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(71) Applicant: **KAO CORPORATION, S.A.**
08210 Barberà del Vallès,
Barcelona (ES)

(72) Inventors:
• **PI BOLEDA, Bernat**
08210 Barberà del Vallès (ES)
• **PEY GUTIÉRREZ, Carmen Maria**
08210 Barberà del Vallès (ES)
• **NOGUÉS LÓPEZ, Blanca**
08210 Barberà del Vallès (ES)

(74) Representative: **Hoffmann Eitle**
Hoffmann Eitle S.L.U.
Paseo de la Castellana 140, 3a planta
Edificio LIMA
28046 Madrid (ES)

(54) **SOFTENER FORMULATIONS WITH BIOCIDAL ACTIVITY**

(57) The present invention provides formulations including a mixture of cationic surfactants and a biocidal component, the weight of the mixture of cationic surfactants in the composition being equal or higher than the

weight of the biocidal component.

Advantageously the formulations are stable single-phase formulations, clear, and with a remarkable dual effect in softening and sanitizing fabrics.

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Description**FIELD OF THE INVENTION**

[0001] The present invention generally relates to stable and clear softener compositions comprising mixtures of quaternary ester ammonium compounds and one or more biocidal agents; as well as to uses and methods for softening and sanitizing fabrics.

BACKGROUND OF THE INVENTION

[0002] It has become common in the consumer and residential sector to use fabric softening compositions that include surfactants and low quantities of optional ingredients such as perfumes, stabilisers, preservatives and colorants.

[0003] There are two main types of fabric softener; those that use cationic surfactants and those that use anionic surfactants. The choice of softener can vary depending on the fabric to be treated.

[0004] Many commercial fabric softeners are based on quaternary ester ammonium salts with one or two long alkyl chains, for example, dipalmitoylethyl hydroxyethylmonium methosulfate. Other cationic compounds can be derived from imidazolium, substituted amine salts, or quaternary alkoxy ammonium salts. Early formulations commonly used dihydrogenated tallow dimethyl ammonium chloride (DHTDMAC). Fabric softeners containing quaternary ammonium salts operate well in conventional residential wash and dryer cycles and provide softness to textiles that are both woven and non-woven.

[0005] On the other hand, adhesion of microorganisms to surfaces is undesirable, particularly when the microorganisms are pathogenic. Adhering microorganisms frequently lead to infections or reinfection in humans, animals and plants.

[0006] The use of disinfecting compositions that can eliminate such microorganisms is becoming more extensive, especially in underwear or delicate clothing, sportswear, household linen (towels, cloths, sheets, blankets, covers, bath mats, shower curtains), or workwear. To effectively eliminate such microorganisms, it is recommended to the consumer that the disinfecting compositions are not used together with a softening agent.

[0007] Additionally, delicate textiles such as silk or microfibers are increasingly being processed into clothing which can only be washed at cooler temperatures of 30 to 40° C. As a result, microorganisms are not killed.

[0008] In addition to a lower washing temperature, it is also common today to use liquid detergents which are generally free of bleaching agents.

[0009] Thus, as a result of changing washing behaviour, textiles contaminated with viruses, bacteria, molds or yeasts cannot be rendered microbe-free to the required extent and so (re)infection may possibly take place on renewed contact of the consumer with the supposedly clean laundry.

[0010] In view of the above, the present invention aims at the problem of providing clear and stable softener formulations which, when mixed with water below 40 °C, preferably at room temperature, are able to provide the softening as well as the biocidal effect. Additionally, it is preferable that such formulations exhibit advantageous storage stability under various conditions, advantageous handleability (simple handling), and/or advantageous softening properties.

SUMMARY OF THE INVENTION

[0011] The present inventors have found that the above problems can be solved when the biocidal component is mixed with a mixture of cationic surfactants obtainable as provided below.

[0012] Particularly, as it is shown below, formulating a liquid composition comprising the mixture of cationic surfactants in an amount equal or higher than the amount of the biocidal component, the resulting formulation is a single-phase composition (i.e., is a continuous liquid phase including both components), clear, stable (i.e, there is no separation of the biocidal agent(s) and the cationic mixture with time) and biocidal-efficient.

[0013] Thus, in an aspect the invention provides a composition comprising:

- (i) a mixture of cationic surfactants; and
- (ii) a biocidal component,

the % by weight of the mixture of cationic surfactants with respect to the total weight of the composition being equal or higher than the % weight of the biocidal component with respect to the total weight of the composition, and

wherein:

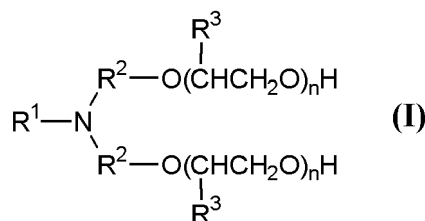
the mixture of cationic surfactants is obtainable by a process comprising the steps:

Step I: esterification of a) with b), and

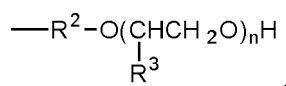
Step II: cation formation from the reaction products of Step I,
wherein:

a) is a hydroxyl group-containing compound or a mixture of hydroxyl group-containing compounds comprising a.1 and optionally a.2, wherein:

- a.1 is an alkanolamine or a mixture of alkanolamines of the general formula (I):



in which R¹ is selected from hydrogen, a C₁-C₆ alkyl group, and the residue



R² is a C₁-C₆ alkylene group, R³ is hydrogen or methyl, n is 0 or an integer from 1 to 20; and

- a.2 is a polyol, which can be optionally alkoxyated, and is characterized by a MW in the range 60 to 190 g/mol;

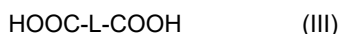
b) is a mixture of compounds containing one or more carboxylic groups comprising b.1 and b.2, wherein:

- b.1 is a monocarboxylic acid or a mixture of monocarboxylic acids of formula (II):



in which R⁶ is a linear or branched C₆-C₂₃ alkyl or alkenyl group; or an alkyl ester or glyceride thereof, preferably a linear or branched C₆-C₂₃ alkyl or alkenyl ester; and

- b.2 is a dicarboxylic acid or a mixture dicarboxylic acids of the general formula (III), or reactive derivative(s) thereof:



wherein L is a saturated or unsaturated, linear, branched or cyclic group having 1 to 10 carbon atoms, each of which carbon atoms is optionally substituted by a C₁-C₆ saturated or unsaturated group; and is preferably represented by (CH(R⁷))_m or by (C₆-C₁₀ arylene) optionally substituted by one or more R⁷, in which each R⁷ is independently a hydrogen, OH or a C₁-C₆ saturated or unsaturated group, m is 0 or an integer from 1 to 10, wherein for m ≥ 2, the chain (CH)_m optionally contains one or more double bonds and/or cyclic group(s);

wherein a.1), a.2), b.1) and b.2) are introduced in the reaction system of Step I in amounts resulting in the following molar ratios:

- the molar ratio of monoacid(s)/diacid(s) (b.1/b.2) is 0.10 to 1.0;
- the molar ratio between organic carboxylic groups and organic hydroxyl groups (COOH/OH) present in the system is 0.30 to 0.80; and
- the molar ratio between the compound(s) within the definition a.2 and the compound/s under definition a.1 is 0 to 0.5.

[0014] The present invention provides, in a further aspect, a process for preparing the composition of the first aspect of

the invention, comprising the step of mixing the mixture of cationic surfactants as provided herein, and the biocidal component.

[0015] In a further aspect, the invention provides the use of the composition of the invention for softening and/or sanitizing fabrics.

[0016] In a final aspect the invention provides a method for softening and/or sanitizing textiles or fabrics, the method comprising the step of:

(a1) contacting one or more textiles or fabrics with the composition of the invention at one or more points during the laundering process, or, alternatively,

(a2) when the composition is in the form of a sprayable form, the method comprises spraying (dispensing) the composition directly on the fabric.

DETAILED DESCRIPTION OF THE INVENTION

[0017] Terms not specifically defined herein should be given the meanings that would be given to them by one of skill in the art in light of the disclosure and the context. As used in the specification, however, unless specified to the contrary, the following terms have the meaning indicated and the following conventions are adhered to.

[0018] Throughout the present specification and the accompanying clauses, the words "comprise" and variations such as "comprises", "comprising" are to be interpreted inclusively. That is, these words are intended to convey the possible inclusion of other elements or integers not specifically recited, where the context allows. The word "comprise" also includes the term "consists of".

[0019] For the purposes of the present invention, any ranges given include both the lower and the upper endpoints of the range.

[0020] The present inventors have surprisingly found that particular mixtures of cationic surfactants (esterquats (EQ)) obtainable by reacting a combination of mono- and di-carboxylic acids with alkanolamine(s) and optionally polyol(s), and subsequent cation formation, form clear, optically transparent, single phase stable solutions when formulated with one or more biocidal agents. These effects can be observed without the necessity to use high EQ or solvent concentrations.

Mixture of cationic surfactants

[0021] The cationic surfactant mixtures suitable in the context of the invention can be directly dissolved in water, thereby providing softener compositions that are optically transparent and stable upon storage under various conditions. No additives are necessary for achieving the optical transparency and stability of the final compositions.

[0022] The cationic surfactant mixtures of the present invention can be used to formulate clear fabric biocidal softener compositions at a temperature between 20°C and 40°C, preferably between 25°C and 35°C. Addition of non-ionic surfactants and solvents is optional, not necessary for, and not affecting the optical transparency of the final composition. Optical transparency is an attractive and desirable feature of the products. Using less additives is advantageous from of environmental, bio- and skin compatibility, and economical perspective.

