse or solubilize oils and other non-polar substances. In addition to their ability to modify surface tension, surfactants can also act as detergents, emulsifiers, foaming agents, wetting agents, and dispersants. Surfactants are used in a wide range of applications, including personal care products (such as shampoo and body wash), cleaning products, paints and coatings, food processing, and many other industrial processes.

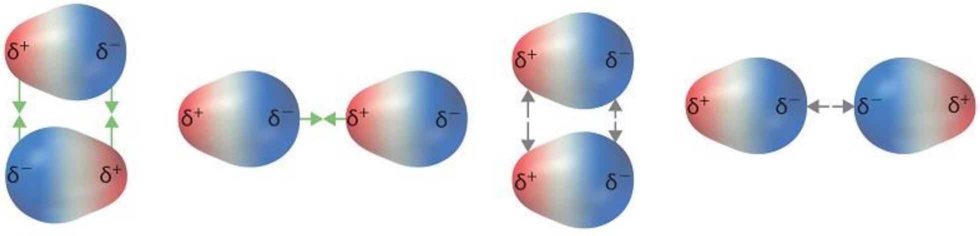


There are many different types of surfactants, including anionic, cationic, non-ionic, and amphoteric surfactants, each with unique properties and uses. The choice of surfactant depends on the specific application and the desired outcome.



The Influence of Atomic Bonds and Molecular Attractive Forces on Interfaces

The influence of atomic bonds and molecular attractive forces on interfaces is an important aspect of surface and interfacial science. At the atomic and molecular level, the interactions between different phases (such as a solid and a liquid or two liquids) are governed by the attractive and repulsive forces that exist between the constituent atoms and molecules. These forces include covalent bonds, ionic bonds, hydrogen bonds, Van der Waals forces, and electrostatic interactions.



(a) Attraction **(b) Attraction** **(c) Repulsion** **(d) Repulsion**

At interfaces between different phases, these forces can cause a variety of phenomena such as adsorption, wetting, capillary forces, and interfacial tension. The nature and strength of the forces between the constituent atoms and molecules in the different phases determine the extent to which the phases can mix and interact with each other. For example, in the case of a solid-liquid interface, the surface of the solid is typically covered with a layer of adsorbed molecules due to the attractive forces between the molecules and the surface atoms. This layer can influence the wetting behaviour of the liquid on the solid surface, as well as the adhesion and friction between the two phases.

In the case of two immiscible liquids, the interfacial tension between the two phases is determined by the relative strengths of the cohesive forces within each liquid and the adhesive forces between the two liquids. This interfacial tension can influence the behaviour of emulsions and foams, as well as the stability and coalescence of droplets.

Here are some additional details on the influence of atomic bonds and molecular attractive forces on interfaces:

Covalent bonds: Covalent bonds are strong chemical bonds that are formed by the sharing of electrons between atoms. At interfaces, covalent bonds between surface atoms and adsorbing molecules can result in the formation of a tightly bound layer of molecules on the surface. This layer, known as the adsorbed layer or monolayer, can affect the surface properties of the solid and the wetting behaviour of the liquid on the surface.

Ionic bonds: Ionic bonds are electrostatic forces that exist between ions of opposite charges. At interfaces, ionic bonds between surface atoms and ions in solution can lead to the adsorption of ions on the surface, which can affect the surface charge and the electrokinetic behavior of the solid-liquid interface.

Hydrogen bonds: Hydrogen bonds are strong dipole-dipole interactions that occur between molecules containing hydrogen and a highly electronegative atom such as oxygen, nitrogen, or fluorine. At interfaces, hydrogen bonding can result in the formation of ordered structures of molecules on the surface, which can affect the wetting behavior of the liquid on the surface.

Van der Waals forces: Van der Waals forces are weak intermolecular forces that arise from fluctuations in electron density. At interfaces, Van der Waals forces can lead to the adsorption of molecules on the surface, which can affect the surface properties of the solid and the wetting behaviour of the liquid on the surface.

Electrostatic interactions: Electrostatic interactions are attractive or repulsive forces that arise from the interaction between charged species. At interfaces, electrostatic interactions can affect the adsorption of charged species on the surface, the electrokinetic behaviour of the solid-liquid interface, and the stability of emulsions and foams.

In general, the strength and nature of the attractive and repulsive forces between atoms and molecules at interfaces depend on a variety of factors such as the chemical nature of the phases involved, the temperature, the pressure, and the presence of other species in the system. Understanding the influence of these forces on interfaces is important for a variety of applications in fields such as materials science, colloid science, and biophysics.

In summary, the atomic bonds and molecular attractive forces between different phases play a critical role in determining the behaviour of interfaces between these phases. The study of these forces and their effects on interfacial phenomena is an important field of research in surface and interfacial science.

Surface Activity

Surface activity refers to the ability of a substance to adsorb at the interface between two immiscible phases, typically a liquid and a gas or a liquid and a solid. The substance that adsorbs at the interface is known as a surfactant, and it can affect the surface tension, wetting behaviour, and stability of the system.

Surfactants are molecules that have both a hydrophobic and a hydrophilic region. When a surfactant is added to a system, the hydrophobic region of the molecule adsorbs at the interface, while the hydrophilic region remains in the bulk phase. This reduces the interfacial tension between the two phases and promotes the formation of stable emulsions, foams, and other complex fluid structures.

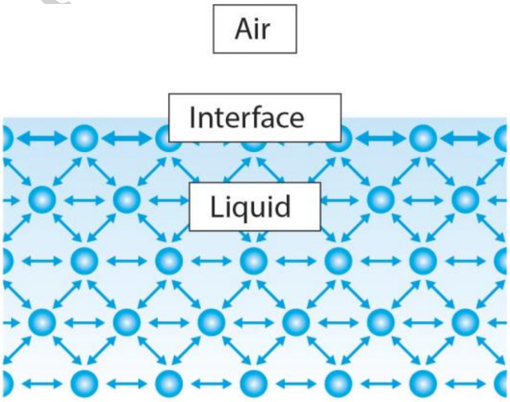
Surfactants can also affect the wetting behaviour of a liquid on a solid surface. If the surfactant is more attracted to the solid surface than to the bulk liquid phase, it will preferentially adsorb at the solid-liquid interface and reduce the contact angle between the liquid and the solid. This can result in improved wetting and spreading of the liquid on the surface.

In addition to their effects on surface tension and wetting behaviour, surfactants can also play a role in the stability of colloidal systems such as emulsions and suspensions. By adsorbing at the interface between the two phases, surfactants can prevent the coalescence of droplets or particles and stabilize the system.

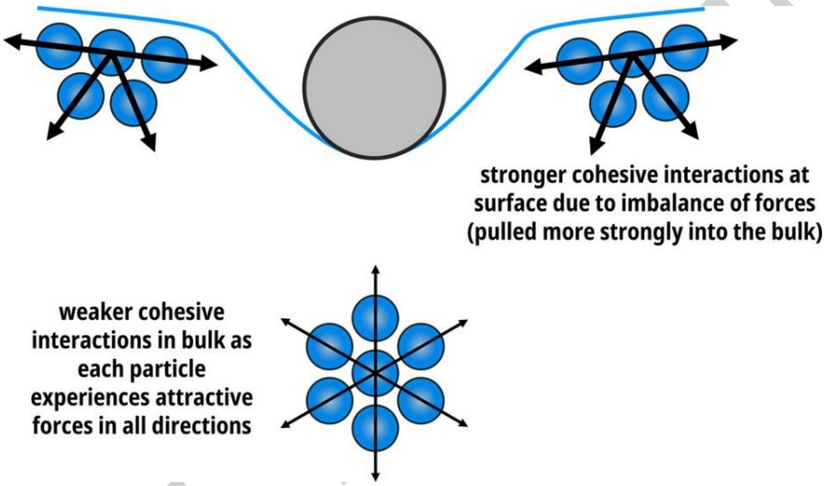
Overall, the surface activity of a surfactant is a complex interplay of its molecular structure, the nature of the phases involved, and the environmental conditions such as temperature and pH. Understanding and controlling surface activity is important for a wide range of applications, including detergency, cosmetics, pharmaceuticals, food processing, and oil recovery.

Surface Tension

Surface tension is a fundamental property of liquids that arises from the intermolecular forces between the molecules that make up the liquid. These forces can be classified into two categories: cohesive forces and adhesive forces. Cohesive forces are the attractive forces between the molecules of the same liquid, while adhesive forces are the attractive forces between the molecules of the liquid and a different surface or material.



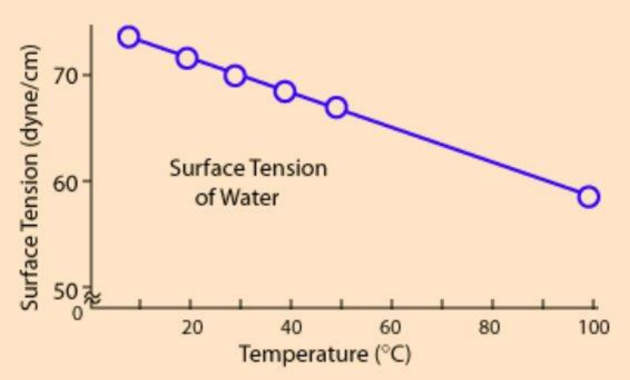
At the surface of a liquid, the molecules experience a net inward force due to the lack of neighbouring molecules above them. This results in a higher density of molecules at the surface and a consequent tendency to minimize the surface area. The surface tension can be thought of as the amount of work required to overcome this cohesive force and increase the surface area.



