

TITLE OF THE INVENTION

ORAL COMPOSITIONS COMPRISING SILOXANE POLYMERS

CROSS REFERENCE TO RELATED APPLICATION

[0001] This application claims the benefit of United States Provisional Patent Application No. 60/796,384 filed May 1, 2006, the contents of which is incorporated herein by reference.

BACKGROUND OF THE INVENTION

[0002] Dental plaque or plaque biofilm is a soft deposit that forms on teeth and is implicated in the occurrence of gingivitis, periodontitis, caries and other forms of periodontal disease. A plaque biofilm provides a locus for calculus or tartar formation, which is a hard mineralized solid formed on the teeth when crystals of calcium phosphate are deposited in the pellicle and extracellular matrix of the dental plaque biofilm and become crystalline hydroxyapatite. While regular brushing helps to prevent rapid build-up of these deposits, even regular brushing is not sufficient to remove all of the calculus deposits which adhere to the teeth.

[0003] Various antibacterial agents have found to have the clinical ability to retard the growth of bacterial and hence have the ability to minimize plaque formation, oral infections and diseases associated therewith. However, many antibacterial agents are incompatible or unstable with other oral care active ingredients, difficult to deliver *in vivo*, or may inactivate other desirable additional oral care ingredients. Some antibacterial agents are difficult to formulate in oral compositions or are expensive.

[0004] It would be desirable to develop highly efficacious oral compositions that prevent or combat plaque formation, as well as other detrimental oral health implications, by using a stable antiplaque and/or antitartar active agent. Thus, there is a need for an oral care composition that effectively reduces the development or progression of oral disease, preferably by having an active ingredient that functions to diminish the effects of oral disease by preventing or reducing multiple etiological factors that contribute to and/or exacerbate oral disease. Further, there is a need to use

stable oral care actives in an oral composition, so that their functionality and bioavailability as delivered to a subject *in vivo* is preserved and stabilized.

DETAILED DESCRIPTION OF THE INVENTION

[0005] The following description is merely exemplary in nature and is not intended to limit the present disclosure, application, or uses.

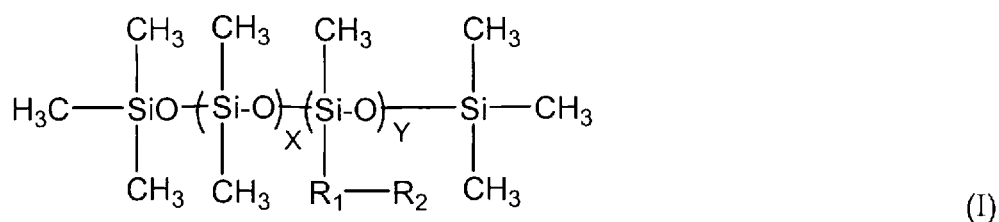
[0006] In various embodiments, oral care compositions are provided with an active ingredient that comprises a siloxane polymer that provides various oral care benefits, such as antiplaque effects and tartar control, among others. A "siloxane polymer" refers to a polymer that has a basic backbone of silicon and oxygen with side constituent groups that may be the same or different, generally described by the structural repeating unit $(-\text{O}-\text{SiRR}')_n$, where R and R' may be the same or different side constituent groups, and n may be any value above 2 designating the repetition of the SRU in the polymer backbone. Siloxane polymers are also known in the art as "silicone" polymers. Siloxane polymers may include polyheterosiloxanes, where side groups and/or structural repeating units may be different entities (having different side constituent groups), such as, for example, the siloxane co-polymer described by the nominal SRU formula, $(-\text{O}-\text{SiRR}')_n - (-\text{O}-\text{Si}-\text{R}''\text{R}''')_m$, wherein R and R' are distinct side groups from R'' and R''' and m is an integer. Further R and R' may be different from one another; likewise the same may be true for R'' and R'''. Such siloxane polymers may terminate in any variety of terminal groups, such as for example, trimethyl silyl $((\text{CH}_3)_3\text{Si})$ terminated siloxane, or ethyl vinyl terminated siloxane. Often, the siloxane polymer is crosslinked, for example, in a hydrosilylation reaction where ethylenically unsaturated groups react with hydride groups.