[0023] The term "obtainable" and "obtained" have the same meaning and are used interchangeably. In any case, the expression "obtainable" encompasses.

[0024] In an embodiment of the invention, the molar ratio of monoacid(s)/diacid(s) (b.1/b.2) is 0.20 to 1.0, preferably 0.30 to 1.0; and/or the molar ratio between organic carboxylic groups and organic hydroxyl groups (COOH/OH) present in the system is 0.40 to 0.70, preferably 0.50 to 0.70; and/or the molar ratio between the compound(s) within the definition a.2 and the compound/s under definition a.1 is 0 or 0.1 to 0.5, preferably 0.1 to 0.5. Without wishing to be bound by theory, each of these particular ratios may even further improve the optical transparency. Additionally, handleability (simple handling), and/or softening properties may be improved.

[0025] In an embodiment of the invention, the amounts of the compounds a.1, a.2, b.1 and b.2 are introduced in the reaction system of Step I in amounts that result in the following molar ratios: the molar ratio of monoacid(s)/diacid(s) (b.1/b.2) is 0.30 to 1.0; the molar ratio between organic carboxylic groups and organic hydroxyl groups (COOH/OH) present in the system is 0.40 to 0.70, preferably 0.50 to 0.70; and the molar ratio between the compound(s) within the definition a.2 and the compound/s under definition a.1 is 0, or is 0.1 to 0.5.

[0026] The particular ratios of the components as in the present invention, it is possible to obtain cationic surfactant mixtures allowing to prepare clear and stable softener formulations when mixed with water at a temperature between 20°C and 40°C, preferably between 25°C and 35°C, even when using a broader variety of monocarboxylic acid(s) than in the prior art.

[0027] The particular mixture of cationic surfactants incorporated in the composition of the invention allows the incorporation of biocides with different antimicrobial activity. The examples provided below are performed with a biocidal component consisting of a mixture of an antifungal+antibacterial substance. On one hand, the composition remains stable

(single-phase composition) and clear, even incorporating the biocidal agents. On the other hand, the mixture of surfactants does not hinder or affect negatively to the biocidal agents, which are formulated, together, in the same composition. On the contrary, the antimicrobial effect, both antibacterial and antifungal are highly notable.

[0028] It is also remarkable that the presence of the antimicrobial agents does not negatively affect to the inherent softener properties of the cationic mixture.

[0029] In an embodiment of the invention, the alkanolamine(s) of formula (I) is/are selected from triethanolamine, N-methyldiethanolamine, N-methyldiisopropanolamine and triisopropanolamine, each of which is optionally alkoxyated with ethylene oxide or propylene oxide, and mixtures thereof.

[0030] In an embodiment of the invention, in the dicarboxylic acid(s) of formula (III), each L is selected from ethane-1,2-diyl, 1-hydroxyethane-1,2-diyl, *cis*-ethene-1,2-diyl, *trans*-ethene-1,2-diyl, propane-1,2-diyl, propane-1,3-diyl, butane-1,4-diyl, pentane-1,5-diyl, hexane-1,6-diyl, cyclohexane-1,4-diyl, octane-1,8-diyl and 1,4-phenylenyl; preferably butane-1,4-diyl, hexane-1,6-diyl or octane-1,8-diyl.

[0031] In an embodiment of the invention, the dicarboxylic acid of formula (III) is selected from succinic, malic, glutaric, adipic, sebacic, pimelic, suberic, maleic and terephthalic acid, acids obtained by thermal oligomerisation of unsaturated fatty acids, and mixtures thereof.

[0032] In an embodiment of the invention, the reactive derivative(s) of the dicarboxylic acid(s) of the general formula (III) are one or more selected from halide, anhydride, preferably mixed anhydride with acetic acid or cyclic anhydride.

[0033] For example, the monocarboxylic acid(s) of formula (II) are synthetic fatty acids and/or are obtained from fats or oils of natural origin, and are optionally hydrogenated; or are derived from oils of vegetal origin which are optionally hydrogenated.

[0034] In an embodiment of the invention, the monocarboxylic acid(s) of formula (II) are selected from those which are obtained from tallow, palm, olive, coconut, sunflower, soya, rapeseed, grape marc and grape, each of which can be hydrogenated, partially hydrogenated, or non-hydrogenated.

[0035] In an embodiment of the invention, the iodine value of the carboxylic monoacid(s) of formula (II) is from 5 to 280, from 5 to 180, from 5 to 100, from 5 to 80, from 5 to 60, from 10 to 10 to 60, from 10 to 50, from 20 to 50, from 20 to 40. Without wishing to be bound by theory, using carboxylic monoacid(s) having such iodine values may contribute to even further improving the optical transparency at various temperatures, and/or the storage stability of the aqueous formulations obtained from the mixture of cationic surfactants according to the present invention.

[0036] In an embodiment of the invention, the carboxylic monoacid(s) of formula (II) is one or more selected from caproic acid, caprylic acid, 2-ethylhexanoic acid, capric acid, lauric acid, isotridecanoic acid, myristic acid, palmitic acid, palmoleic acid, stearic acid, isostearic acid, oleic acid, elaidic acid, petroselinic acid, linoleic acid, linolenic acid, eleostearic acid, arachic acid, gadoleic acid, behenic acid and erucic acid, and mixtures thereof which are obtained for example by pressure splitting of natural fats and oils, in the reduction of aldehydes from Roelen's oxosynthesis or dimerization of unsaturated fatty acids, stearic acids, isostearic acid, palmitic acid, myristic acid, lauric acid, capric acid, caprylic acid, 2-ethylhexanoic acid, 2-octyldodecanoic acid, capric acid, oleic acid, linoleic acid, linolenic acid, partially hydrogenated coconut fatty acid, palm fatty acid, partially hydrogenated distilled palm fatty acid, hydrogenated distilled palm fatty acid, palm kernel fatty acid, tallow fatty acid, distilled tallow fatty acid, and rapeseed fatty acid.

[0037] In an embodiment of the invention, the compounds corresponding to a.1 and/or a.2 can be from natural origin or from synthetic origin.

[0038] In an embodiment of the invention, the polyol a.2 is one or more selected from trimethylolpropane (TMP), glycerine, neopentyl glycol (NPG) and sorbitol, each of which can be optionally alkoxyated, preferably ethoxyated; wherein the polyol a.2 is more preferably trimethylolpropane (TMP), or is absent.

[0039] Step I is an esterification step of reacting a) with b). In an exemplary embodiment, monoacid b.1 and diacid b.2 are combined with alkanolamine a.1 and optionally the polyol b.2. The obtained mixture is heated. Preferably, the mixture is heated to reflux under atmospheric pressure, e.g., for 1-5, preferably 2-4 hours at 140-200 °C, preferably 160-180 °C. Preferably, step I is performed until no more water is distilled off the reaction mixture.

[0040] The reaction product obtained from step I is subjected to cation formation in step II. Preferably, an organic solvent is added before step II. Step II can correspond to the formation of the addition salts of the alkanolamine esters obtained from Step I with mineral or organic acids, preferably wherein the mineral or organic acids are one or more selected from hydrochloric, sulphuric, phosphoric, citric and lactic acid. Alternatively, Step II can correspond to the quaternisation of reaction mixtures of Step I with alkylating agent(s), preferably wherein the alkylating agents are one or more selected from methyl chloride, methyl bromide, dimethyl sulphate, diethyl sulphate and dimethyl carbonate. Step II can be performed at room temperature or elevated temperature, e.g., 40-100 °C, preferably 50-90 °C; preferably for 1-5, more preferably 2-4 hours, or until the virtually complete absence of amine value was verified by acid/base assay.

[0041] In an embodiment of the invention, the mixture further comprises an organic solvent, preferably an alcohol, more preferably ethanol, n-propanol or isopropanol, butanols, glycol, propane or butanediol, glycerol, diglycol, propyl or butyl diglycol, ethylene glycol methyl ether, ethylene glycol ethyl ether, ethylene glycol propyl ether, ethylene glycol mono-n-butyl ether, diethylene glycol methyl ether, diethylene glycol ethyl ether, propylene glycol methyl, ethyl or propyl ether,

dipropylene glycol methyl or ethyl ether, methoxy, ethoxy or butoxy triglycol, 1-butoxyethoxy-2-propanol, 3-methyl-3-methoxybutanol, or propylene glycol t-butyl ether. For instance, such solvent may be added during the preparation step, e.g., before, during and/or after II, preferably before Step II.

[0042] In an embodiment of the invention, the content of the organic solvent in the cationic surfactant mixture is 0-30%, preferably 0-20%, more preferably 10-20% by weight.

[0043] In an embodiment of the invention, the mixture is essentially water-free.

[0044] In an embodiment of the invention, the mixture essentially consists of the reaction products of steps I and II, and optionally an organic solvent. Preferably, the mixture consists of the reaction products of steps I and II and solvent, if any, and unreacted starting materials as well as inevitable impurities from the production process, if any.

Biocidal component

[0045] In the context of the invention, the term "biocidal component" refers to a single substance with biocidal activity (hereinafter referred as "biocide", "biocidal agent" or "biocidal active substance"), but also to mixtures including two or more biocides, biocidal agents or biocidal active substance.

[0046] In the context of the invention a "biocide", "biocidal agent" and "biocidal active substance" have the same meaning, can be used interchangeably, and refer to a chemical substance or microorganism intended to destroy, deter, render harmless, or exert a controlling effect on any harmful organism.

[0047] Biocides can be mainly classified in synthetic and natural biocides.