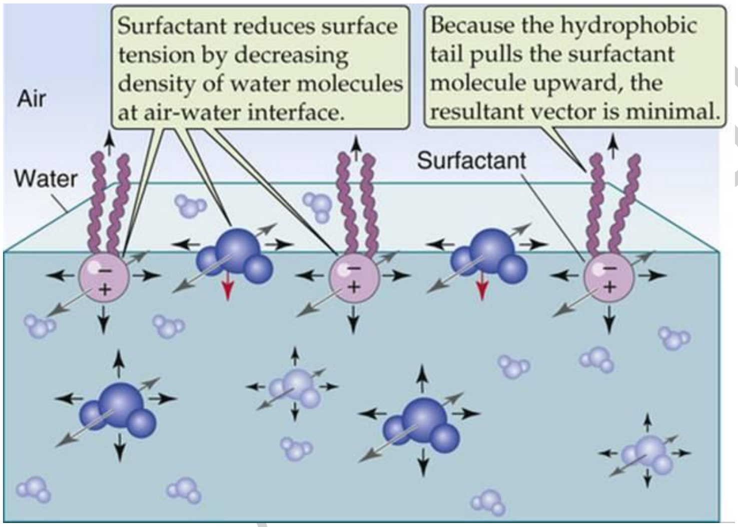
Factors affected on surface tension:

The surface tension of a liquid depends on several factors. One of the most important factors is **the nature of the liquid** itself. The strength of the intermolecular forces in the liquid determines the magnitude of the surface tension. For example, liquids with strong intermolecular forces, such as water, typically have higher surface tensions than liquids with weaker intermolecular forces, such as organic solvents.

The temperature and pressure also have an effect on the surface tension. Generally, the surface tension of a liquid decreases as the temperature increases. This is because the thermal motion of the molecules at the surface reduces the cohesive forces between them. Pressure can also affect the surface tension, with higher pressures generally leading to higher surface tensions.



The presence of other substances can also influence the surface tension of a liquid. Surfactants, for example, are molecules that preferentially adsorb at the surface of a liquid, disrupting the cohesive forces between the liquid molecules and reducing the surface tension. Other substances that can influence the surface tension of a liquid include solutes, gases, and suspended particles. Surface tension has several important applications in everyday life and technology. For example, it is responsible for the formation of droplets and bubbles, and can influence the wetting behaviour of liquids on surfaces. In industrial processes such as oil recovery and foam fractionation, surface tension plays a critical role in separating different components of a mixture. The study of surface tension and its applications is an important area of research in chemistry, physics, and engineering.



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Surface Tension Measuring Methods

Surface tension is the property of a liquid that determines the magnitude of the force required to deform its surface. There are several methods to measure the surface tension of liquids, including:

Capillary rise method: In this method, a liquid is allowed to rise in a capillary tube due to surface tension. The height of the liquid in the capillary tube is measured, and the surface tension can be calculated using the formula: $\gamma = (2\rho gh)/d$, where γ is the surface tension, ρ is the density of the liquid, g is the acceleration due to gravity, h is the height of the liquid in the capillary tube, and d is the diameter of the capillary tube.

Drop weight method: In this method, a drop of liquid is allowed to fall from a capillary tube, and the time taken for the drop to fall a known distance is measured. The surface tension can be calculated using the formula: $\gamma = (4mgh)/(\pi d^2t^2)$, where γ is the surface tension, m is the mass of the drop, g is the acceleration due to gravity, h is the height of the fall, d is the diameter of the capillary tube, and t is the time taken for the drop to fall the known distance.

Pendant drop method: In this method, a drop of liquid is suspended from a needle or a capillary tube, and the shape of the drop is analyzed to determine the surface tension. The shape of the drop is recorded using a camera, and the surface tension can be calculated using the formula: $\gamma = (mg)/(4\pi r^2)$, where γ is the surface tension, m is the mass of the drop, g is the acceleration due to gravity, and r is the radius of the drop.

Wilhelmy plate method: In this method, a thin plate or wire is dipped into a liquid, and the force required to remove the plate from the liquid is measured. The surface tension can be calculated using the formula: $\gamma = F/2L$, where γ is the surface tension, F is the force required to remove the plate from the liquid, and L is the length of the plate in contact with the liquid.

These methods can be used to measure the surface tension of a wide range of liquids and are widely used in research and industrial applications.

Surface Pressure and transport

Surface pressure refers to the atmospheric pressure at a given location on the Earth's surface. It is typically measured in units of millibars (mb) or hectopascals (hPa). Surface pressure is affected by a variety of factors, including the temperature, humidity, and density of the air, as well as the presence of weather systems such as high and low-pressure systems.

Transport refers to the movement of various atmospheric variables, such as heat, moisture, and pollutants, through the atmosphere. Transport can occur on a variety of scales, from local to global, and is influenced by a variety of factors, including wind patterns, atmospheric stability, and the presence of natural and human-made barriers.

Surface pressure and transport are closely related because surface pressure gradients can drive atmospheric transport. When there is a difference in surface pressure between two locations, air will flow from the high-pressure region to the low-pressure region, resulting in atmospheric transport. This can result in the movement of heat, moisture, and pollutants, among other things.

Additionally, the transport of atmospheric variables can affect surface pressure patterns. For example, the transport of moisture can lead to the formation of clouds and precipitation, which can in turn affect surface pressure patterns. Similarly, the transport of heat can lead to the formation of weather systems, such as fronts and cyclones, which can also influence surface pressure patterns.

The importance of surfactants

Surfactants are a diverse group of compounds that have a wide range of important functions in many different industries and applications. Here are some key reasons why surfactants are important:

Emulsification: Surfactants can help to emulsify immiscible liquids, such as oil and water. This is important in the production of food products, such as salad dressings, as well as in industrial applications, such as the production of paints and coatings.

Wetting: Surfactants can lower the surface tension of a liquid, allowing it to spread more easily over a surface. This is important in cleaning applications, where surfactants can help to wet surfaces and remove dirt and grime.

Foaming: Surfactants can help to stabilize foams, which are important in many industrial and consumer products, such as shampoos, detergents, and cosmetics.

Dispersing: Surfactants can help to disperse solids in a liquid, which is important in the production of suspensions, such as paint and ink.

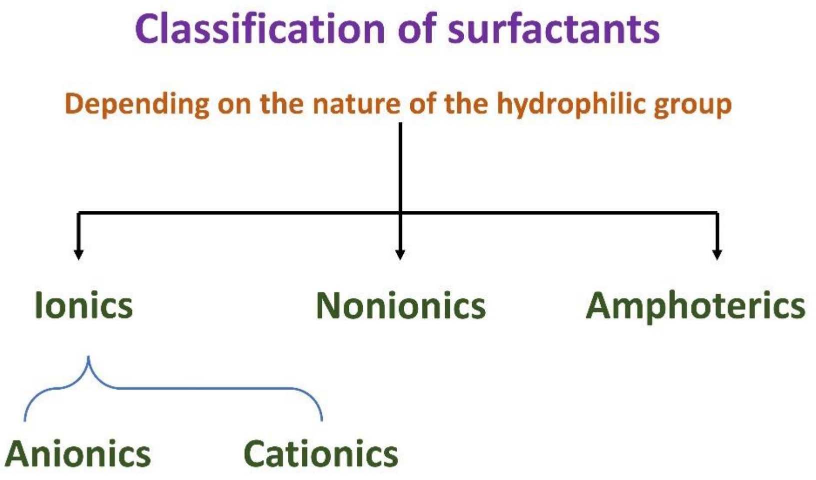
Lubrication: Surfactants can reduce friction between surfaces, which is important in the production of lubricants for machinery and engines.

Biocompatibility: Some surfactants have good biocompatibility, meaning that they are safe to use in personal care products, pharmaceuticals, and food products.

Overall, surfactants play a critical role in many different industries and applications. They help to improve the efficiency and effectiveness of many processes, and they enable the production of a wide range of products that are used in our daily lives.

Surfactant Types and Structures

There are several types of surfactants, each with unique chemical structures and properties. The most common types of surfactants include:



Anionic surfactants:

Anionic surfactants are the most commonly used type of surfactant. These surfactants have a negatively charged head group and are typically used as detergents and cleaning agents. Examples of anionic surfactants include sodium lauryl sulfate and sodium dodecylbenzenesulfonate.

Cationic surfactants:

These surfactants have a positively charged head group and are often used as disinfectants and fabric softeners. Examples of cationic surfactants include cetyltrimethylammonium bromide and benzalkonium chloride.

Nonionic surfactants:

These surfactants have an uncharged head group and are often used as emulsifiers, solubilizers, and wetting agents in industrial applications. Examples of nonionic surfactants include polyethylene glycol (PEG) and alkyl polyglucosides.

Amphoteric surfactants:

These surfactants have both a positively and negatively charged head group and are often used as mild detergents and personal care products. Examples of amphoteric surfactants include cocamidopropyl betaine and disodium cocoamphodiacetate.

Surfactants are amphiphilic, meaning they have both hydrophilic and hydrophobic properties. The hydrophilic head group is usually polar or charged, while the hydrophobic tail is typically a long hydrocarbon chain. The structure of the surfactant is designed to allow it to interact with both polar and non-polar substances, which gives it its unique surface-active properties.

Surfactants work by adsorbing onto the surface of a liquid or solid to reduce its surface tension. This can help to facilitate the spreading, wetting, or emulsification of the substance. The effectiveness of a surfactant depends on its concentration, chemical structure, and the properties of the substances it is interacting with. Surfactants are used in a wide range of applications, including personal care products (such as shampoos, soaps, and lotions), household and industrial cleaning products, paints and coatings, food processing, and agricultural products.

