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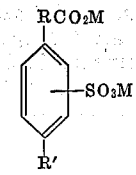
SURFACE ACTIVE AGENTS

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ABSTRACT OF THE DISCLOSURE

Novel surface active agents are provided having the general formula:



wherein R is a linear alkyl group containing from about 1 to 30 carbon atoms, R′ is an acyclic alkyl group containing from about 1 to 30 carbon atoms, the sum of R plus R′ being at least 7, and M is a cation selected from the group consisting of Li, Na, K, Rb, Cs, Ca, Mg, NH_4 and substituted ammonium.

BACKGROUND OF THE INVENTION

Field of the invention

This invention relates to surface active agents. In one aspect this invention relates to novel surface active agents having easily varied hydrophobic characteristics. In another aspect this invention relates to novel surface active agents containing 2 functional groups per molecule, namely, a carboxylate and a sulfonate moiety.

Brief description of the prior art

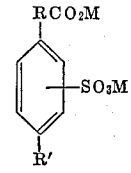
Alkyl benzene sulfonates, e.g., dodecylbenzene sulfonate, have been known for many years to be excellent surface active agents, as have the alkali metal salts of fatty acids. However, in order to obtain the benefit of the sulfonate and the alkali metal carboxylate groups in a composition, it has been necessary to admix two different compounds, one containing the sulfonate group and the other containing the carboxylate group. Thus, it would be desirable to produce a surface active agent having both the sulfonate and carboxylate moiety in the same molecule. Further, it would be desirable to obtain a surface active agent wherein a phenyl group is located down the alkyl chain toward the end removed from the carboxylate group, while at the same time providing for a sulfonate group to be attached to the phenyl ring. In addition, it would be desirable to vary the hydrophobic-hydrophilic balance in the molecule in order to obtain surface active agents having both water and oil solubility characteristics.

OBJECTS OF THE INVENTION

An object of the invention is to provide a novel surface active agent. Another object of the invention is to provide a surface active agent containing a carboxylate and sulfonate group in one molecule. Yet another object of the invention is to provide a surface active agent in which the hydrophobic-hydrophilic balance of said surface active agent can be readily varied. These and other objects, advantages and features of the present invention will become apparent to those skilled in the art from a reading of the following detailed disclosure and the appended claims.

SUMMARY OF THE INVENTION

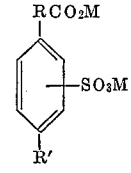
According to the present invention novel surface active agents are provided having the general formula:



wherein R is a linear alkyl group containing from about 1 to 30 carbon atoms, R′ is an acyclic alkyl group containing from about 1 to 30 carbon atoms, the sum of R plus R′ being at least 7, and M is a cation selected from the group consisting of Li, Na, K, Rb, Cs, Ca, Mg, NH_4 and substituted ammonium. The phenyl group is distributed along the alkyl chain represented by R, but concentrated toward the end away from the carboxylate group.

DESCRIPTION OF PREFERRED EMBODIMENTS

The novel surface active agents of the present invention are those having the general formula:



wherein R is a linear alkyl group containing from about 1 to 30 carbon atoms, R′ is an acyclic alkyl group containing from about 1 to 30 carbon atoms, the sum of R plus R′ being at least 7, and M is a cation selected from the group consisting of Li, Na, K, Rb, Cs, Ca, Mg, NH_4 and substituted ammonium. Suitable substituted ammonium cations are alkyl ammonium, such as methyl ammonium, dimethyl ammonium, and the like; and alkanol ammonium, such as monoethanol, diethanol, triethanol ammonium and the like. Likewise, any combination of linear alkyl groups and acyclic alkyl groups can be employed as R and R′, respectively, the only requirement being that the sum of R plus R′ must be at least 7 to provide the surface active properties of the composition. The term "acyclic," as used in this specification, is to include both linear and branched alkyl groups. The term "surface active agent," as used in this specification, is a compound which lowers the surface tension of water. It is well known that such surface active agents are employed in detergent formulations and are used as wetting agents to improve the wettability of substances. Especially desirable results have been obtained wherein R and R′ are both linear alkyl groups, the sum of R plus R′ is between about 18 and 22 carbon atoms and M is Na.

Suitable linear alkyl groups which can be employed as R in the formula described above are methyl, ethyl, propyl, butyl, pentyl, hexyl, heptyl, octyl, nonyl, decyl, dodecyl, tetradecyl, hexadecyl, octadecyl, isosyl, tetracosyl, octacosyl, nonacosyl, triacontyl, and the like. Examples of suitable acyclic alkyl groups which can be employed as R′ are methyl, ethyl, propyl, butyl, pentyl, hexyl, heptyl, octyl, nonyl, decyl, dodecyl, tetradecyl, hexadecyl, octadecyl, icosyl, tetracosyl, octacosyl, nonacosyl, triacontyl, and the like.