[0048] Illustrative non-limitative examples of natural biocides are: extracts of natural oils with biocide activity, such as Agastache Rugosa Stem Oil, Azadirachta Indica Bark/Seed Extract, Azadirachta Indica Leaf Extract, Eucalyptus Globulus Leaf Oil, Eugenia Uniflora Leaf Oil, Eugenol, Illicium Verum Oil, Melia Azadirachta Bark Extract, Melia Azadirachta Extract, Melia Azadirachta Leaf Powder, P-chloro-m-cresol, Tanacetum Cinerariifolium (Pyrethrum) Root Extract, Vitex Negundo Flower/Leaf/Seed Oil

[0049] Illustrative examples of synthetic biocides are the non-oxidant biocides, particularly cationic biocides. Cationic biocides (CBs) have been in use for surface disinfection and topical antisepsis. Broad-spectrum activity and relatively low toxicity have led to increased deployment of these compounds in medicated dressings, in contact lens cleaning solutions, in swimming pools to control microbial growth, and in domestic cleaning products. Their mode of action normally involves interaction with the cell envelope, displacing divalent cations. Subsequent interactions with membrane proteins and the lipid bilayer depend upon the specific nature of the biocide, but generally CB exposure results in membrane disruption and lethal leakage of cytoplasmic materials. CBs have a range of structures that can be categorized according to the number of cationic groupings per molecule. The quaternary ammonium compounds are often monocationic surfactants generally containing one quaternary nitrogen associated with at least one major hydrophobic component.

[0050] Illustrative non-limitative examples of synthetic biocides not included within the cationic biocides group are BHAP (2-Bromo-4-hydroxyacetophenone), Bronopol (2-Bromo-2-nitropropane-1,3-diol), DBNPA (2-2-Dibromo-3-nitrilopropionamide), DTEA (2-(Decylthio)ethanamine), Glutaraldehyde, and Isothiazolines, among others.

[0051] In one embodiment, the biocidal component comprises one or more quaternary ammonium compound(s). In another embodiment, the biocidal component comprises at least two biocides, particularly quaternary ammonium compound(s). In another embodiment, the biocidal component consists of two biocides. In another embodiment, the biocidal component consists of two biocides, wherein one or both are quaternary ammonium compound(s)

[0052] In the context of the invention, the term "quaternary ammonium compound" refers to a salt of a quaternary ammonium cation, wherein the protonated nitrogen atom (N⁺) is covalently bonded to four radicals, such as alkyl and/or aryl groups. Preferably, the quaternary ammonium compound is of general formula (IV):



wherein R⁴ to R⁷ are the same or different, each independently being selected from the group consisting of: a (C₁-C₂₀) straight or branched alkyl chain, (C₃-C₂₀) cycloalkyl optionally substituted with a straight or branched alkyl having from 1 to 6 carbon atoms, (C₆-C₂₀) aryl optionally substituted with a straight or branched alkyl having from 1 to 6 carbon atoms, and benzyl; and X⁻ is an anionic counterion.

[0053] Examples of (C₁-C₂₀) straight or branched alkyl chain include, but are not limited to: methyl, ethyl, n-propyl, isopropyl, n-butyl, sec-butyl, isobutyl, tert-butyl, n-pentyl, isopentyl, tert-pentyl, neopentyl, n-hexyl, n-heptyl, n-octyl, n-decyl, n-dodecyl, n-hexadecyl and n-octadecyl.

[0054] The term "cycloalkyl" as used herein refers to cyclic alkyl groups having the indicated number of ring carbon atoms. Examples, of substituted or unsubstituted (C_3 - C_{20})cycloalkyl groups include, but are not limited to: cyclopropyl, cyclopentyl, cyclohexyl, 4-methylcyclohexyl, 4-ethylcyclohexyl, 4-n-propylcyclohexyl and 4-n-butylcyclohexyl.

[0055] The term "aryl" as used herein refers to an aromatic hydrocarbon radical having the indicated number of ring carbon atoms such as phenyl, naphthyl or anthracyl. The aryl group may be unsubstituted or substituted with a straight or branched alkyl group having from 1 to 6 carbon atoms, preferably from 1 to 3 carbon atoms, such as methyl or ethyl. Examples (C_6 - C_{20}) of substituted or unsubstituted aryl groups include, but are not limited to: phenyl, naphthyl, 4-methylphenyl and 4-ethylphenyl.

[0056] The term "anionic counterion" includes any ion that can form a salt with quaternary ammonium. Examples of suitable counterions include halides (such as chlorides and bromides), propionates, methosulphates, saccharinates, ethosulphates, hydroxides, acetates, phosphates, carbonates, and nitrates. Preferably, the anionic counterion is chloride.

[0057] In one embodiment, the composition of the invention comprises one quaternary compound of formula (IV). In another embodiment, the composition of the invention comprises at least two quaternary ammonium compounds of formula (IV), which are the same or different. In another embodiment, the composition of the invention comprises two different quaternary ammonium compounds of formula (IV).

[0058] In any of the embodiments provided above, the quaternary ammonium compound of formula (IV) is one wherein R^4 , R^5 , R^6 and R^7 are the same or different, each independently being selected from the group consisting of (C_1 - C_{20}) straight or branched alkyl chain, and benzyl; and X^- is a halide. Preferably, at least two of R^4 , R^5 , R^6 and R^7 are methyl, and the other two of R^4 , R^5 , R^6 and R^7 are selected from the group consisting of (C_1 - C_{20}) straight or branched alkyl chain, and benzyl; and X^- is a halide, particularly Cl^- . Preferably, two or three of R^4 , R^5 , R^6 and R^7 are methyl, and the other(s) are selected from the group consisting of (C_1 - C_{20}) straight or branched alkyl chain, and benzyl; and X^- is a halide, particularly Cl^- (chloride).

[0059] In one embodiment, quaternary ammonium compounds of formula (IV) are selected from:

-->Dialkyldimethylammonium chloride types: (C_8 - C_{18}) dialkyldimethylammonium chloride (examples: didecyl dimethylammonium chloride, dialkyl C_{8-10} dimethylammonium chloride);

--> Alkyldimethylbenzylammonium types: (C_8 - C_{18}) alkyldimethylbenzylammonium chloride (examples: alkyl C_{12-16} dimethylbenzylammonium chloride, alkyl (C_{12-18})dimethylbenzylammonium chloride).

[0060] In one embodiment of the present invention, the quaternary ammonium compound(s) of formula (IV) are selected from the group consisting of (C_8 - C_{18}) alkyl dimethylbenzylammonium salt and di-(C_1 - C_{10}) alkyl dimethylammonium salt.

[0061] Examples of quaternary ammonium compounds of formula (IV) include but are not limited to, alkyl C_{12-16} dimethylbenzylammonium chloride, alkyl C_{12-18} dimethylbenzylammonium chloride, octyl decyl dimethyl ammonium chloride, dioctyl dimethyl ammonium chloride, and didecyl dimethyl ammonium chloride, to name few.

Softener compositions

[0062] Further provided is a softener composition, preferably a fabric-softening, comprising the cationic surfactant mixture as defined above together with the biocidal component. The composition preferably further comprises water.

[0063] In one embodiment of the present invention the weight ratio between the mixture of cationic surfactants and the biocidal component is from 1:1 to 5:1, particularly from 2:1 to 4:1. In the context of the invention, the term "weight ratio" refers to ratio between the weight (expressed in grams, g) of the mixture of cationic surfactants and weight (expressed in grams, g) of the biocidal component.

[0064] The "weight", when the biocidal component comprises two or more biocides or biocidal agents, will be understood, in context of the invention, as the total weight, summing the weight of each one of the biocides forming the biocidal component.

[0065] In one embodiment, the mixture of cationic surfactants is at a % by weight, with respect to the total weight of the composition, from 0.5 to 20%, particularly from 0.5 to 3 or from 3 to 15%.

[0066] The amount of the one or more biocidal agents selected to form the biocidal component of the composition can be easily and routine established by the skilled person in art. In the context of the invention, the amount would be, in the context of the invention, suitable to be used and be in contact with mammals, particularly human beings.

[0067] In another embodiment, the composition comprises a biocidal component: (ii) comprising or consisting of one or more quaternary ammonium biocide compounds as defined in any of the embodiments provided above; and (ii) it is at a % by weight, with respect to the total weight of the composition, from 0.5 to 5%, particularly from 1 to 4%, with respect to the total weight of the composition.

[0068] In another embodiment, the composition comprises a biocidal component (ii) comprising at least a dialkyldimethylammonium chloride compound, wherein the content of dialkyldimethylammonium chloride compound is from 0.5 to 5%, particularly from 1 to 4%, with respect to the total weight of the composition.

[0069] In another embodiment, the composition comprises a biocidal component (ii) comprising at least an alkyl-dimethylbenzylammonium compound, wherein the content of alkyl-dimethylbenzylammonium compound is from 0.5 to 5%, particularly from 0.5 to 3%, with respect to the total weight of the composition.

[0070] In another embodiment, the composition comprises a biocidal component: (ii) comprising at least a dialkyl-dimethylammonium chloride compound and at least an alkyl-dimethylbenzylammonium compound, wherein the sum of dialkyl-dimethylammonium chloride and alkyl-dimethylbenzylammonium compound is from 0.5 to 5, particularly from 1 to 4%, with respect to the total weight of the composition.

[0071] In another embodiment, the composition comprises a biocidal component: (ii) comprising at least a dialkyl-dimethylammonium chloride compound and at least an alkyl-dimethylbenzylammonium compound, wherein the content of dialkyl-dimethylammonium compound is from 0.5 to 2%, preferably from 0.5 to 1.5%, with respect to the total weight of the composition; and wherein the content of alkyl-dimethylbenzylammonium compound is from 0.5 to 3.5%, preferably from 1.5 to 3% wt, with respect to the total weight of the composition.