[0007] Conventional polyorganosiloxane polymers are hydrophobic. However, in accordance with various aspects of the disclosure, the active ingredient comprises a siloxane polymer that has at least one hydrophilic region. In various embodiments, the hydrophilic region comprises one or more hydrophilic moieties, such as alkylene oxides, amines or phosphorus-containing groups. In certain embodiments, the hydrophilic region includes a moiety comprising phosphorus. Exemplary

phosphorus containing moieties include, by way of example, phosphates, phosphonates, phospholipids, and the like, as will be described in more detail below.

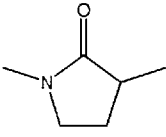
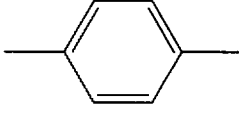
[0008] In certain embodiments, the siloxane polymer comprises has pendent alkyl groups. The siloxane polymer further comprises a phosphorus-containing moiety, for example, a phosphate. In this regard, a suitable siloxane polymer for use as an oral care active ingredient comprises a phosphate and one or more alkyl groups, and is broadly referred to as an alkyl phosphate siloxane polymer. In certain embodiments, the alkyl groups are selected to be methyl groups and the siloxane polymer comprises a polydimethylsiloxane having a phosphate group.

[0009] In certain embodiments, the siloxane polymer comprises a compound according to the nominal general formula (I):



where R₁ is selected from the group consisting of: alkyl, aryl, amide, ester, pyrrolidone, vinyl, acrylate, siloxane, urethane, carbonate, vinyl alcohol, alkylene oxide, and combinations thereof; and R₂ comprises a moiety selected from the group consisting of: phosphate, phosphonate, phospholipids, a phosphate-containing group, and combinations thereof. In certain embodiments, R₁ alkyl and/or aryl groups range from (C₁ - C₅₀), and in some embodiments have lower alkyl/aryl groups, for example having from C₂ - C₁₀, optionally from C₂ - C₆. In certain embodiments, alkylene oxides can range from C₂ - C₄, thus including ethylene oxide, propylene oxide, and butylene oxide, of which multiple groups may be provided. "x" ranges from 0 to 100 and "y" from 1 to 100.

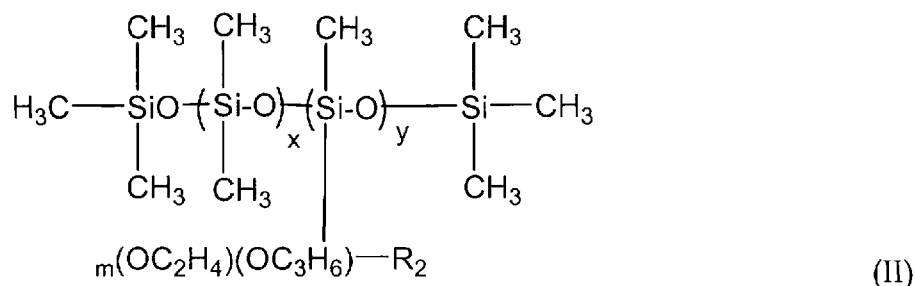
[0010] In certain embodiments, R₁ comprises -(CH₂)_v-(Q)_z, where Q is at least one group selected from: an alkylene oxide having C₂ - C₃, such as C₂H₂O or C₃H₆O;

CH₂CH(OH); CONH, CO₂, NH, CONH,  and , wherein v and z are respectively 1 to 16. For example, R₂ can be selected from PO₃H₂, PO₃K₂, PO₃Na₂, PO₃Li₂ and PO₃(NH₄)₂, from phospholipids, such as phosphatidyl choline, phosphatidic acid, phosphatidyl inositol, phosphatidyl ethanolamine, and the like.