Overall, surfactants play an important role in many everyday products and industrial processes, and their properties and structures can be carefully designed and tailored to suit specific applications and outcomes.

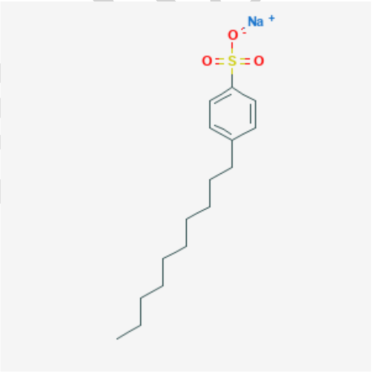
In our course, we will focus on every type of the surfactant in some details.

Anionic surfactants:

Anionic surfactants are a type of surfactant that contains a negatively charged ion in the hydrophilic (water-loving) part of the molecule. **This charge is usually provided by a sulfonate, sulfate, or carboxylate group,** which makes the molecule water-soluble and able to form stable micelles in water.

1- Sulfonates surfactants: -SO_3^-

A- Alkylbenzene sulfonates (LABS)



Linear alkylbenzene sulfonate (LABS): This is a common anionic surfactant that is used in a wide range of applications, including laundry detergents, dishwashing liquids, and household industrial cleaners. It is effective at removing dirt and oil and is compatible with hard water.

Synthesis of LABS:

Here are the general production steps of LABS:

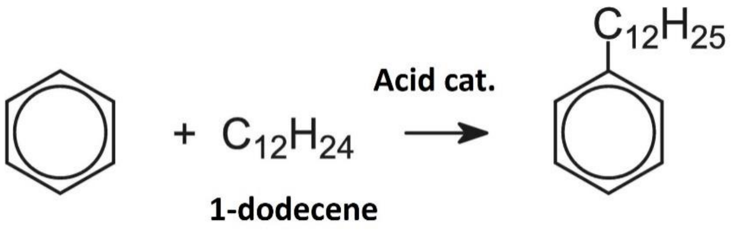
Alkylation: In this step, benzene is alkylated with a linear alkyl chain, usually derived from an olefin (e.g. propyl**ene**, butyl**ene**) *via* a catalytic process. The alkyl chain length typically ranges from 10 to 14 carbon atoms. The process of alkylation is typically carried out in a liquid-phase reactor containing benzene and the olefinic feed, along with a suitable catalyst (e.g. hydrofluoric acid, aluminum chloride). The catalyst promotes the reaction between benzene and the olefin, leading to the formation of LAB. The resulting LAB stream is then neutralized to remove any unreacted acid or catalyst.

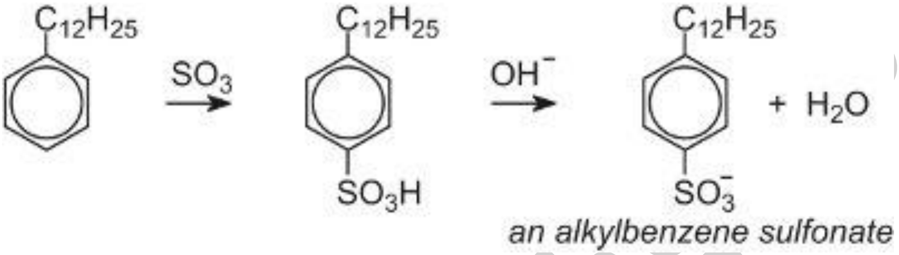
Sulfonation: The LAB is then sulfonated to produce sulfonic acid, which is then neutralized to form LABSA. The sulfonation reaction is typically carried out using concentrated sulfuric acid as a catalyst and sulfur trioxide (SO_3) as the sulfonating agent. The reaction is typically carried out in a reactor at temperatures ranging from 90 to 120°C, and the reaction time is carefully controlled to ensure that the desired level of sulfonation is achieved. After sulfonation, the reaction mixture is cooled and neutralized with an alkali, usually sodium hydroxide, to form the sodium salt of LABSA.

Separation and purification: The LABSA is then separated from the reaction mixture by a series of steps, including neutralization, filtration, and drying. In this step, the LABSA is separated from the reaction mixture by adding an alkali (usually sodium hydroxide), which neutralizes the sulfuric acid and precipitates the LABSA. The precipitate is then washed with water to remove any residual sulfuric acid and sodium sulfate, which is a by-product of the neutralization reaction. The LABSA is then dried and the resulting powder is milled to the desired particle size.

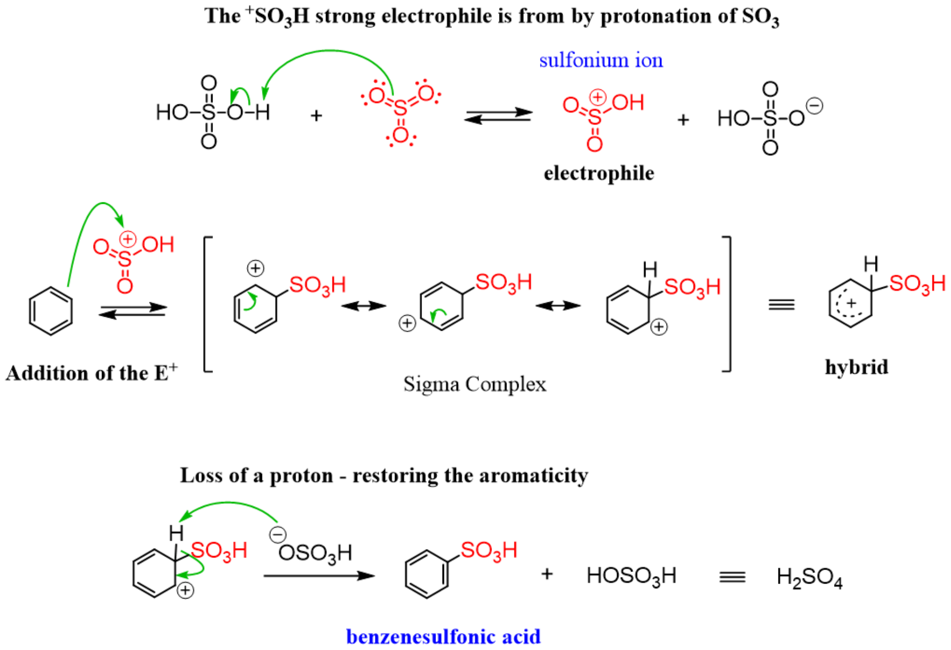
Optional steps: Depending on the specific application of the LABSA, additional steps may be carried out to modify its properties. For example, LABSA used in liquid laundry detergents may be subjected to an ethoxylation process to increase its solubility in water and improve its performance in cold water. In this process, the LABSA is reacted with ethylene oxide, which adds ethylene oxide molecules to the LABSA molecule, resulting in an ethoxylated LABSA (or "AELAS"). The degree of ethoxylation can be controlled to modify the physical properties of the resulting AELAS.

Overall, the production of LABSA is a complex process that requires careful control of the reaction conditions and the separation and purification steps to ensure a high-quality product.





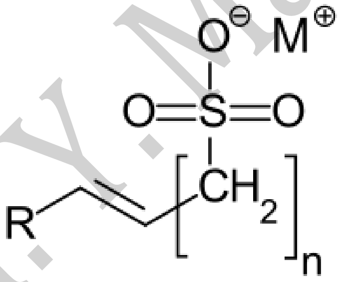
The reaction mechanism of Benzene sulphonic acid formation:



B- Alpha Olefin Sulfonates (AOS):

These are anionic surfactants that are commonly used in laundry detergents and household cleaning products. They are effective at removing tough stains and grease, and can work well in hard water conditions.

The compounds contain a - mostly linear, primary - alkyl R and a monovalent cation M, preferably sodium. The most frequently used example of this group of substances is sodium α-olefin sulfonate (INCI: Sodium C14-16 Olefin Sulfonate).



General chemical structure of α-olefin sulfonates

R= Alkyl, M= Na+, n = 1 or 2

<u>Description</u>

In addition to a longer hydrocarbon chain in which there must be at least one double bond (hence the name "olefin"), it has an anionic sulfonate headgroup with a sodium ion as a counterion. The sulfonate group is negative in aqueous solution, which is why the α-olefin sulfonates are among the anionic surfactants. In contrast to most other surfactants in which the C12-alkyl chains have the highest surface activity, olefin sulfonates shows maximal activity when using C14 and C16-olefins.

Production and composition

α-Olefin sulfonates are produced by sulfonation of alpha-olefins, typically using sulfur trioxide. Subsequent alkaline hydrolysis gives a mixture of alkene sulfonates (60-65%) and hydroxyalkane sulfonates (35-40%). The commercially available olefin sulfonates are mostly solutions with about 40% active ingredient content.

Usage

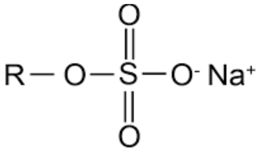
α-Olefin sulfonates with linear alkenyl radicals from C12 to C18 are used as anionic surfactants in various areas of application due to their pronounced foam formation and foam stability (even with high water hardness), excellent fat-dissolving power and oil dissolving power as well as a favorable ecological profile and low aquatic toxicity and human toxicity. They are typically used in detergents and cleaning agents, for degreasing, in the emulsion polymerization, the conditioning of concrete and mortar as well as in the **formulation of pesticides**.

Sodium C14-16 olefin sulfonate is being introduced in some shampoos as an alternative to sodium laureth sulfate. Some groups and sellers suggest that it is better for someone's health, but this claim lacks evidence.