[0072] The compositions of the invention may exhibit advantageous storage stability (remains in a single phase) under various conditions, as well as further advantageous properties, such as handleability (simple handling) and/or softening properties.

[0073] Such compositions are clear solutions at RT, and can be stable upon storage at RT, or at 40°C, e.g., for at least 2 months.

[0074] In an embodiment of the invention, the composition is optically transparent at room temperature, and preferably also at temperatures of 10-45°C, 15-35°C or 20-30 °C.

[0075] The compositions of the invention provide a potent antimicrobial effect at low laundry temperatures, together with a softening effect of the fabrics. Examples below show that using water at 20°C, a remarkable antifungal and antibacterial effects were achieved.

[0076] In the composition, the water content is preferably higher than 50%, more preferably higher than 80%, most preferably higher than 85% w/w, preferably higher than 90% w/w, alternatively, water content is from 80 to 98% w/w.

[0077] In an embodiment of the invention, the composition further comprises a perfume. The perfume consists of one or more substance(s). The average logP of the perfume substance(s) is from 1 to 6, preferably from 1 to 4, preferably from 2 to 4. The weight ratio between the cationic surfactant mixture according to the invention, as defined hereinabove, and the perfume is from 99:1 to 90:10, from 99:1 to 80:20.

[0078] In an embodiment of the invention, the composition further comprises a non-ionic surfactant. The weight ratio between the cationic surfactant mixture and the non-ionic surfactant is preferably from 100:0 (i.e., no non-ionic surfactant is present) to 70:30. A non-ionic surfactant can advantageously improve solubility of a perfume in the composition, especially when high amounts of perfume are used (e.g., > 1%, optionally up to 3% by weight of the composition, or more). Preferably, when the amount of perfume in the composition is 0.3% by weight or less, no non-ionic surfactant is used; otherwise, a non-ionic surfactant may optionally be used. Additionally, the addition of a non-ionic surfactant can even further improve the good stability of the formulation upon storage.

[0079] In an embodiment of the invention, the composition further comprises a thickener, e.g., a thickening polymer. The weight ratio the cationic surfactant mixture to the thickener is preferably from 100:0 to 10:5, more preferably from 100:1 to 10:2. A thickener may be added to increase the viscosity of the composition. Suitable thickeners are, e.g., PEG-150 distearate, Hydroxyethyl cellulose, hydroxymethyl cellulose and derivatives thereof, PEG-120 Methyl Glucose Dioleate, PEG-120 Methyl Glucose Trioleate (and) propanediol, ethoxylated Sorbitan Triisostearate (e.g., PEG-160 Sorbitan Triisostearate, such as Kaopan TW IS-559S from Kao Chemicals Europe, S.L.), and copolymers of acrylamide and dimethyl amino ethyl methacrylate methyl chloride cross-methylene bisacrylamide (such as FLOSOFT 222 manufactured by SNF).

[0080] In an embodiment of the invention, the composition further comprises a chelating agent. The chelating agent plays the role of providing detergency through a mechanism of destroying hardness components within a washing liquid by chemically bonding to a multivalent cation (hardness component) to form a metal ion complex, and favorably satisfies conditions of a) fast chelating speed, b) high chelating ability, c) chelate stability, d) high security, e) good biodegradability, and f) good solubility.

[0081] To give examples of available substances as the organic chelating agent according to the present invention, sodium salt of organic carboxylic acid such as oxalic acid (OA), citric acid (CA), tartaric acid (TA), or gluconic acid (GA), a hydroxyamino carboxylic acid chelating agent, which is sodium salt of N-(2-hydroxyethyl) glycine (DEG), triethanolamine (TEA), N-(2-hydroxyethyl) iminodiacetic acid (HEIDA), or N-(hydroxyethyl)ethylenediamine tetraacetic acid (HEDTA), an ether carboxylic acid chelating agent, which is sodium salt of O-carboxymethyltartronic acid (CMT) or O-carboxymethylsuccinic acid (CMOS), a vinyl polyelectrolyte chelating agent, which is sodium salt of a copolymer of acrylic acid/maleic acid and polyacrylic acid, or a carboxylic acid chelating agent, which is sodium salt of Nitrilo Triacetic Acid (NTA), Diethylene Triamine Pentaacetic Acid (DTPA), Hydroxyethyl Ethylene Diamine Triacetic Acid (HEDTA), Ethylene Diamine Tetraacetic Acid (EDTA), MethylglycineDiacetic Acid (MGDA), Dicarboxymethylglutamic Acid (GLDA), Aspartate Diacetic Acid (ASDA), Ethylenediamine Disuccinic Acid (EDDS), Hydroxye Iminodisuccinic Acid (HIDS), or Iminodisuc-

cinic Acid (IDS) are preferably used. Of these, MGDA, GLDA, ASDA, EDDS, HIDS, and IDS with good biodegradability are preferred in terms of environmental burden.

[0082] Some of quantitative conditions for when selecting an appropriate organic chelating agent for use in the present invention are i) pH of a 1% aqueous chelating agent solution is 9 or greater, preferably within a range of 10 and 12.5, and ii) maximum calcium trapping ability (number of milligrams of CaCO₃ per gram for pH 11) is 200 mg/g or greater, preferably 300 mg/g or greater.

[0083] Particularly, the chelating agent such as tetrasodium ethylene diamine tetraacetic acid (may be referred to as "EDTA-4Na" hereafter): Trilon B powder (registered trademark, manufactured by BASF Corporation), or trisodium methylglycinediacetic acid (may be referred to as "MGDA-3Na" hereafter): Trilon M powder (registered trademark, manufactured by BASF Corporation) may be given as an example of a substance satisfying such quantitative conditions. For comparison, with EDTA-4Na, the pH of a 1% aqueous EDTA-4Na solution is 10.5 to 12.5 and maximum calcium trapping ability is 225 mg/g, and with MGDA-3Na, the pH of a 1% aqueous MGDA-3Na solution is 10.5 to 12.5 and maximum calcium trapping ability is 327 mg/g.

[0084] The weight ratio of the cationic mixture and the chelating agent is from 100:0 to 75:25.

[0085] In an embodiment of the invention, the softener composition further comprises:

A) a perfume, preferably wherein:

- (i) the perfume consists of one or more substance(s); and/or
- (ii) the average logP of the perfume substance(s) is from 1 to 6; and/or

B) a non-ionic surfactant, which is preferably characterised in that the weight ratio of the described components are values according to the following ratios:

P:C is a value from 0:100 to 20:80 NI:C is from 0:100 to 30:70
 P corresponds to the perfume;
 C corresponds to the cationic surfactant mixture;
 NI corresponds to the non-ionic surfactant.

[0086] In another embodiment of the invention, the softener composition further comprises:

A) a perfume, preferably wherein:

- (i) the perfume consists of one or more substance(s); and/or
- (ii) the average logP of the perfume substance(s) is from 1 to 6; and/or
- (iii) optionally the perfume can be an encapsulated perfume, preferably the perfume is encapsulated in a biodegradable microcapsule, more preferably the microcapsule is based on chitosan; and/or

B) a non-ionic surfactant, which is preferably characterised in that the weight ratio of the described components are values according to the following ratios:

P:C is a value from 0:100 to 20:80 NI:C is from 0:100 to 30:70
 P corresponds to the perfume, optionally microencapsulated perfume;
 C corresponds to the cationic surfactant mixture;
 NI corresponds to the non-ionic surfactant.

[0087] As used herein, the non-ionic surfactant(s) can be selected from fatty acids, linear or branched, alkoxyated or non-alkoxyated esters of fatty acids, especially those containing from 8 to 18 carbon atoms, alkoxyated or non-alkoxyated Guerbet alcohols, optionally alkoxyated glycerol and polyglycerol esters, xylitol esters, alkoxyated or non-alkoxyated sorbitan esters, esters of sugars, such as glucose, fructose, galactose, mannose, xylose, arabinose, ribose, 2-deoxyribose and sucrose, C₈₋₁₈ fatty alcohols, alkyl polyglucosides, non-ionic surfactants with amide groups derived from amines, such as glucamine, and the derivatives of methylethanolamine, diethanolamine, isopropanolamine and monoethanolamine, with linear or branched fatty acids, especially those containing from 8 to 18 carbon atoms, waxes, such as paraffins, microcrystalline waxes derived from petroleum, and synthetic waxes, and pentaerythritol esters, especially having a tallow, hydrogenated tallow, palm, behenic or oleic chain, preferably non-ionic surfactants are selected from glycerine esters that are ethoxyated, sorbitan monoesters and pentaerythritol esters, especially those having a

tallow, hydrogenated tallow, palm, behenic or oleic chain.

[0088] Suitable non-ionic surfactants are Glycereth-6 Cocoate (e.g., Levenol F-200), Glycereth-17 Cocoate (e.g., Levenol C-201), ethoxylated C₁₃₋₁₅ alcohol (e.g., with 7EO, such as Findet 1315/19), ethoxylated C₁₆₋₁₈ alcohol (e.g., with 23 EO, such as Findet 1618/35); particularly suitable is ethoxylated hydrogenated castor oil (e.g., with 40 EO, such as Findet ARH-52).

[0089] The softener composition may have a viscosity at 20 °C of 2-500cps, as measured on a Brookfield LVT viscometer with spindle 2 at 60 rpm.. Preferably, such compositions have a viscosity of 2 to 200 mPas as measured on a Brookfield LVT viscometer with spindle 4 at 12 rpm. For example, diluted formulations (from 2% active to 50% active) can have viscosity values between 2 and 500 mPa·s.