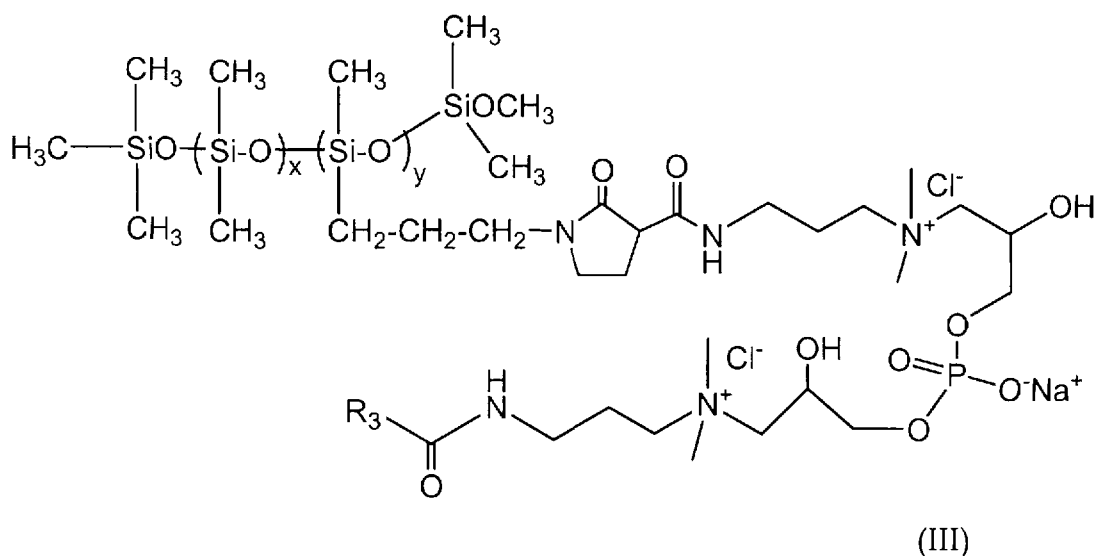
[0011] Suitable siloxane polymers are disclosed in United States Patent Nos. 5,530,084 to Ihara *et al.*; 5,070,171 and 6,175,028 both to O'Lenick; 6,124,490 to Gormley *et al.*; 6,225,489, 5,849,313, and 5,688,496 all to Fost *et al.*; and 5,859,161 to Imperante *et al.* All references cited in the detailed description, including those listed above, are expressly incorporated by reference in their entireties.

[0012] In some embodiments, the siloxane polymer having a phosphate-containing moiety comprises a dimethicone copolyol phosphate of the type disclosed in United States Patent No. 5,070,171. Such siloxane polymers have a pendant phosphate functional group and are prepared by reacting a hydroxyl-containing silicone with a phosphating reagent.

[0013] In certain embodiments, the siloxane polymer comprising a phosphate moiety is a compound having the formula (II):



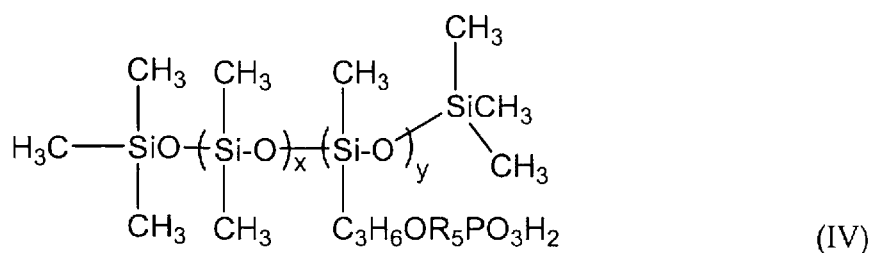
where R₂ is a pendant phosphate group, such as -PO₃H₂ or -(CH₃CH₂H₃O)_nPO₃H₂, "x" is 0 to 100, "y" is 1 to 100, "m" is 0 to 15. In other embodiments, the siloxane polymer comprises at least one phosphate and at least one amine group. An example of a suitable compound of such a siloxane polymer comprising a phospholipid as the phosphorus-containing moiety has the formula (III):



where R₃ is an alkyl group ranging from C₁ to C₅₀, "x" is 0 to 100, "y" is 1 to 100. In some embodiments, R₃ is a C₁₈ alkyl group.