2- Sulfate surfactants: -OSO_3^-

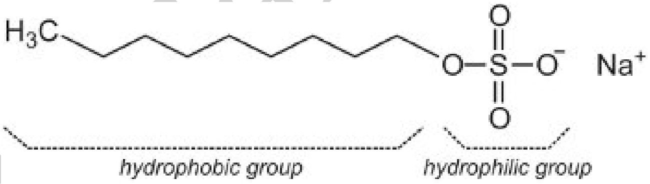
A- Alkyl sulphate:

These are anionic surfactants that are commonly used in personal care products, such as shampoo and body wash. They are effective at removing dirt and oil from the skin and hair but can also be harsh and irritating if used at high concentrations.

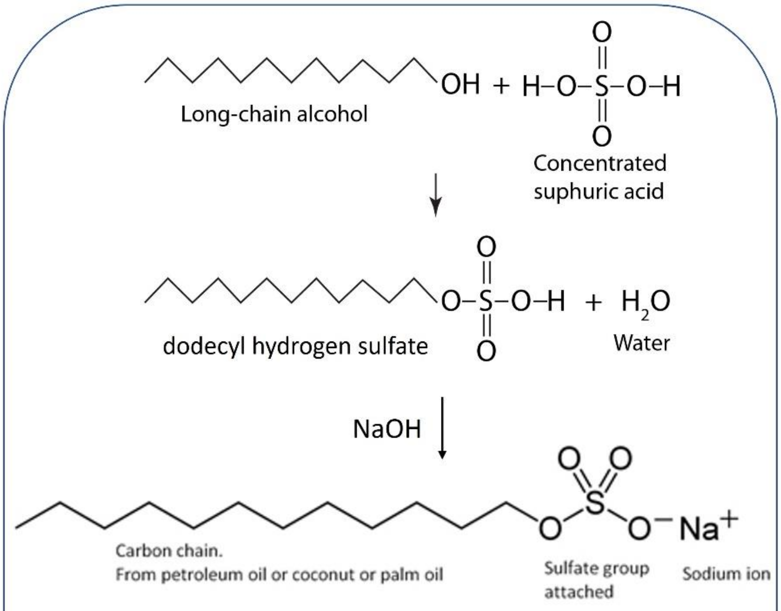


$R-O-S(=O)_2-O^-\,Na^+$

Sodium Alkyl Sulphate (Detergent)



an alkyl sulfate



Sodium Lauryl Sulfate (SLS)

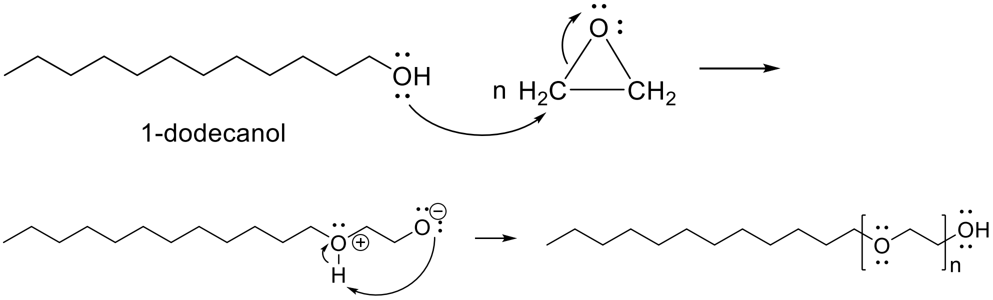
Sodium Dodecyl Sulfate (SDS)

B- Sodium lauryl ether sulfate (SLES):

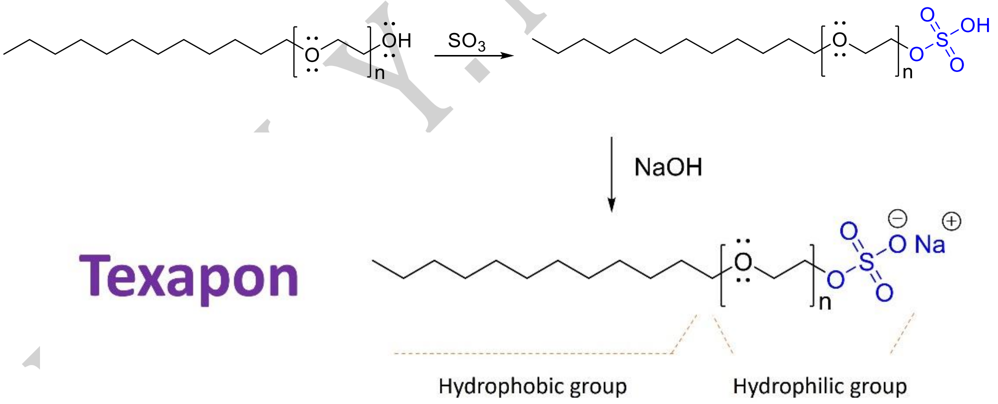
This is a milder form of anionic surfactant that is often used in personal care products such as shampoos and body washes. It has good foaming properties and is effective at removing dirt and oil but is less harsh on the skin than some other anionic surfactants.

<u>Sodium lauryl ether sulfate (SLES) production steps</u>

Ethoxylation: In this step, lauryl alcohol is ethoxylated by reacting with ethylene oxide in the presence of a catalyst. The reaction is typically carried out in a stirred-tank reactor at elevated temperatures and pressures. The degree of ethoxylation is carefully controlled to achieve the desired level of ethoxylation.



Sulfation: The ethoxylated lauryl alcohol is then sulfated by reacting with sulfur trioxide gas or sulfuric acid. The sulfation reaction is typically carried out in a falling-film reactor, where a thin film of the ethoxylated lauryl alcohol is exposed to the sulfating agent. The reaction conditions are carefully controlled to ensure that the desired level of sulfation is achieved.



Sodium Lauryl Ether Sulfate (SLES)

Neutralization: The resulting sulfated product is then neutralized with an alkali, typically sodium hydroxide or ammonium hydroxide, to form the sodium or ammonium salt of SLES. The neutralization reaction is typically carried out in a mixing tank, where the sulfated product is mixed with the alkali.

Concentration and purification: The resulting SLES solution is then concentrated and purified to remove any impurities. This is typically achieved by a combination of heat, vacuum, and filtration. The purified SLES is then dried and milled to the desired particle size.

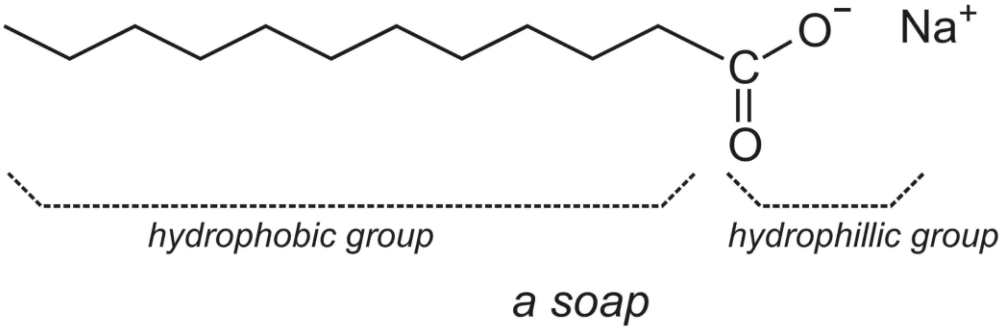
Optional steps: Depending on the desired properties of the SLES, additional steps may be carried out. For example, the SLES may be further ethoxylated or propoxylated to modify its physical properties. It may also be formulated with other surfactants, such as betaines or sulfosuccinates, to improve its performance in specific applications.

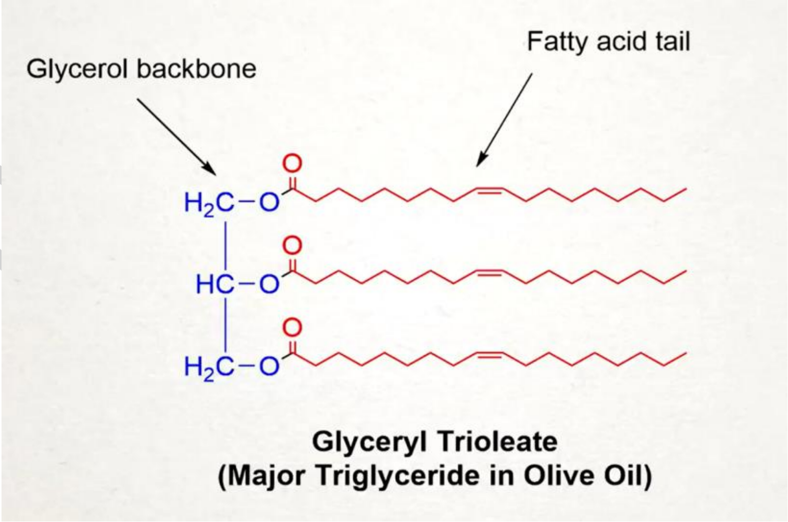
Overall, the production of SLES is a complex process that requires careful control of the reaction conditions and the separation and purification steps to ensure a high-quality product.

Note: It's worth mentioning that the production process for SLES may vary slightly depending on the specific manufacturer and production method. The steps mentioned above represent a general overview of the process.