[0090] In a further embodiment the present invention, the composition of the invention comprises the following:

(i) the mixture of cationic surfactants, as defined herein, at a % by weight from 0.5 to 15 % w/w, particularly from 0.5 to 3 or from 3 to 15% w/w,

(ii) the one or more biocidal agent(s) at a % by weight from 0.5 to 5 %, particularly from 1 to 4% w/w, and

(iii) optionally the one or more ingredients selected from the group consisting of:

non-ionic surfactants at a % by weight from 0 to 5% w/w;

thickeners at a % by weight from 0 to 1% w/w;

chelating agents at a % by weight from 0 to 5% w/w; and

perfume is at a % by weight from 0 to 2% w/w,

all the percentages being expressed with respect to the total weight of the composition.

[0091] Depending on the particular use, the skilled person, using the general knowledge, can easily and routinely select those ingredients and amounts to be incorporated into the composition of the invention, comprising the mixture of cationic surfactants and the biocidal component.

[0092] Once added these further ingredients, the skilled person just needs to mix all the ingredients, including water, using any of the well-known means.

[0093] In one embodiment, the process for preparing the composition of the invention comprises:

(a) mixing the mixture of cationic surfactants and the biocidal component;

(b) adding one or more of the surfactants, thickeners, chelating agents or fragrances as provided in any of the above embodiments; and

(c) repeating the mixing; or, alternatively,

the process comprising mixing at the same time the mixture of cationic surfactants, the biocidal component, water and the one or more ingredients selected from of the surfactants, thickeners, chelating agents or fragrances as provided in any of the above embodiments.

[0094] The present invention further provides the following aspects.

1. A composition comprising:

(i) a mixture of cationic surfactants; and

(ii) a biocidal component,

the weight of the mixture of cationic surfactants in the composition being equal or higher than the weight of the biocidal component, and

wherein:

the mixture of cationic surfactants is obtainable by a process comprising the steps:

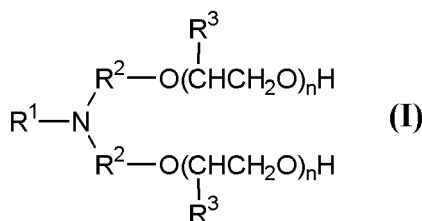
Step I: esterification of a) with b), and

Step II: cation formation from the reaction products of Step I,

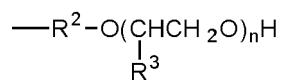
wherein:

a) is a hydroxyl group-containing compound or a mixture of hydroxyl group-containing compounds comprising a.1 and optionally a.2, wherein:

- a.1 is an alkanolamine or a mixture of alkanolamines of the general formula (I):



in which R¹ is selected from hydrogen, a (C₁-C₆)alkyl group, and the residue



R² is a (C₁-C₆) alkylene group, R³ is hydrogen or methyl, n is 0 or an integer from 1 to 20; and

- a.2 is a polyol, which can be optionally alkoxyated, and is characterized by a MW in the range 60 to 190 g/mol;

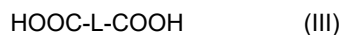
b) is a mixture of compounds containing one or more carboxylic groups comprising b.1 and b.2, wherein:

- b.1 is a monocarboxylic acid or a mixture of monocarboxylic acids of formula (II):



in which R⁶ is a linear or branched (C₆-C₂₃) alkyl or alkenyl group; or an alkyl ester or glyceride thereof, preferably a linear or branched (C₆-C₂₃) alkyl or alkenyl ester; and

- b.2 is a dicarboxylic acid or a mixture dicarboxylic acids of the general formula (III), or reactive derivative(s) thereof:



wherein L is a saturated or unsaturated, linear, branched or cyclic group having 1 to 10 carbon atoms, each of which carbon atoms is optionally substituted by a (C₁-C₆) saturated or unsaturated group; and is preferably represented by (CH(R⁷))_m or by (C₆-C₁₀) arylene optionally substituted by one or more R⁷, in which each R⁷ is independently a hydrogen, OH or a (C₁-C₆)saturated or unsaturated group, m is 0 or an integer from 1 to 10, wherein for m ≥ 2, the chain (CH)_m optionally contains one or more double bonds and/or cyclic group(s);

wherein a.1), a.2), b.1) and b.2) are introduced in the reaction system of Step I in amounts resulting in the following molar ratios:

- the molar ratio of monoacid(s)/diacid(s) (b.1/b.2) is 0.10 to 1.0;
- the molar ratio between organic carboxylic groups and organic hydroxyl groups (COOH/OH) present in the system is 0.30 to 0.80; and
- the molar ratio between the compound(s) within the definition a.2 and the compound/s under definition a.1 is 0 to 0.5.

2. The composition according to aspect 1, wherein the molar ratio of monoacid(s)/diacid(s) (b.1/b.2) is 0.20 to 1.0, preferably 0.30 to 1.0.

3. The composition according to any one of the preceding aspects, wherein the molar ratio between organic carboxylic groups and organic hydroxyl groups (COOH/OH) present in the system is 0.40 to 0.70, preferably 0.50 to 0.70.

4. The composition according to any one of the preceding aspects, wherein the molar ratio between the compound(s) within the definition a.2 and the compound/s under definition a.1 is 0 or 0.1 to 0.5, preferably 0.1 to 0.5.

5. The composition according to any one of the preceding aspects, wherein the amounts of the compounds a.1, a.2, b.1 and b.2 are introduced in the reaction system of Step I in amounts that result in the following molar ratios:

- the molar ratio of monoacid(s)/diacid(s) (b.1/b.2) is 0.30 to 1.0;
- the molar ratio between organic carboxylic groups and organic hydroxyl groups (COOH/OH) present in the system is 0.40 to 0.70, preferably 0.50 to 0.70; and
- the molar ratio between the compound(s) within the definition a.2 and the compound/s under definition a.1 is 0, or is 0.1 to 0.5.

6. The composition according to any one of the preceding aspects, wherein the alkanolamine(s) of formula (I) is/are selected from triethanolamine, N-methyldiethanolamine, N-methyldiisopropanolamine and triisopropanolamine, each of which is optionally alkoxylated with ethylene oxide or propylene oxide, and mixtures thereof.

7. The composition according to any one of the preceding aspects, wherein in the dicarboxylic acid(s) of formula (III), each L is selected from ethane-1,2-diyl, 1-hydroxyethane-1,2-diyl, *cis*-ethene-1,2-diyl, *trans*-ethene-1,2-diyl, propane-1,2-diyl, propane-1,3-diyl, butane-1,4-diyl, pentane-1,5-diyl, hexane-1,6-diyl, cyclohexane-1,4-diyl, octane-1,8-diyl and 1,4-phenylenyl; preferably butane-1,4-diyl, hexane-1,6-diyl or octane-1,8-diyl.

8. The composition according to any one of the preceding aspects, wherein the dicarboxylic acid of formula (III) is selected from succinic, malic, glutaric, adipic, sebacic, pimelic, suberic, maleic and terephthalic acid, acids obtained by thermal oligomerisation of unsaturated fatty acids, and mixtures thereof.

9. The composition according to any one of the preceding aspects, wherein the reactive derivative(s) of the dicarboxylic acid(s) of the general formula (III) are one or more selected from halide, anhydride, preferably mixed anhydride with acetic acid or cyclic anhydride.

10. The composition according to any one of the preceding aspects, wherein the monocarboxylic acid(s) of formula (II) are synthetic fatty acids and/or are obtained from fats or oils of natural origin, and are optionally hydrogenated.

11. The composition according to any one of the preceding aspects, wherein the monocarboxylic acid(s) of formula (II) are derived from oils of vegetal origin which are optionally hydrogenated.

12. The composition according to any one of the preceding aspects, wherein the monocarboxylic acid(s) of formula (II) are selected from those which are obtained from tallow, palm, olive, coconut, sunflower, soya, rapeseed, grape marc and grape, each of which can be hydrogenated, partially hydrogenated, or non-hydrogenated.

13. The composition according to any one of the preceding aspects, wherein the iodine value of the carboxylic monoacid(s) of formula (II) is preferably ≥ 5 , more preferably ≥ 35 , even more preferably ≥ 45 , most preferably ≥ 50 ; and/or preferably ≤ 280 , more preferably ≤ 180 , even more preferably ≤ 100 , most preferably ≤ 80 .

14. The composition according to any one of the preceding aspects, wherein the iodine value of the carboxylic monoacid(s) of formula (II) is from 5-280, from 5 to 180, from 5 to 100, from 5 to 80, from 5 to 60, from 10 to 10 to 60, from 10 to 50, from 20 to 50, from 20 to 40.

15. The composition according to any one of the preceding aspects, wherein the carboxylic monoacid(s) of formula (II) is one or more selected from caproic acid, caprylic acid, 2-ethylhexanoic acid, capric acid, lauric acid, isotridecanoic acid, myristic acid, palmitic acid, palmoleic acid, stearic acid, isostearic acid, oleic acid, elaidic acid, petroselinic acid, linoleic acid, linolenic acid, eleostearic acid, arachic acid, gadoleic acid, behenic acid and erucic acid, and mixtures thereof which are obtained for example by pressure splitting of natural fats and oils, in the reduction of aldehydes from Roelen's oxosynthesis or dimerization of unsaturated fatty acids, stearic acids, isostearic acid, palmitic acid, myristic acid, lauric acid, capric acid, caprylic acid, 2-ethylhexanoic acid, 2-octyldodecanoic acid, capric acid, oleic acid, linoleic acid, linolenic acid, partially hydrogenated coconut fatty acid, palm fatty acid, partially hydrogenated distilled palm fatty acid, hydrogenated distilled palm fatty acid, palm kernel fatty acid, tallow fatty acid, distilled tallow fatty acid, and rapeseed fatty acid.