[0014] Non-limiting examples of siloxane polymers comprising a moiety comprising phosphorus suitable for use in oral care and/or personal care compositions include phosphated silicone polymers that are available commercially from Phoenix Chemical of Somerville, New Jersey, United States of America under the trade designations PECOSIL® PS-100 (a dimethicone polyethylene glycol (PEG-7) phosphate), PS-200 (a dimethicone polyethylene glycol (PEG-10) phosphate), WDS-100 (a dimethicone polyethylene glycol/polypropylene glycol (PEG/PPG-7/4) phosphate), WDS-200 dimethicone polyethylene glycol/polypropylene glycol (PEG/PPG-12/4) phosphate), and PECOSIL® PSQ-418 (Steardimonium hydroxypropyl PEG-7 dimethicone).

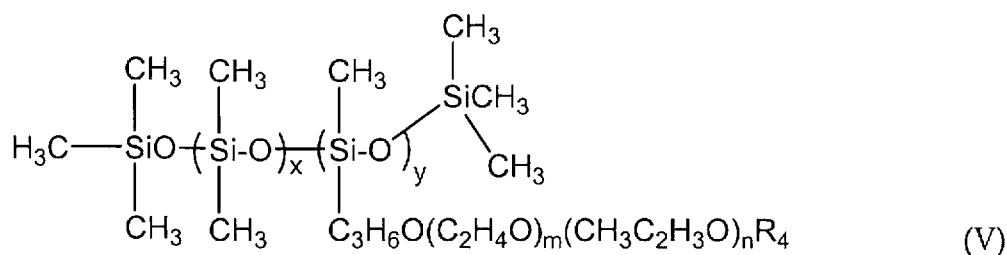
[0015] These commercially available phosphated siloxane polymers generally have the following structural formulas (IV):



where R_5 is $(C_2H_4O)_a$ where "a" varies based on the desired ethylene glycol (PEG) chain length/desired molecular weight; and PECOSIL® WDS-100 and WDS-200 are $(CH_3C_2H_3O)_b(C_2H_4O)_c$ where "b" and "c" vary based on the selected chain length of the propylene glycol (PPG) and ethylene glycol (PEG) respectively. Polymers of this general class have "x" of 0 to 100 and "y" of 1 to 100.

[0016] Another siloxane polymer having a hydrophilic region including a phosphorus-containing moiety useful as active ingredients for oral compositions is linoleamidopropyl PG-dimonium chloride phosphate dimethicone available commercially under the trade name MONASIL™ PLN (also available as ARLASILK™ Phospholipid PLN) from Uniqema Inc., of Wilmington, Delaware, United States of America. This polymer has the structure previously shown in Formula III above, and polymers of this general class include in certain embodiments, R_3 representing C_{18} , "x" from 0 to 100, and "y" from 1 to 100.

[0017] In some embodiments, the hydrophilic region of the siloxane polymer comprises one or more hydrophilic groups, such as alkylene oxides and/or amines, where the siloxane polymer comprises a compound having the formula (V):



where R_4 is selected from H or $-\text{PO}_3\text{H}_2$, "x" is 0 to 100, "y" is 1 to 100, and "m" is 0 to 15, and "n" is 0 to 15. For example, a siloxane polymer having R_4 selected to be H is commercially available as DC-190 and is available from the Dow-Corning Company, Midland, Michigan, United States of America. Other suitable siloxane polymers having hydrophilic regions are commercially available under the trade names DC-193 (polyethylene methylpolysiloxane copolymer or PEG-12 dimethicone) and DC-5103

(siloxylated polyether surfactants with ethylene oxide and/or propylene oxide from Dow-Corning Company, Midland, Michigan, United States of America.