3- Carboxylate surfactants: (R-COO$^-$)

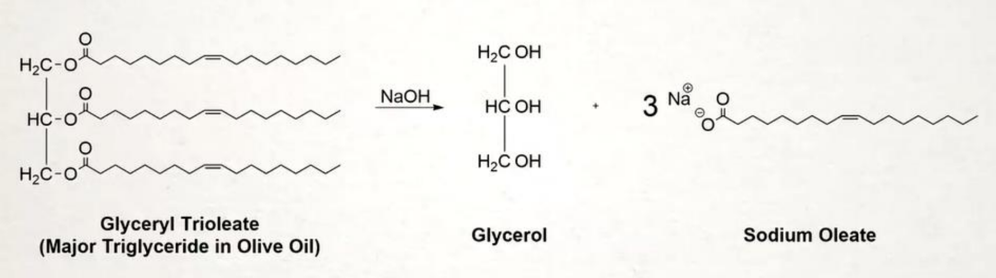
Fatty acid soaps: These are anionic surfactants that are commonly used in bar soaps and liquid hand soaps. They are mild and gentle on the skin, but can also leave a residue if not rinsed off properly.

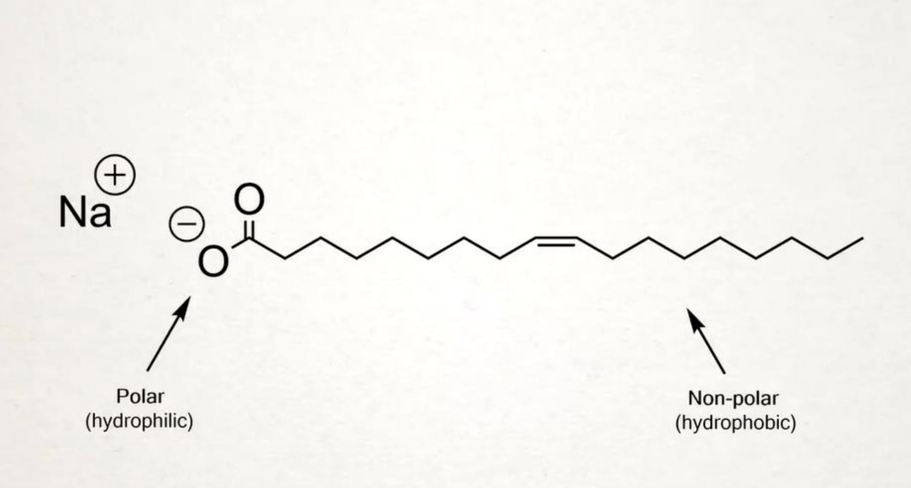




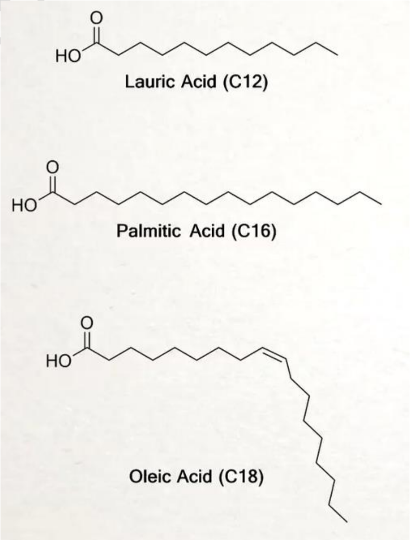
Glyceryl Trioleate
(Major Triglyceride in Olive Oil)

Saponification reaction:



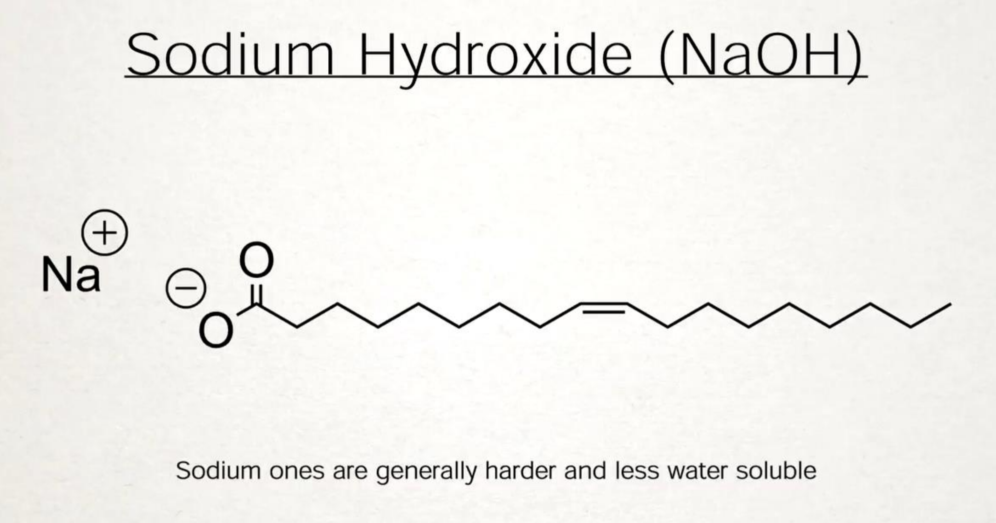


Examples of Fatty acids:



The final product of fatty acid salt is depending on the base used as follow:

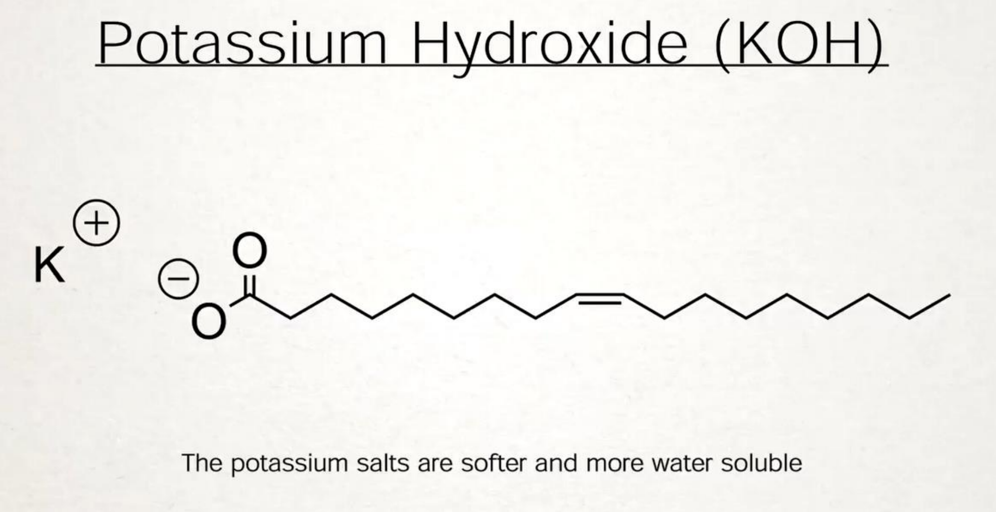
Sodium salt is suitable for making solid bar soap.



Sodium Hydroxide (NaOH)

Sodium ones are generally harder and less water soluble

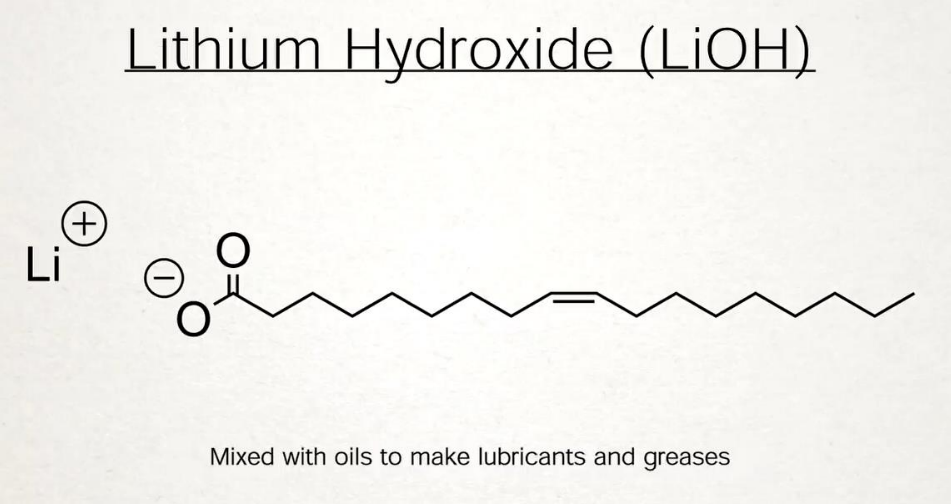
Potassium salt is suitable for making liquid soap.



Potassium Hydroxide (KOH)

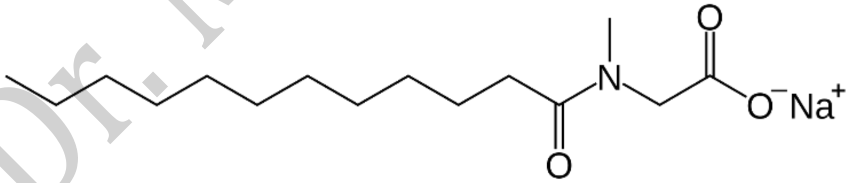
The potassium salts are softer and more water soluble

Lithium salt is suitable for making lubricants and greases.


Lithium Hydroxide (LiOH)

Mixed with oils to make lubricants and greases

Sodium lauroyl sarcosinate, also known as sarcosyl, is an anionic surfactant derived from sarcosine used as a foaming and cleansing agent in shampoo, shaving foam, toothpaste, and foam wash products. It is mild and gentle on the skin, and produces a mild foam.