16. The composition according to any one of the preceding aspects, wherein the compounds corresponding to a.1 and/or a.2 are from natural origin.

17. The composition according to any one of the preceding aspects, wherein the compounds corresponding to a.1 and/or a.2 are from synthetic origin.

18. The composition according to any one of the preceding aspects, wherein Step II corresponds to the formation of the addition salts of the alkanolamine esters obtained from Step I with mineral or organic acids, preferably wherein the mineral or organic acids are one or more selected from hydrochloric, sulphuric, phosphoric, citric and lactic acid.

19. The composition according to any one of aspects 1-17, wherein Step II corresponds to the quaternisation of reaction mixtures of Step I with alkylating agent(s), preferably wherein the alkylating agents are one or more selected from methyl chloride, methyl bromide, dimethyl sulphate, diethyl sulphate and dimethyl carbonate.

20. The composition according to any one of the preceding aspects, wherein the polyol a.2 is one or more selected from trimethylolpropane (TMP), glycerine, sorbitol and neopentyl glycol (NPG), each of which can be optionally alkoxyated, preferably ethoxyated; wherein the polyol a.2 is more preferably trimethylolpropane (TMP), or is absent.

21. The composition according to any one of the preceding aspects, wherein the mixture of cationic surfactants further comprises an organic solvent, preferably an alcohol, more preferably ethanol, n-propanol or isopropanol, butanols, glycol, propane or butanediol, glycerol, diglycol, propyl or butyl diglycol, ethylene glycol methyl ether, ethylene glycol ethyl ether, ethylene glycol propyl ether, ethylene glycol mono-n-butyl ether, diethylene glycol methyl ether, diethylene glycol ethyl ether, propylene glycol methyl, ethyl or propyl ether, dipropylene glycol methyl or ethyl ether, methoxy, ethoxy or butoxy triglycol, 1-butoxyethoxy-2-propanol, 3-methyl-3-methoxybutanol, or propylene glycol t-butyl ether.

22. The composition according to aspect 21, wherein the mixture of cationic surfactants has a content of organic solvent of 0-30%, preferably 0-20%, more preferably 10-20% by weight.

23. The composition according to any one of the preceding aspects, wherein the mixture of cationic surfactants is essentially water-free.

24. The composition according to any one of the preceding aspects, wherein the mixture of cationic surfactants essentially consists of the reaction products of steps I and II, and optionally an organic solvent.

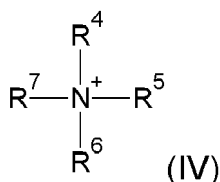
25. The composition according to any one of the preceding aspects, wherein the mixture of cationic surfactants consists of the reaction products of steps I and II and solvent, if any, and unreacted starting materials as well as inevitable impurities from the production process, if any.

26. The composition according to any one of the preceding aspects, wherein the biocidal component comprises one or more cationic biocidal agents.

27. The composition according to aspect 26, wherein the biocidal component comprises or consists of a mixture of cationic biocidal agents, wherein at least one is a quaternary ammonium compound.

28. The composition according to any one of the preceding aspects 26-27, wherein the biocidal component comprises or consists of a mixture of two quaternary ammonium compounds as biocidal agents.

29. The composition according to any one of the preceding aspects 26-28, wherein the biocidal agent is a quaternary ammonium compound is of formula (IV):



wherein R⁴ to R⁷ are the same or different, each independently being selected from the group consisting of: a (C₁-C₂₀)

straight or branched alkyl chain, (C₃-C₂₀)cycloalkyl optionally substituted with a straight or branched alkyl having from 1 to 6 carbon atoms, (C₆-C₂₀)aryl optionally substituted with a straight or branched alkyl having from 1 to 6 carbon atoms, and benzyl; and X⁻ is an anionic counterion.

30. The composition according to aspect 29, wherein two or three of R⁴, R⁵, R⁶ and R⁷ are methyl, and the other(s) are selected from the group consisting of (C₁-C₂₀) straight or branched alkyl chain, and benzyl.

31. The composition according to any one of the preceding aspects 29-30, wherein the anionic counterion is halide, particularly chloride.

32. The composition according to any of the aspects 29-34, wherein the biocidal component comprises one or more quaternary ammonium biocide compounds selected from (C₈-C₁₈)alkyldimethylbenzylammonium chloride or (C₈-C₁₈)dialkyldimethylammonium chloride; particularly the biocidal component consists of a mixture of two compounds selected from (C₈-C₁₈)alkyldimethylbenzylammonium chloride or (C₈-C₁₈)dialkyldimethylammonium chloride.

33. The composition according to any of the preceding aspects, wherein the weight ratio between the mixture of cationic surfactants and the one or more biocidal agent(s) is from 1:1 to 5:1, more particularly from 2:1 to 4:1.

34. The composition according to any one of the preceding aspects, wherein the mixture of cationic surfactants is at a % by weight, with respect to the total weight of the composition, from 0.5 to 20%, particularly from 0.5 to 3 or from 3 to 15%.

35. The composition according to any one of the preceding aspects, wherein the biocidal component is at a % by weight, with respect to the total weight of the composition, from 0.5 to 5, particularly from 1 to 4%.

36. The composition according to any one of the preceding aspects, wherein the biocidal component (ii) comprises at least a dialkyldimethylammonium chloride compound and is at a weight, with respect to the total weight of the composition, from 0.5 to 5%, particularly from 1 to 4%.

37. The composition according to any one of the preceding aspects, wherein the biocidal component (ii) comprises at least an alkyldimethylbenzylammonium compound, and is at a weight, with respect to the total weight of the composition, from 0.5 to 5%, particularly from 0.5 to 3%.

38. The composition according to any one of the preceding aspects, wherein the biocidal component (ii) comprises at least a dialkyldimethylammonium chloride compound and at least an alkyldimethylbenzylammonium compound, wherein the sum of dialkyldimethylammonium chloride and alkyldimethylbenzylammonium compound is at a weight, with respect to the total weight of the composition from 0.5 to 5, particularly from 1 to 4%.

39. The composition according to any one of the preceding aspects, wherein the biocidal component (ii) comprising at least a dialkyldimethylammonium chloride compound and at least an alkyldimethylbenzylammonium compound, wherein the content of dialkyldimethylammonium compound is from 0.5 to 2%, preferably from 0.5 to 1.5%; and wherein the content of alkyldimethylbenzylammonium compound is at a weight, with respect to the total weight of the composition from 0.5 to 3.5%, preferably from 1.5 to 3% wt.

40. The composition according to any one of the preceding aspects, further comprising water, preferably wherein the water content is from 80 to 98%.

41. The composition according to any one of the preceding aspects, which is optically transparent at room temperature, and preferably at temperatures of 10-45°C, 15-35°C or 20-30 °C.

42. The composition according to any one of the preceding aspects, wherein the composition comprises the following:

- (i) the mixture of cationic surfactants, as defined herein, at a % by weight from 0.5 to 15 % w/w, particularly from 0.5 to 3 or from 3 to 15% w/w,
- (ii) the one or more biocidal agent(s) at a % by weight from 0.5 to 5 %, particularly from 1 to 4% w/w, and
- (iii) optionally the one or more ingredients selected from the group consisting of:

non-ionic surfactants at a % by weight from 0 to 5% w/w;
 thickeners at a % by weight from 0 to 1% w/w;
 chelating agents at a % by weight from 0 to 5% w/w; and
 perfume is at a % by weight from 0 to 2% w/w, all the percentages being expressed with respect to the total weight of the composition.

43. The composition according to aspect 42, wherein the non-ionic surfactant(s) are selected from fatty acids, linear or branched, alkoxylated or non-alkoxylated esters of fatty acids, especially those containing from 8 to 18 carbon atoms, alkoxylated or non-alkoxylated Guerbet alcohols, optionally alkoxylated glycerol and polyglycerol esters, xylitol esters, alkoxylated or non-alkoxylated sorbitan esters, esters of sugars, such as glucose, fructose, galactose, mannose, xylose, arabinose, ribose, 2-deoxyribose and sucrose, C₈₋₁₈ fatty alcohols, alkyl polyglucosides, non-ionic surfactants with amide groups derived from amines, such as glucamine, and the derivatives of methylethanolamine, diethanolamine, isopropanolamine and monoethanolamine, with linear or branched fatty acids, especially those containing from 8 to 18 carbon atoms, waxes, such as paraffins, microcrystalline waxes derived from petroleum, and synthetic waxes, and pentaerythritol esters, especially having a tallow, hydrogenated tallow, palm, behenic or oleic chain, preferably non-ionic surfactants are selected from glycerine esters that are ethoxylated, sorbitan monoesters and pentaerythritol esters, especially those having a tallow, hydrogenated tallow, palm, behenic or oleic chain.

44. The composition according to any one of the preceding aspects, characterised in having a viscosity at 20 °C of 2 to 500 cps, as measured on a Brookfield LVT viscometer with spindle 2 at 60.

45. The composition according to any one of the preceding aspects, which is a sprayable composition.

46. A process for preparing a composition as defined in any one of the preceding aspects, which comprises mixing: the mixture of cationic surfactants, the biocidal component, , and, optionally, the one or more the ingredients as defined in any of the previous aspects.