[0018] In various embodiments, the siloxane polymers comprising at least one hydrophilic region are believed to function as an antiattachment or antiadhesion agent. While not limiting as to the present invention, antiattachment oral care active ingredients are generally believed to operate by either (or both) of two predominant anti-attachment mechanisms. Biofilms (also referred to as pellicle) are a matrix formed on an oral surface, typically on a hard tissue surface, comprising bacteria (generally about 60-70% of the biomatrix), bacterial extracellular byproducts, proteins, lipids, and glycolipids. The term "oral surface" encompasses hard and soft tissues within the oral cavity. Hard tissues include the teeth, periodontal support, and the like. Soft tissues comprise gums, the tongue, surfaces of the buccal cavity, and the like. The oral compositions of the various embodiments can be used in a mammalian subject, which includes humans and other warm blooded higher level vertebrate animals, such as felines and canines.

[0019] Without being bound by theory, it is believed that early stages of biofilm formation include an initial bacteria layer that attaches to an oral surface, generally believed to be attached by ligands or adhesins on the bacterial cell wall that interact with receptors on an oral surface. It is believed that the bacterial cells attach to the salivary glycoproteins on the oral surface, *e.g.*, enamel. The bacteria appear to form a stronger attachment by generating extracellular glucan polymers to adhere to the oral surface. The bacteria then grow and divide to form a dense layer on the oral surface. After a specific density is reached, it is believed that the bacteria reorganize and begin to form pillars and irregular surface structures. Further, the biofilm matrix is believed to have a complex association of multi-layered and diverse species that form cell clusters attached to the anchoring bacteria of the first layer.

[0020] Without being bound by any particular theory, it is believed that one mechanism by which anti-attachment oral care agents are believed to operate is where the anti-attachment agent interacts with the bacteria itself to disable it from attaching to

the oral surface, likely by interacting with the adhesins, ligands, or other moieties on the surface of the bacteria that would ordinarily facilitate a linkage with a receptor or other moiety on the oral surface.

[0021] Another anti-attachment mechanism is one where agents interact with an oral surface to form a protective layer, such that the bacteria and biofilm components cannot adhere to the oral or tooth surface, thereby preventing an initial anchoring layer from forming on the oral surface. Such an anti-attachment agent may substantially cover an oral surface, and prevent attachment of the bacteria and other components of the biofilm matrix. While not limiting as to any particular mechanism by which the invention operates, it is believed that the siloxane polymer active agents of the various embodiments of the disclosure operate via such a mechanism, coating a tooth surface, altering its surface energy, and inhibiting bacterial attachment.

[0022] Thus, while not wishing to be limited to any particular mechanism it is believed that oral care compositions comprising a siloxane having a hydrophilic region as an active ingredient, *e.g.*, a phosphorus-containing moiety, function via an anti-attachment mechanism that substantially inhibits bacterial attachment to a tooth surface. By “substantially inhibit” it is meant that the biofilm generation or proliferation is impeded; however the extent to which the inhibition occurs depends upon concentration and distribution of the active ingredient as delivered *in vivo* to the oral surface, as well as the amount of biofilm present prior to treatment with the active ingredient. It appears that certain siloxane polymers having hydrophilic regions alter the surface energy of hard tissues, such as enamel (by reducing the surface energy), and in turn, prevent or reduce adherence and attachment of microorganisms that may form a plaque biofilm on the tooth surface. Preferred siloxane polymers have substantivity on the tooth surface, such that they remain attached for a sufficient period of time to effectively prevent or reduce microorganisms’ growth and or adherence to the tooth surface, thereby preventing or reducing biofilm formation.