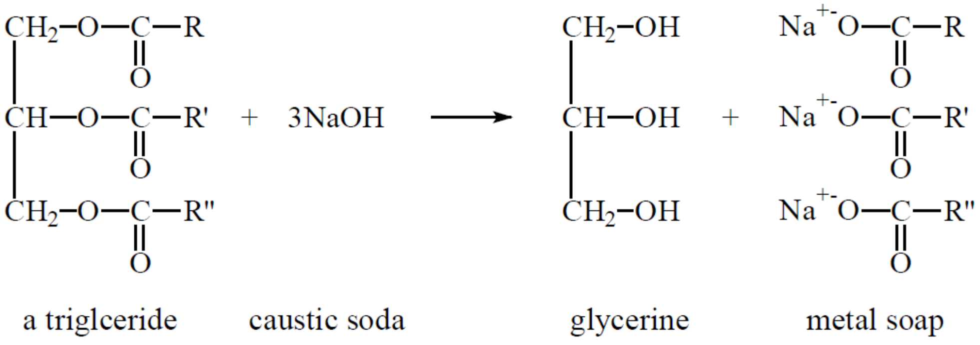
This surfactant is amphiphilic due to the hydrophobic 12-carbon chain (lauroyl) and the hydrophilic carboxylate. Since the nitrogen atom is in an amide linkage, the nitrogen is not pH active and is neutrally charged in all aqueous solutions regardless of pH. The carboxylate has a pKa of about 3.6 and is therefore negatively charged in solutions of pH greater than about 5.5.

Soap production

Soap production typically involves a reaction between a fatty acid and an alkali. Here are the basic steps involved in soap production:

Weighing and mixing the ingredients: The fatty acids (such as coconut oil, palm oil, or tallow) are first weighed and mixed in a large container. Then, the alkali (such as sodium hydroxide or potassium hydroxide) is added to water and dissolved to form a solution.

Saponification: The fatty acids are then heated and the alkali solution is slowly added to them while stirring continuously. This initiates the saponification reaction, which results in the formation of soap and glycerol.



Salting out: After saponification, salt (such as sodium chloride) is added to the mixture. This causes the soap to separate from the glycerol and other impurities, and rise to the top.

Settling and separation: The mixture is left to settle and the soap is separated from the glycerol and other impurities. The impurities are drained off, and the remaining soap is washed with water to remove any residual impurities.

Finishing: The soap is then shaped, cut, stamped, and dried to give it its final form. This may involve the use of molds or extruders, and the addition of fragrances or colors.

It is important to note that soap production is a complex process that can involve variations in the specific ingredients and methods used. Additionally, there are many different types of soap that can be produced, each with its own unique characteristics and production methods.

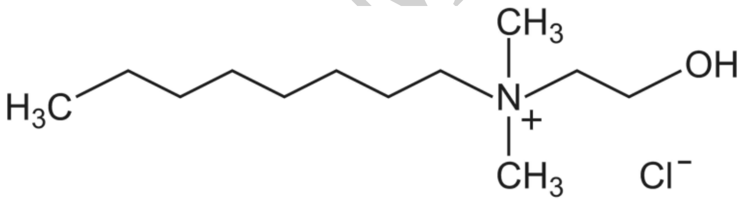
Sulfosuccinates: These are anionic surfactants that are often used in personal care products such as shampoos and body washes. They are mild and gentle, and produce a rich, creamy lather.

Cationic surfactants:

The hydrophilic head is positively charged, have quaternary ammonium (quats) as the polar end.

A) Alkyl quaternary systems

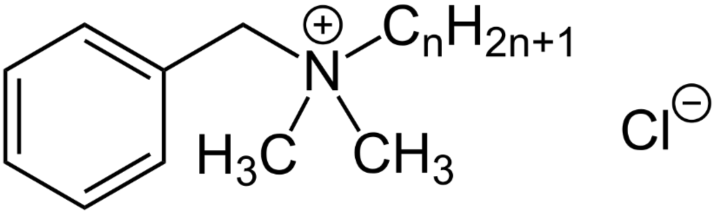
Quaternary ammonium compounds (quats): These are cationic surfactants that are commonly used as disinfectants in household cleaning products, as well as in personal care products such as hair conditioners and fabric softeners. They are effective against a wide range of bacteria and viruses, but can also be toxic to aquatic life if not disposed of properly.



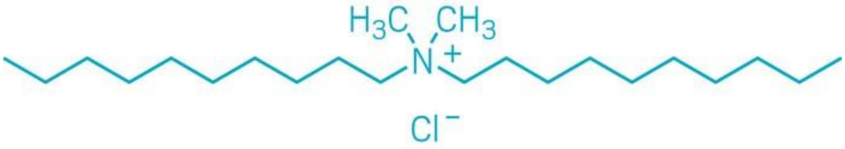
an alkyl quaternary system

Benzalkonium chloride: commonly used as a disinfectant and antiseptic in medical and personal care products.

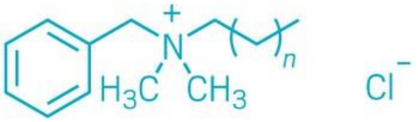
Cetyltrimethylammonium bromide: commonly used as a fabric softener and in hair conditioning products.



$n = 8, 10, 12, 14, 16, 18$



Didecyldimethylammonium chloride (DDAC)



Alkyldimethylbenzylammonium chloride (ADBAC)

$n = 6, 8, 10, 12, 14, 16$

1-Cetylpyridinium chloride (CPC)

Production of Quaternary ammonium compounds (quats)

The production of quats typically involves the following steps:

Alkylation: The first step in the production of quats is the alkylation of a tertiary amine with an alkyl halide or sulfate. This reaction is typically carried out in the presence of a strong base, such as sodium hydroxide or potassium hydroxide. The resulting product is a quaternary ammonium salt.

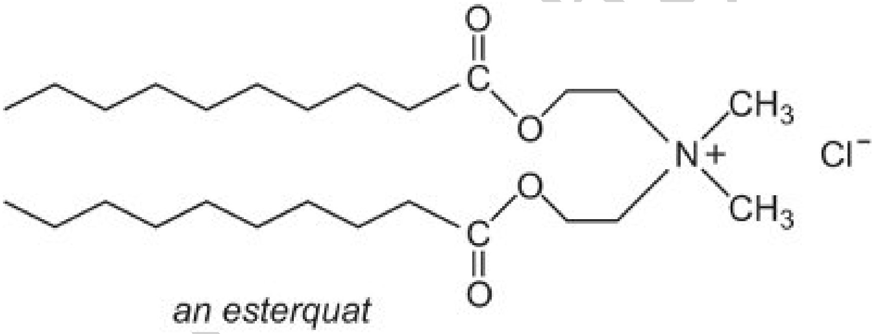
Neutralization: The quaternary ammonium salt is then neutralized with an acid, such as hydrochloric acid, to produce the corresponding quaternary ammonium compound. This step is necessary to convert the salt to the free base form.

Purification: The quaternary ammonium compound is then purified to remove any impurities or unreacted starting materials. Purification methods may include distillation, extraction, or chromatography.

Formulation: The purified quaternary ammonium compound can then be formulated into a variety of products, such as fabric softeners, hair conditioners, or antimicrobial agents. Formulation may involve blending the quaternary ammonium compound with other ingredients, such as emulsifiers, preservatives, or fragrances.

The specific process for producing quats may vary depending on the type of quat and the intended application. For example, some quats may be synthesized using different alkylating agents or purification methods. However, the general steps outlined above are commonly used in the production of many different quats.

Cationic surfactant esters (Esterquats): There is an ester linkage between the alkyl chains and the quaternary head-group. These are cationic surfactants that are commonly used in hair conditioners and other personal care products. They can help to smooth and detangle hair, but can also be heavy and greasy if used at high concentrations.



an esterquat

<u>Here are some examples of formulations that contain quats:</u>

Fabric softeners: Quats are commonly used in fabric softeners to provide a soft, smooth feel to fabrics. In these formulations, the quat is typically blended with a carrier, such as water or a solvent, and may be combined with other ingredients, such as emulsifiers, fragrances, or colorants.

Disinfectants: Quats are effective antimicrobial agents and are used in a variety of disinfectant formulations, including sprays, wipes, and foams. In these formulations, the quat is typically blended with a carrier, such as water or a solvent, and may be combined with other ingredients, such as fragrances, surfactants, or chelating agents.

Hair conditioners: Quats are commonly used in hair conditioners to provide conditioning and detangling benefits. In these formulations, the quat is typically blended with a carrier, such as water or a solvent, and may be combined with other ingredients, such as emollients, humectants, or proteins.

Shampoos: Quats can also be used in shampoo formulations to provide conditioning benefits and improve wet combability. In these formulations, the quat is typically blended with other surfactants, such as sulfates or betaines, and may be combined with other ingredients, such as thickeners, fragrances, or preservatives.

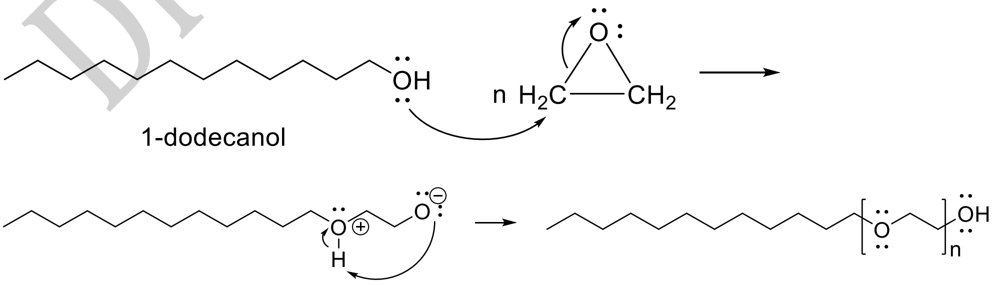
Industrial formulations: Quats are used in a wide range of industrial formulations, including oilfield chemicals, water treatment chemicals, and agricultural chemicals. In these formulations, the quat is typically blended with a carrier, such as water or a solvent, and may be combined with other ingredients, such as surfactants, dispersants, or corrosion inhibitors.