47. A process as defined in aspect 43, further comprising mixing: the mixture of cationic surfactants, the biocidal component, water, and, optionally, the one or more ingredients as defined in any of the previous aspects.

48. Use of the composition as defined in any of the preceding aspects 1-48, for softening and/or sanitizing fabrics

49. A method for softening and/or sanitizing textiles of fabrics, the method comprising the step of:

- (a1) contacting one or more fabric articles with the composition of the invention at one or more points during the laundering process, or, alternatively,
- (a2) when the composition is in the form of a sprayable form, the method comprises spraying (dispensing) the composition directly on the fabric.

[0095] As used herein, "clear" or "optically transparent" appearance of a mixture/composition/formulation refers to essentially complete optical transmittance, e.g., preferably $\geq 90\%$, more preferably $\geq 95\%$, even more preferably $\geq 98\%$, most preferably $\geq 99\%$. Preferably, and unless specified otherwise, the optical transmittance of such mixture/composition/formulation is measured at $\lambda = 600$ nm (1 cm thickness, 20 °C).

[0096] As used herein, in cases where a ratio (e.g., molar ratio) "x/y" between compound(s) within a first definition "x" and compound(s) under a second definition "y" is 0, this means that compounds within the first definition "x" are absent or essentially absent.

[0097] As used herein, and unless specified otherwise, "stable" or "stable upon storage" refer to compositions comprising the cationic surfactant mixture according to the present invention which maintain essentially complete optical transmittance and single-phase appearance, as described above immediately after their preparation and after storage. Preferably, the compositions are stable over at least 7 days at 20 °C; over at least 14 d at 20 °C; over at least 28 days at 20 °C; or over at least 28 days at 40 °C.

[0098] As used herein, viscosity is measured on a Brookfield LVT viscometer at 20 °C with a spindle 2 at 30 or 60 rpm (preferably: for low viscosities), or with a spindle 4 at 12 rpm (preferably: for high viscosities).

[0099] As used herein, "iodine number" (or "iodine value", IV) describes the degree of unsaturation, e.g., of a fatty acid, and can be determined according to EN 14111:2003.

[0100] As used herein, "room temperature (RT)" is understood as a temperature from 10 to 40°C, preferably from 20 to 40°C.

EXAMPLES**Example 1: preparation of the mixture of cationic surfactants****Synthetic procedure**(i) Esterification:

[0101] 115.1 grams (0.42 mol) of tallow fatty acid and 202.9 grams (1.39 mol) of Adipic acid were introduced in an inert atmosphere into a glass reactor. Then, 292.3 g (1.96 mol) of triethanolamine, together with 65.8 grams of Trimethylolpropane (0.49 mol) were introduced, which were added with stirring. The mixture was heated for at least 4 hours at 160-180°C in order to remove water from the reaction. The final point of the reaction is monitored by an acid value assay until the value was below 2 mg KOH/g.

[0102] A yellowish liquid product from the esterification was obtained, consisting essentially of a mixture of unesterified fatty acids and adipic acid, mono-, di- and triesterified triethanolamine with fatty acids, mono-, di- and triesterified triethanolamine with adipic acid or a combination thereof, mono-, di- and triesterified trimethylolpropane with fatty acids, mono-, di- and triesterified trimethylolpropane with adipic acid or a combination thereof, together with unreacted triethanolamine and trimethylolpropane.

(ii) Quaternisation:

[0103] 611.5 grams of the product from esterification step (containing 1.94 mol of amine equivalent product) are mixed with 149.0 g of Ethanol (3.23 mol), then, 232.4 grams (1.84 mol) of dimethyl sulphate were added with stirring at a temperature of 50-90 °C.

[0104] After four hours of digestion, the virtually complete absence of amine value was verified by acid/base assay. 992.9 grams of the final product was obtained.

Calculations

[0105] Molar ratio monocarboxylic acid / dicarboxylic acid:

$$0.42 \text{ mol tallow fatty acid} / 1.39 \text{ mol adipic acid} = 0.30$$

[0106] Equivalents ratio COOH / OH:

$$(1 \text{ eq} * 0.42 \text{ mol tallow fatty acid} + 2 \text{ eq} * 1.39 \text{ mol adipic acid}) / (3 \text{ eq} * 1.96 \text{ mol triethanolamine} + 3 \text{ eq} * 0.49 \text{ mol trimethylolpropane}) = 0.44$$

[0107] Molar ratio polyol / triethanolamine:

$$0.49 \text{ mol trimethylolpropane} / 1.96 \text{ mol triethanolamine} = 0.25$$

Example 2: preparation of the biocidal softener compositions of the invention**Formulation 1**

[0108] 91.6 g of distilled water were added at room temperature to a flask. Then, 4 g of the cationic mixture resulting from Example 1 were added on, and provided with proper stirring at room temperature. Mixture was left stirring for 15 minutes. Afterwards 0.75 g of trisodium methylglycinediacetic was added to the mixture under stirring. After 15 minutes, 0.9 g of Benzalkonium chloride and 2.7g of Didecyltrimethylammonium chloride were added to the mixture under stirring.

Formulation 2

[0109] 85.6 g of distilled water were added at room temperature to a flask. Then, 7 g of the cationic mixture were added on, and provided with proper stirring at room temperature. Mixture was left stirring for 15 minutes. Afterwards 0.75 g of

trisodium methylglycinediacetic was added to the mixture under stirring. Then, 3 g of hydrogenated castor oil (40EO) was added under constant stirring. Once incorporated, 0.5g of fragrance was added to the mixture under stirring. After 15 minutes, 0.9 g of Benzalkonium chloride and 2.7g of Didecyltrimethylammonium chloride were added to the mixture under stirring.

Example 3: Preparation of the comparative formulation

Preparation of the mixture of cationic surfactants (comparative process)

Esterification

[0110] 750.0 grams (2.76 mol) of palm fatty acid and 250.0 grams (0.92 mol) of hydrogenated palm fatty acid were introduced in an inert atmosphere into a stainless steel reactor together with 332.0 g (2.23 mol) of triethanolamine, which were added with stirring. The mixture was heated for at least 4 hours at 160-180°C in order to remove water from the reaction. The final point of the reaction is monitored by an acid value assay until the value was below 2 mg KOH/g.

[0111] A yellowish liquid product from the esterification was obtained, comprising a mixture of unesterified fatty acids, mono-, di- and triesterified triethanolamine and unreacted triethanolamine.

Quaternization

[0112] 153.09 grams of isopropyl alcohol were added with stirring to 1140.27 grams of the product from esterification step (containing 2.00 mol of esterified product). Then 237.50 grams (1.88 mol) of dimethyl sulphate were added with stirring at a temperature of 50-90°C. After four hours of digestion, the virtually complete absence of amine value was verified by acid/base assay. 1530.86 grams of the final product were obtained. "

Comparative Formulation

[0113] 91.6 g of distilled water were added at 36°C to a flask. Then, 4 g of the cationic mixture (comparative) were added on, and provided with proper stirring at room temperature. Mixture was left stirring for 15 minutes. Afterwards 0.75 g of trisodium methylglycinediacetic was added to the mixture under stirring. After 15 minutes, 0.9 g of Benzalkonium chloride and 2.7g of Didecyltrimethylammonium chloride were added to the mixture under stirring.

Example 4: tests

[0114] BACTERICIDAL ACTIVITY was determined following UNE-EN 1276:2020.

- Conditions: 5 minutes, 2% dilution, clean conditions, T 20°C, *Pseudomonas aeruginosa* ;
- For norm 1276, there must be at least a reduction of 5 log.

[0115] ANTIFUNGAL ACTIVITY was determined following UNE EN 1650:2020

- Conditions: 15 minutes, 2% dilution, clean conditions, T 20°C, *Candida Albicans*
- For norm 1650 there must be at least a reduction of 4 log for disinfection for general use.

SENSORIAL SOFTNESS

[0116] Softening performance of fabric softener compositions was determined by means of a sensorial test carried out by a panel of experts using pieces of terry cotton towel treated with the corresponding aqueous dispersions of the fabric softener active compositions.

[0117] Fabric treatment consists of a consecutive sequence of washing and softening step, carried out in hard water of 20°HF. Previously scoured terry cotton towels were washed at 40°C with a heavy duty powder detergent (at a dosage of 2.7% on weight fabric), rinsed twice and spinning dried. Wet towels were treated for 10 minutes at 25°C with the corresponding aqueous dispersions diluted in water to provide a dosage of 0.12% fabric softener active composition on weight fabric, for a bath ratio of 1/10. Treated cotton towels were finally spun dried and let dry by hanging, and left still for 24 hours under controlled atmospheric conditions (60%HR and 20°C).

[0118] Softening effect was determined by comparison in pairs, by 12 panelists,. The comparative evaluation was made

according to the following criteria: the softness scale went from 0 to 5, with 0 being not soft (so the higher the number the better).

[0119] Appearance was assessed by visual evaluation.

[0120] Table 1 shows results for appearance, bactericidal activity, fungicidal activity and sensorial softness for prepared formulations:

Table 1

	Comparative	Formulation 1	Formulation 2
Appearance	X	○	○
Bactericidal Activity (1276:2020), logR has to be >5	-	5.6	5.5
Fungicidal Activity (1650:2020), logR should be >4	-	4.1	4.1
Sensorial Softness (0-5)	-	2.5	3.0

[0121] The results show that the cationic mixture (comparative) cannot be mixed with the biocide, since the formula shows phase separation.

[0122] Bactericidal, fungicidal and sensorial softness could not be evaluated as formulation was not stable to perform the evaluation.