[0023] In some embodiments, an oral composition comprises an anti-plaque and/or antitartar active ingredient that is a siloxane polymer comprising at least one

hydrophilic region that is believed to be an anti-attachment agent that substantially inhibits bacteria from forming a biofilm on a tooth surface. The hydrophilic region comprises a moiety selected from the group consisting of: alkylene oxides, phosphates, phosphonates, phospholipids, amines, and combinations thereof. Such siloxane polymers include those described above, *inter alia*. The efficacy of the siloxane polymer as delivered in an oral composition is sufficient such that there is no need for an additional antibacterial agent. For example, in certain embodiments, the oral composition is substantially free of lipophilic active ingredients, such as halogenated diphenyl ethers, eucalyptol, thymol, menthol and the like. In this regard, the compositions have high antiplaque efficacy, while requiring fewer active ingredients, which can be costly and complex to formulate. By "substantially free" it is meant that the component or compound is absent to the extent that it cannot be detected or it is still suitable to use the item for its intended purpose (where the absence of the desired characteristic or property is required). In certain embodiments, substantially free means that there is less than about 3% by weight of the non-ionic or lipophilic active ingredients, optionally less than about 2%; optionally less than about 1%, and preferably entirely free of the active ingredient. In certain embodiments, the oral composition consists essentially of an anti-plaque and/or antitartar active ingredient that is a siloxane polymer comprising at least one hydrophilic region.

[0024] Such oral compositions can optionally comprise other active ingredients that are less complex to formulate in an oral composition or provide particular desirable oral care benefits, for example, polyphosphate anticalculus compounds or anticaries agents, as will be discussed in more detail below. In certain embodiments, the oral composition comprises an antiplaque or antitartar agent that consists essentially of a siloxane polymer having at least one hydrophilic region.

[0025] In various embodiments, such an antiattachment effect is obtained at relatively low concentrations. For example, the oral composition comprises an active ingredient having a siloxane polymer having one or more hydrophilic regions that is present in the oral composition at about 0.001 to about 3% by weight, more preferably

between about 0.5 to about 2.5% by weight. In certain embodiments, the oral composition comprises a siloxane polymer having one or more hydrophilic regions at about 1% by weight.

[0026] In accordance with various embodiments, the application of oral compositions having an active ingredient comprising a siloxane polymer with a hydrophilic region, as provided in the various embodiments of the present disclosure, promotes longer and more effective anti-plaque benefits at lower concentrations in comparison with many other antimicrobial ingredients which are washed away in the aqueous oral cavity. Such a reduction in plaque, in turn, provides calculus or tartar control, as well.

[0027] In various embodiments, a highly efficacious antiplaque and anticalculus oral care composition contains the siloxane polymers having a hydrophilic region as the sole antiplaque/antibacterial ingredient. However, in certain embodiments, one or more additional active ingredients may be included in the oral care compositions. Any additional active agents for use with the siloxane polymer should be carefully selected. If added, the additional active ingredients should not react with or detract from the efficacy and bioavailability of the siloxane polymer agents.

[0028] Non-limiting examples of oral care active ingredients for oral compositions, include for example, tooth whitening agents, antimicrobial agents, anti-caries agents, antitartar agents, anti-plaque agents, anti-adhesion agents, desensitizing agents, anti-inflammatory agents, malodor control agents, flavoring agents, coloring agents, anti-aging agents, salivary stimulants, periodontal actives, conditioning agents, moisturizing agents, including emollients, occlusive reagents and humectants, natural extracts and essential oils, nutrients, enzymes, proteins, amino acids, vitamins, analgesics, antibiotics, and mixtures thereof. Exemplary oral care actives among those useful herein are disclosed in United States Patent Nos. 4,894,220 to Nabi *et al.*, 5,288,480 and 5,776,435, both to Gaffar *et al.*, 5,681,548 to Esposito *et al.*, 5,912,274 and 5,723,500 both to Stringer *et al.*, 6,290,933 to Durga *et al.*, and 6,685,921 to Lawlor, as well as in United States Patent Application Publication No. 2003/0206874 to Doyle *et al.* Further,

a wide variety of suitable active ingredients for both oral and personal care compositions are listed in Gottschalk *et al.* eds., International Cosmetic Ingredient Dictionary and Handbook, Tenth Edition, Volume 3 (2004). Such active ingredients are well known to one of skill in the art.