Nonionic surfactants:

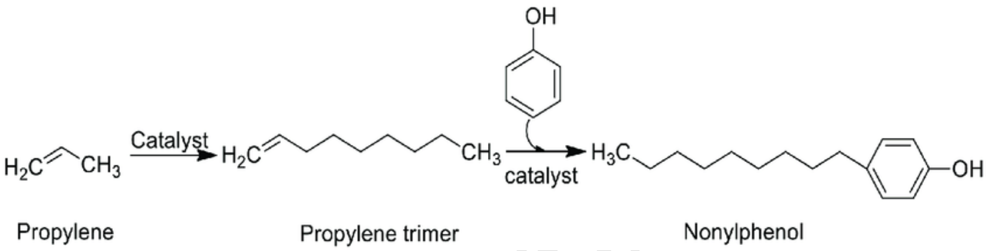
These surfactants do not bear an electrical charge and are often used together with anionic surfactants. The major group of nonionics are the ethoxylates.

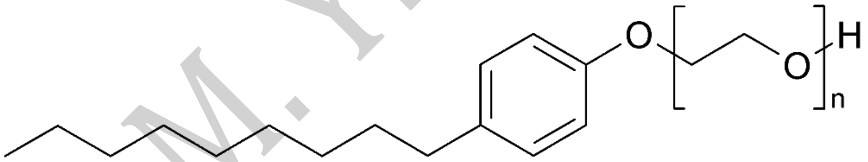
Ethoxylated alcohols: These are nonionic surfactants that are commonly used in laundry detergents and industrial cleaners. They are effective at removing oily and greasy stains, and can work well in hard water conditions.

Silicone surfactants: These are nonionic surfactants that are commonly used in personal care products, such as hair conditioners and skin lotions. They can help to smooth and soften the hair and skin, but can also be expensive and difficult to formulate.



Alkyl phenol ethoxylates: Alkyl phenol ethoxylates are another class of nonionic surfactants that are derived from alkyl phenols. They are similar to alkyl ethoxylates, but have a hydrophobic alkyl phenol group instead of a fatty alcohol. Alkyl phenol ethoxylates are often used in industrial formulations, such as emulsion polymerization, as well as in agricultural and oilfield chemicals.





Polysorbate 20: commonly used as an emulsifier and solubilizer in personal care products, such as facial cleansers and lotions.

Alkyl polyglucosides (APGs): commonly used in household cleaning products and as a foaming agent in personal care products.

As the temperature of the surfactant solution is increased the hydrogen bonds gradually break causing the surfactant to come out of solution. This is commonly referred to as the cloud point and is characteristic for each nonionic surfactant. Nonionics are more surface active and better emulsifiers than anionics at similar concentrations. They are less soluble than anionics in hot water and produce less foam. They are also more efficient in removing oily and organic dirt than anionics.

Alkyl ethoxylates production steps

Here are the general production steps for alkyl ethoxylates:

Raw material preparation: The first step in the production of alkyl ethoxylates is to obtain the starting materials, which are typically linear or branched alcohols and ethylene oxide. The alcohols are typically obtained from natural fats and oils, such as coconut oil or palm kernel oil, and are then purified and distilled to obtain the desired chain length.

Ethoxylation: The alcohols are then reacted with ethylene oxide in the presence of a catalyst, such as potassium hydroxide, to produce the alkyl ethoxylate. The reaction takes place in a stirred reactor under controlled temperature and pressure conditions.

The amount of ethylene oxide used in the reaction can be varied to produce alkyl ethoxylates with different levels of ethoxylation.

Neutralization: The alkyl ethoxylate is then neutralized with an acid, such as phosphoric acid, to remove any residual catalyst and adjust the pH of the product.

Purification: The alkyl ethoxylate is then purified to remove any impurities and byproducts, such as unreacted alcohol or ethylene oxide. This can be done through a variety of methods, such as distillation or crystallization.

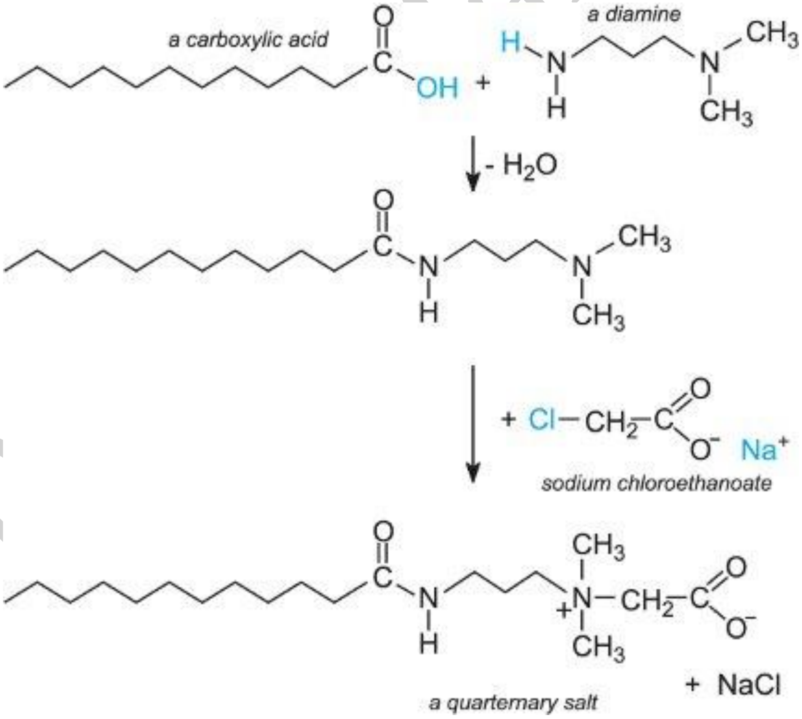
Formulation: The purified alkyl ethoxylate can then be formulated into a final product, such as a detergent or personal care product, by blending it with other ingredients, such as other surfactants, builders, and fragrances.

The specific production steps and conditions for alkyl ethoxylates can vary depending on the specific product and application, but the general process involves the preparation of raw materials, ethoxylation, neutralization, purification, and formulation.

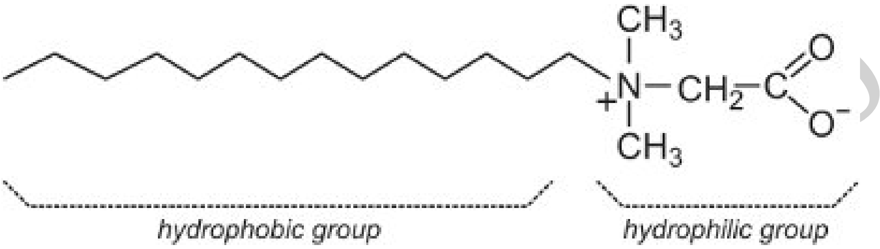
Amphoteric (Zwitterionic) Surfactants:

The head-group carries both a negative and positive charge. The positive charge is almost quaternary ammonium ion and negatively charged group can be carboxylate, $-CO_2^-$, sulfate, $-OSO_3^-$ or sulfonate, $-SO_3^-$.

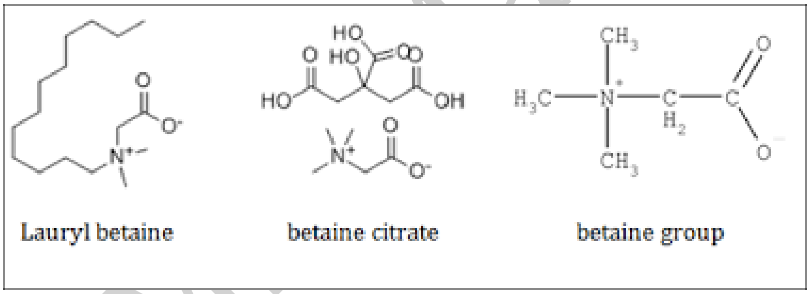
Amphoteric: These are amphoteric surfactants that are commonly used in industrial cleaners and hard surface cleaners. They are effective at removing dirt and grime from a wide range of surfaces, and can work well in hard water conditions.



Cocamidopropyl betaine: commonly used as a mild detergent and conditioner in personal care products, such as shampoo and body wash. Betaines are neutral compounds with a cationic and an anionic group which are not adjacent to one another.



an alkyl betaine



Lauryl betaine betaine citrate betaine group

<u>Here are the general steps involved in the production of betaines:</u>

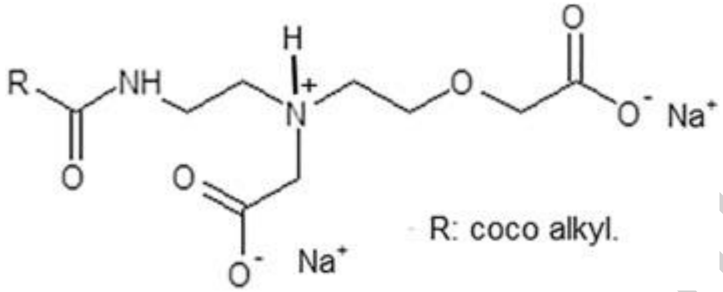
Synthesis of amine: The first step is to synthesize the amine that will be used as a starting material. This can be done by reacting an alkyl halide or an alkyl sulfonate with ammonia or a primary amine, using conditions such as high temperature and pressure or the presence of a catalyst.