[0123] The cationic mixture of the invention is stable and clear when mixed with the biocides, and the combination of the cationic mixture of the invention with the biocide does not affect the final bactericidal and fungicidal activity, while also providing softness to fabrics.

Claims

1. A composition comprising:

(i) a mixture of cationic surfactants; and

(ii) a biocidal component,

the weight of the mixture of cationic surfactants in the composition being equal or higher than the weight of the biocidal component in the composition, and wherein:

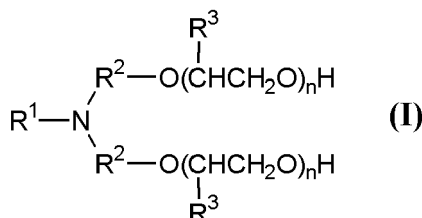
the mixture of cationic surfactants is obtainable by a process comprising the steps:

Step I: esterification of a) with b), and

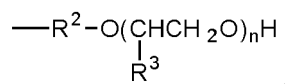
Step II: cation formation from the reaction products of Step I, wherein:

a) is a hydroxyl group-containing compound or a mixture of hydroxyl group-containing compounds comprising a.1 and optionally a.2, wherein:

- a.1 is an alkanolamine or a mixture of alkanolamines of the general formula (I):



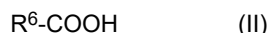
in which R¹ is selected from hydrogen, a C₁-C₆ alkyl group, and the residue



R² is a C₁-C₆ alkylene group, R³ is hydrogen or methyl, n is 0 or an integer from 1 to 20; and
- a.2 is a polyol, which can be optionally alkoxyated, and is **characterized by** a MW in the range
60 to 190 g/mol;

b) is a mixture of compounds containing one or more carboxylic groups comprising b.1 and b.2,
wherein:

- b.1 is a monocarboxylic acid or a mixture of monocarboxylic acids of formula (II):



in which R⁶ is a linear or branched (C₆-C₂₃) alkyl or alkenyl group; or an alkyl ester or glyceride
thereof, preferably a linear or branched (C₆-C₂₃) alkyl or alkenyl ester; and
- b.2 is a dicarboxylic acid or a mixture dicarboxylic acids of the general formula (III), or reactive
derivative(s) thereof:



wherein L is a saturated or unsaturated, linear, branched or cyclic group having 1 to 10 carbon
atoms, each of which carbon atoms is optionally substituted by a (C₁-C₆) saturated or
unsaturated group; and is preferably represented by (CH(R⁷))_m or by (C₆-C₁₀ arylene) option-
ally substituted by one or more R⁷, in which each R⁷ is independently a hydrogen, OH or a
(C₁-C₆) saturated or unsaturated group, m is 0 or an integer from 1 to 10, wherein for m ≥ 2, the
chain (CH)_m optionally contains one or more double bonds and/or cyclic group(s);

wherein a.1), a.2), b.1) and b.2) are introduced in the reaction system of Step I in amounts resulting in the
following molar ratios:

- the molar ratio of monoacid(s)/diacid(s) (b.1/b.2) is 0.10 to 1.0;
- the molar ratio between organic carboxylic groups and organic hydroxyl groups (COOH/OH) present in
the system is 0.30 to 0.80; and
- the molar ratio between the compound(s) within the definition a.2 and the compound/s under definition
a.1 is 0 to 0.5.

2. The composition according to claim 1, wherein the amounts of the compounds a.1, a.2, b.1 and b.2 are introduced in
the reaction system of Step I in amounts that result in the following molar ratios:

- the molar ratio of monoacid(s)/diacid(s) (b.1/b.2) is 0.30 to 1.0;
- the molar ratio between organic carboxylic groups and organic hydroxyl groups (COOH/OH) present in the
system is 0.40 to 0.70, preferably 0.50 to 0.70; and
- the molar ratio between the compound(s) within the definition a.2 and the compound/s under definition a.1 is 0, or
is 0.1 to 0.5.

3. The composition according to claim 1 or 2, wherein:

- A) the alkanolamine(s) of formula (I) is selected from triethanolamine, N-methyldiethanolamine, N-methyldiiso-
propanolamine and triisopropanolamine, each of which is optionally alkoxyated with ethylene oxide or propylene
oxide, and mixtures thereof; and/or
- B) the dicarboxylic acid(s) of formula (III) is selected from succinic, malic, glutaric, adipic, sebacic, pimelic,
suberic, maleic and terephthalic acid, acids obtained by thermal oligomerisation of unsaturated fatty acids, and
mixtures thereof; and/or
- C) the monocarboxylic acid(s) of formula (II) are synthetic fatty acids or are obtained from fats or oils of natural
origin and are optionally hydrogenated, preferably from oils of vegetal origin which are optionally hydrogenated,
preferably wherein the monocarboxylic acids of formula (II) are selected from those which are obtained from

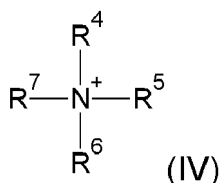
tallow, palm, olive, coconut, sunflower, soya, rapeseed, grape marc and grape, each of which can be hydrogenated, partially hydrogenated, or non-hydrogenated; and/or
D) the compounds corresponding to a.1 and/or a.2 are from natural origin.

4. The composition according to any one of the preceding claims, wherein:

A) Step II corresponds to the formation of the addition salts of the alkanolamine esters obtained from Step I with mineral or organic acids,
preferably wherein the mineral or organic acids are one or more selected from hydrochloric, sulphuric, phosphoric, citric and lactic acid; or
B) Step II corresponds to the quaternisation of reaction mixtures of Step I with alkylating agent(s), preferably wherein the alkylating agents are one or more selected from methyl chloride, methyl bromide, dimethyl sulphate, diethyl sulphate and dimethyl carbonate.

5. The composition according to any one of the preceding claims, wherein the biocidal component comprises one or more cationic biocidal agents; particularly comprises or consists of two cationic biocidal agents, wherein one or both are quaternary ammonium biocide compound (s).

6. The composition according to claim 5, wherein the quaternary ammonium compound is of formula (IV):



wherein R^4 to R^7 are the same or different, each independently being selected from the group consisting of: a C_1 - C_{20} straight or branched alkyl chain, C_3 - C_{20} cycloalkyl optionally substituted with a straight or branched alkyl having from 1 to 6 carbon atoms, C_6 - C_{20} aryl optionally substituted with a straight or branched alkyl having from 1 to 6 carbon atoms, and benzyl; and X^- is an anionic counterion.

7. The composition according to claim 6, wherein two or three of R^4 , R^5 , R^6 and R^7 are methyl; the other(s) are selected from the group consisting of C_1 - C_{20} straight or branched alkyl chain, and benzyl; and the anionic counterion is halide.

8. The composition according to any of the preceding claims 5-7, wherein the biocidal agent(s) are selected from (C_8-C_{18}) alkyldimethylbenzylammonium chloride or (C_8-C_{18}) dialkyldimethylammonium chloride.

9. The composition according to any of the preceding claims 1-8, wherein:

the weight ratio between the mixture of cationic surfactants and the biocidal component is from 1:1 to 5:1, more particularly from 2:1 to 4:1; and/or
the mixture of cationic surfactants is at a % by weight, with respect to the total weight of the composition, from 0.5 to 20% w/w, particularly from 0.5 to 3 or from 3 to 15% w/w; and/or
the biocidal component is at a % by weight, with respect to the total weight of the composition, from 0.5 to 5, particularly from 1 to 4% w/w.

10. The composition according to any one of the preceding claims 1-9, further comprising water, preferably wherein the water content is from 80 to 98%.

11. The composition according to any one of the preceding claims 1-10, further comprising one or more ingredients selected from the group consisting of:

A) a perfume, preferably wherein:

- (i) the perfume consists of one or more substance(s); and/or
- (ii) the average logP of the perfume substance(s) is from 1 to 6; and/or
- (iii) the weight ratio between the cationic surfactant mixture and the perfume is from 99:1 to 80:20;

B) a non-ionic surfactant, the weight ratio between the cationic surfactant mixture and the non-ionic surfactant is from 100:0 to 70:30;

C) a thickener, wherein the weight ratio of the cationic mixture and the thickener is from 100:0 to 10:5, preferably from 100:1 to 10:2; and

D) a chelating agent, wherein the weight ratio of the cationic mixture and the chelating agent is from 100:0 to 75:25.

12. The composition according to any one of the preceding claims 1-11 comprising:

(i) the mixture of cationic surfactants as defined in any one of claims 0.5 to 15, particularly from 0.5 to 3 or from 3 to 15% w/w,

(ii) the biocidal component at a % by weight from 0.5 to 5 w/w%, particularly from 1 to 4% w/w, and

(iii) optionally the one or more ingredients selected from the group consisting of:

non-ionic surfactants at a % by weight from 0 to 5% w/w;

thickeners at a % by weight from 0 to 1% w/w;

chelating agents at a % by weight from 0 to 5% w/w; and

perfume is at a % by weight from 0 to 2% w/w,

all the percentages being expressed with respect to the total weight of the composition.

13. The composition according to any one of the preceding claims 1-12, which is a sprayable composition.

14. Use of the composition as defined in any of the claims 1 to 13, for softening and/or sanitizing fabrics.

15. A method for softening and/or sanitizing textiles of fabrics, the method comprising the step of:

(a1) contacting one or more fabric articles with the composition as defined in any of the claims 1 to 13 during the laundering process, or, alternatively,

(a2) when the composition is in the form of a sprayable form, the method comprises spraying (dispensing) the composition directly on the fabric.



EUROPEAN SEARCH REPORT

Application Number

EP 23 38 3375

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Place of search		Date of completion of the search	Examiner
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