[0029] Mixtures of additional oral care active ingredients, even within the same classification, are contemplated by the present disclosure. In various embodiments, the additional active ingredients comprise from about 0.0001% to about 10%, preferably from about 0.001% to about 5%, more preferably from about 0.01% to about 3% by weight of the oral composition, depending on the concentration of the active compounds and form of the oral composition.

[0030] In various embodiments, it is preferred that the additional active ingredients are non-lipophilic or non-ionic. However, for certain embodiments, a non-ionic antibacterial agent is optionally included in oral compositions, and may include phenolic and/or bisphenolic compounds, such as, halogenated diphenyl ethers, including triclosan (2,4,4'-trichloro-2'-hydroxy-diphenylether, triclocarban (3,4,4-trichlorocarbanilide), 2-phenoxyethanol, benzoate esters, carbanilides, phenols, thymol, eugenol, hexyl resorcinol and 2,2'-methylene bis (4-chloro-6-bromophenol).

[0031] The active ingredient may also optionally comprise a cationic active ingredient. In certain embodiments, the siloxane polymer comprises an anionic group or moiety and it is desirable to avoid strongly cationic active ingredients, because such anionic compounds can bind to the cationic active ingredient potentially reducing its bioavailability. In such embodiments, the oral composition containing an anionic siloxane polymer, such as an anionic siloxane polymer having a pendant phosphorus-containing moiety, is substantially free of cationic active ingredients.

[0032] However, in other embodiments, cationic active ingredients can be suitable for use in oral compositions, particularly when the siloxane polymer is only mildly anionic or the cationic active is only slightly cationic. In various embodiments, suitable cationic actives include, for example, quaternary ammonium compounds, such as, benzalkonium chloride and benzethonium chloride; pyridinium and isoquinolinium

compounds, including hexadecylpyridinium chloride; pyrimidine derivatives such as hexetidine; amidine derivatives such as hexamidine isethionate; bispyridine derivatives such as octenidine. Other cationic actives include guanides, such as bis-biguanides include chlorhexidine and alexidine. Other optional active ingredients that are cationic compounds include N^{α} -acyl amino acid alkyl esters and salts, including ethyl lauroyl arginine ester hydrochloride (ELAH).

[0033] In some embodiments, the additional active ingredient comprises an oral care active that is a biofilm disruption agent. A biofilm disruption agent is generally a compound that prevents formation of and/or attacks a biofilm (or pellicle) already formed on an oral surface and includes enzymes that can hydrolyze proteins, starch and lipids, which form a part of a biofilm matrix. In certain embodiments, such active ingredients are enzymes, including by way of example, protease enzymes, such as cysteine proteases or serine proteases. Examples are most desirably selected from the group: papain (for example, isolated from the latex of the green fruit and leaves of *Carica papaya*), ficin (for example, isolated from the latex of tropical fig trees *Ficus glabrata*), krillase (for example, isolated from Antarctic krill), other cysteine and serine proteases, glucoamylase, dextranase, mutanase, lysozyme, plant lipase, gastric lipase, pancreatic lipase, tannase, bromelain, chymotrypsin, alcalase, amalysecs, lactoferrin, gingipains, glucose oxidase, elastases and/or cellulases pectinase, and mixtures thereof. Other exemplary biofilm disruption agents for the oral cavity include synthetic histatin, furanone, derivatives of furanone, and mixtures of any of the above.

[0034] Other useful oral active ingredients include fluoride ion sources, preferably present in an amount sufficient to supply about 25 ppm to about 5,000 ppm of fluoride ions, such as sodium fluoride, potassium fluoride, sodium fluorosilicate, ammonium fluorosilicate, sodium monfluorophosphate (MFP), and amine fluorides, including olaflur (N' -octadecyltrimethylendiamine- $\text{N},\text{N},\text{N}'$ -tris(2-ethanol)-dihydrofluoride). Actives can also include stannous and/or zinc ion sources. Suitable stannous ion sources include without limitation stannous fluoride, other stannous halides such as stannous chloride dihydrate, stannous pyrophosphate, organic stannous

carboxylate salts such as stannous formate, acetate, gluconate, lactate, tartrate, oxalate, malonate and citrate, stannous ethylene glyoxide and the like. Zinc ion sources, such as zinc acetate, zinc chlorite, zinc citrate, zinc gluconate, zinc glycinate, zinc oxide, zinc sulfate, sodium zinc citrate and the like are also suitable for use in oral compositions.