Reaction with carboxylic acid: The amine is then reacted with a carboxylic acid such as glycine or sarcosine, which has a carboxylate group and a hydrogen atom that can be substituted by the amine. The reaction is typically carried out in the presence of a strong base such as sodium hydroxide, and may require a coupling agent or an activating reagent such as dicyclohexylcarbodiimide (DCC) or 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC) to facilitate the reaction.

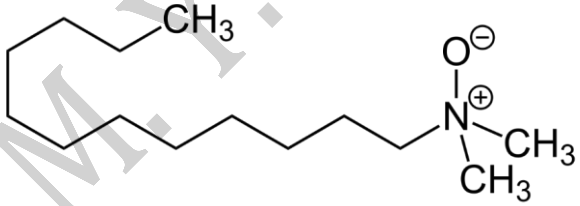
Purification and isolation: The resulting product is a quaternary ammonium compound with both positive and negative charges in its molecular structure, which is typically purified and isolated by methods such as extraction, precipitation, or chromatography.

The specific conditions and reagents used in the production of betaines can vary depending on the desired product, as well as the equipment and resources available in the manufacturing facility.

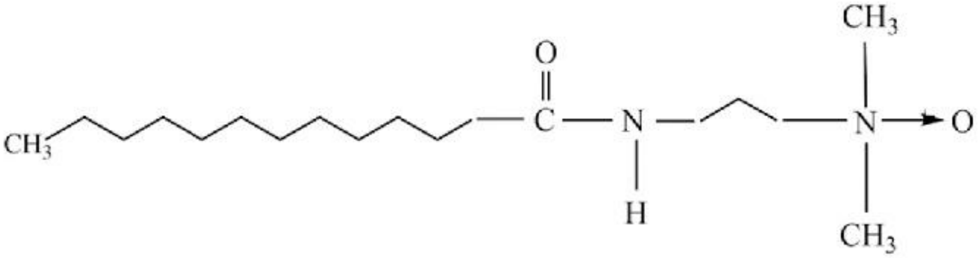
Disodium cocoamphodiacetate: commonly used in personal care products, such as facial cleansers and makeup removers.



Amine oxides: Amine oxides are cationic surfactants that contain an amine group and an oxide group. They are used as foam boosters, viscosity builders, and detergents in a variety of applications. Examples of amine oxides include lauryldimethylamine oxide and cocamidopropylamine oxide.



Lauryldimethylamine oxide



Cocamidopropylamine oxide

These are just a few examples of the many different types of surfactants and their applications. The specific type of surfactant used in a product will depend on its intended use and the desired properties and performance characteristics.

Micelle Formation

Micelle formation is a process by which amphiphilic molecules, which have both hydrophobic (water-repelling) and hydrophilic (water-attracting) regions, arrange themselves in a specific way in a liquid medium, such as water. These amphiphilic molecules include detergents, soaps, and phospholipids, which are important components of cell membranes.

In a liquid medium, such as water, the hydrophobic tails of the amphiphilic molecules tend to cluster together and form a core, while the hydrophilic head groups point outwards towards the surrounding water. The result is the formation of a spherical structure known as a micelle, where the hydrophobic tails are shielded from the water, and the hydrophilic head groups are exposed to the water.

The formation of micelles is driven by the tendency of the system to minimize its free energy, which is achieved by optimizing the interactions between the hydrophobic tails and minimizing their exposure to water, while maximizing the interactions between the hydrophilic head groups and water.

Micelles are important in a variety of biological and industrial processes. In biological systems, micelles play a role in the digestion and absorption of fats and lipids. In industrial applications, micelles are used in detergents to help solubilize and remove dirt and oil, and in pharmaceuticals to help deliver drugs to specific targets in the body.

Surfactants Mechanism of Action

The mechanism of action of surfactants depends on their ability to reduce the surface tension of the interface between two immiscible phases. At the interface, the hydrophilic head groups of the surfactant molecules are attracted to the water molecules, while the hydrophobic tails are repelled by the water and oriented towards the air or oil phase. This reduces the surface tension between the two phases and allows them to mix more easily.

In the case of cleaning applications, such as in detergents, surfactants work by emulsifying oils and greases, which are typically hydrophobic and do not mix well with water. When added to water, surfactants can form micelles, which are spherical structures in which the hydrophobic tails of the surfactant molecules cluster together, while the hydrophilic head groups remain exposed to the surrounding water. This creates a stable structure in which the hydrophobic regions are shielded from the water, allowing the micelles to trap and solubilize the hydrophobic oils and greases.

In addition to their ability to reduce surface tension and emulsify oils, surfactants can also act as wetting agents, helping to spread liquids more evenly over a surface, and as foaming agents, which can help to create stable foam structures in applications such as shampoo or bubble bath.

Overall, the mechanism of action of surfactants is based on their ability to interact with interfaces between different phases, allowing them to reduce surface tension, emulsify hydrophobic substances, and provide other useful properties in a variety of applications.

Foam formation mechanism

Foam is formed when a gas is dispersed in a liquid or solid in the form of bubbles. The formation of foam involves several steps, including nucleation, growth, and stabilization.

Nucleation is the first step in foam formation, and it involves the formation of small gas bubbles in the liquid. Nucleation can occur spontaneously due to fluctuations in pressure and temperature, or it can be induced by mechanical agitation, such as stirring or shaking. The size and number of the bubbles formed during nucleation depend on the properties of the liquid, the gas, and the agitation conditions.

After nucleation, the bubbles start to grow due to the diffusion of gas molecules from the bulk phase to the gas-liquid interface. The rate of bubble growth is determined by the rate of gas diffusion, the surface tension of the liquid, and the viscosity of the liquid. As the bubbles grow, they may coalesce and merge with neighboring bubbles, which can result in an increase in the bubble size.

Finally, the stability of the foam is determined by the balance between the attractive and repulsive forces acting on the bubbles. Attractive forces, such as van der Waals forces and gravity, tend to bring the bubbles together, while repulsive forces, such as electrostatic repulsion and steric hindrance, prevent them from coalescing. The addition of a surfactant, which can adsorb to the gas-liquid interface and form a stable film around the bubbles, can enhance the stability of the foam by reducing the attractive forces between the bubbles.

Overall, the formation of foam is a complex process that is influenced by a range of physical and chemical factors, including the properties of the liquid, the gas, and the surfactant, as well as the agitation conditions and the environmental factors such as temperature and pressure.

Foam Stabilization and De-Stabilization

Foam stabilization refers to the process by which bubbles in a foam are prevented from coalescing or merging with one another, resulting in a stable foam structure that can persist for a long time. On the other hand, foam destabilization is the process by which foam bubbles collapse or merge, resulting in a breakdown of the foam structure.

The stability of a foam depends on the balance between the attractive and repulsive forces between the bubbles. Attractive forces, such as surface tension and van der Waals forces, tend to bring the bubbles together, while repulsive forces, such as electrostatic repulsion and steric hindrance, prevent them from coalescing.

There are several factors that can affect the stability of a foam. These include:

Surfactants: Surfactants are compounds that can lower the surface tension of a liquid, allowing bubbles to form and stabilize. They can also provide a barrier between the bubbles, preventing them from coalescing.

pH: The pH of the liquid can affect the stability of a foam by altering the charge of the surfactant molecules. This, in turn, can affect the repulsive forces between the bubbles.

Temperature: The temperature can affect the stability of a foam by altering the viscosity and surface tension of the liquid.

Mechanical agitation: Mechanical agitation, such as stirring or shaking, can destabilize a foam by breaking down the bubble structure.

In order to destabilize a foam, one can use methods such as adding a destabilizing agent (e.g. salt or acid), reducing the concentration of the surfactant, or increasing the temperature. On the other hand, to stabilize a foam, one can use methods such as increasing the concentration of the surfactant, adjusting the pH, or adding thickening agents to increase viscosity.

Examples of antifoam compounds

Antifoam compounds are substances that can reduce or eliminate the formation and stability of foam. They are used in a variety of industrial and commercial applications where foam can interfere with the performance of the process or product. Here are some common examples of antifoam compounds:

Silicone-based antifoams: Silicone-based antifoams are the most widely used type of antifoam compound, and they are commonly used in industrial processes, such as pulp and paper manufacturing, wastewater treatment, and food processing. Silicone-based antifoams contain a silicone oil that spreads over the surface of the foam bubbles and breaks them down, resulting in the collapse of the foam structure.

Mineral oil-based antifoams: Mineral oil-based antifoams are commonly used in the production of food and beverages, such as beer, soft drinks, and vegetable oils. Mineral oil-based antifoams work by spreading over the surface of the foam bubbles and lowering the surface tension of the liquid, which causes the bubbles to collapse.

Polypropylene glycol-based antifoams: Polypropylene glycol-based antifoams are used in a variety of industrial processes, such as the production of latex and coatings, as well as in the manufacture of personal care products, such as shampoos and lotions. Polypropylene glycol-based antifoams work by adsorbing to the surface of the foam bubbles and reducing the surface tension of the liquid.

Fatty acid-based antifoams: Fatty acid-based antifoams are commonly used in the production of paints and coatings, as well as in the oil and gas industry. Fatty acid-based antifoams work by destabilizing the foam structure through the formation of insoluble complexes with the surfactant molecules that stabilize the foam.

Overall, the selection of an antifoam compound depends on the specific application and the properties of the foam, such as the size and stability of the bubbles, the composition of the liquid, and the environmental factors such as temperature and pressure.

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