In the preparation of the surface active agents of the present invention, it is important that the sulfonate and carboxylate groups be separated and that the sulfonate group be attached to the phenyl group while the carboxylate group is attached to a linear alkyl group, designated as R in the before-mentioned formula. In addition, in order to obtain the desirable surface active properties, the

total carbon atoms represented by R plus R' in the before-described formula must be at least 7, and more desirably between about 18 and 22. Thus, one must carefully choose the reactants and the process in order to produce a compound meeting the above requirements. Desirable results have been obtained where the surface active agents of the present invention, e.g., sulfonated alkyl phenylalkanoic acid dimetal salt compounds, are prepared by alkylation of a phenylalkanoic acid with an olefin in the presence of an alkylation catalyst and carbon disulfide under alkylation conditions which are well known in the art. The resulting alkylate is then sulfonated and neutralized to produce the desired sulfonated alkyl phenylalkanoic acid dimetal salt compounds. As is evident to those skilled in the art, any suitable sulfonating agent, such as sulfuric acid, oleum, and the like, can be employed. Likewise, any suitable alkali can be employed to neutralize the resulting sulfonated product. However, the amount of sulfonating and neutralizing agents and the reaction condition will vary depending upon the particular sulfonating and neutralizing agents being employed.

In order to more fully describe the surface active agents of the present invention, the following specific examples in the preparation and utilization of the novel surface active agents of the present invention are provided. However, it is to be understood that the following example is for illustrative purposes only and the limitations contained therein are not to be construed as unduly limiting the scope of the invention which will be defined in the claims hereinafter.

EXAMPLE

An experiment was conducted to produce sulfodecylphenylundecanoic acid disodium salt. Two hundred and forty-four grams of $AlCl_3$ and 400 ml. of carbon disulfide were introduced and stirred in a flask fitted with a condenser, a mechanical stirrer, a thermometer, and a dropping funnel. Four hundred grams of phenylundecanoic acid and two hundred and thirty-five grams of decene-1 were admixed, placed in the dropping funnel and added dropwise into the flask over a period of 1¾ hours. The contents of the flask were maintained at about 25 to 30° C. One ml. of water, acting as a promoter, was added to the flask prior to the addition of the phenylundecanoic acid and the decene-1 at the halfway point and again after the addition was complete. The resulting reaction mixture was then poststirred for about seventeen hours.

The reaction mixture containing the alkylate was then hydrolyzed by pouring same into a vessel containing 200 ml. of concentrated HCl and ice. This mixture was then stirred and diethyl ether was added to aid hydrolysis. After the hydrolysis was completed the mixture was allowed to separate into an organic phase and a water phase. The organic phase was separated and the water phase washed with ether to extract any remaining organic compounds. The ether wash and the organic phase were combined and washed repeatedly with water until the wash effluent was neutral. The organic phase, e.g., product phase, was then dried over Na_2SO_4 and filtered through diatomaceous earth. The solvent was then removed by distillation at atmospheric pressure. The product was then vacuum distilled through a 6-inch Vigreux column, and a fraction boiling at 215 to 255° C. at 0.6 to 1.5 mm. Hg and weighing 154 grams was collected. Analyses by N.M.R. and IR. indicated that the product was 85 to 90% pure decylphenylundecanoic acid.

One hundred grams, i.e., 0.25 mole, of the decylphenylundecanoic acid and eighty grams of oleum were then placed in a batch-type sulfonation reactor. The reactor was equipped with a thermometer and a condenser which was open to the air. The sulfonation of the decylphenylundecanoic acid was conducted at a temperature of about

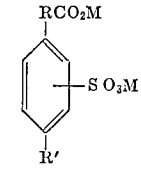
45 to 50° C. After the sulfonation of the decylphenylundecanoic acid was completed, the sulfonation product was neutralized with sodium hydroxide in an isopropyl alcohol-water diluent. The solvent, e.g. diluent, was then evaporated off. A solid was then obtained; the solid was then ground up into a powder.

The powder was then treated to remove unsulfonated decylphenylundecanoic acid. This procedure involved dissolution in aqueous isopropyl alcohol, acidification of the carboxylate group, extraction with hexane, neutralization of the carboxylate group, dilution with isopropyl alcohol to precipitate sodium sulfate, separation of sodium sulfate, and evaporation of solvent to recover a purified powder weighing 93 grams. The purified powder was then analyzed by N.M.R. and acid-base titration and determined to be the sulfodecylphenylundecanoic acid disodium salt.

The cotton wetting properties of the sulfodecylphenylundecanoic acid disodium salt was then compared with an alkali metal salt of a linear alkyl benzene sulfonate, a well known surface active agent designated LAS, and found to be equal to or better than LAS in wetting properties. The result of such comparison is tabulated below.

	Cotton wetting, 75° F.	
Compound	3 g. hook, 0.02% conc.	5 g. skein, 0.1% conc.
Sulfodecylphenylundecanoic acid disodium salt, seconds	50	5-6
LAS, seconds	72	5.5

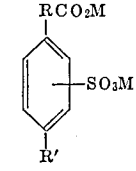
Thus, the above example and data clearly illustrate the preparation of a novel surface active agent having the general formula:



wherein R, R' and M are as previously defined.

Having thus described the invention, I claim:

1. A surface active agent having the general formula:



wherein R is a linear alkyl group containing from about 1 to 30 carbon atoms, R' is an acyclic alkyl group containing from about 1 to 30 carbon atoms, the sum of R plus R' being at least 7, and M is a cation selected from the group consisting of Li, Na, K, Rb, Cs, Ca, Mg, NH_4 and substituted ammonium.

2. The surface active agent of claim **1** wherein said R' is a linear alkyl group and the sum of R plus R' is from about 18 to 22 carbon atoms.

3. The surface active agent of claim **2** wherein said M is Na.

4. The surface active agent of claim **3** wherein said surface active agent is sulfodecylphenylundecanoic acid disodium salt.

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ELBERT L. ROBERTS, Primary Examiner

U.S. Cl. X.R.

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