[0035] Certain types of useful anticalculus active ingredients are linear molecularly dehydrated polyphosphate salts. Polyphosphate salts are generally employed in the form of their wholly or partially neutralized water soluble alkali metal (*e.g.*, potassium, sodium or ammonium salts, and any mixtures thereof). Thus, linear molecularly dehydrated polyphosphate compounds useful as antitartar agents include those such as sodium tripolyphosphate, sodium hexametaphosphate pyrophosphate, dialkali or tetraalkali metal pyrophosphate salts such as $\text{Na}_4\text{P}_2\text{O}_7$, $\text{K}_4\text{P}_2\text{O}_7$, $\text{Na}_2\text{K}_2\text{P}_2\text{O}_7$, $\text{Na}_2\text{H}_2\text{P}_2\text{O}_7$ and $\text{K}_2\text{H}_2\text{P}_2\text{O}_7$, and cyclic phosphates such as sodium tripolyphosphate sodium trimetaphosphate, or mixtures thereof. In various embodiments, such active ingredients are present at concentrations from about 0.001 to about 10%, more preferably between about 1 to about 5% of the composition. Polyphosphates may also be used, for example, as active ingredients in home care and cleansing compositions, as will be discussed in more detail below.

[0036] Synthetic anionic linear polycarboxylates are also well known as efficacy enhancing agents for certain active ingredients, in particular for enhancing efficacy of oral care ingredients, including antibacterial, antitartar or other active agents within the composition. Further, such compounds may also be used to form films, as described below. Such anionic polycarboxylates are generally employed in the form of their free acids, or preferably partially neutralized or more preferably fully neutralized water soluble alkali metal (*e.g.*, potassium and preferably sodium) or ammonium salts. Preferred copolymers are 1:4 to 4:1 copolymers of maleic anhydride or acid with another polymerizable ethylenically unsaturated monomer, preferably methyl vinyl ether (methoxyethylene) having a molecular weight (M.W.) of about 30,000 to about 5,000,000. One preferable copolymer is methylvinylether/maleic anhydride. Examples of these copolymers are available from ISP Corporation, Wayne, New Jersey, United

States of America, under the trade name GANTREZ®, *e.g.*, AN 139 (M.W. 1,100,000), AN 119 (M.W. 200,000); S-97 Pharmaceutical Grade (M.W. 1,500,000), AN 169 (M.W. 2,000,000), and AN 179 (M.W. 2,400,000); wherein the preferred copolymer is S-97 Pharmaceutical Grade (M.W. 1,500,000). In various embodiments where a synthetic anionic polycarboxylate is included in the composition, it is preferably present from about 0.001% to about 5% weight

[0037] Saliva stimulating agents are other conventional active ingredients and include food acids such as citric, lactic, maleic, succinic, ascorbic, adipic, fumaric and tartaric acids, and mixtures thereof. H₂ histamine receptor antagonists are other useful active ingredients. H₂ antagonists useful herein include cimetidine, etintidine, ranitidine, ICIA-5165, tiotidine, ORF-17578, lupitidine, donetidine, famotidine, roxatidine, pifatidine, lamtidine, BL-6548, BMY-25271, zaltidine, nizatidine, mifentidine, BMY-52368, SKF-94482, BL-6341A, ICI-162846, ramixotidine, Wy-45727, SR-58042, BMY-25405, loxidine, DA-4634, bisfentidine, sufotidine, ebrotidine, HE-30-256, D-16637, FRG-8813, FRG-8701, impromidine, L-643728, HB-408.4, and mixtures thereof. Desensitizing agents useful herein include potassium citrate, potassium chloride, potassium tartrate, potassium bicarbonate, potassium oxalate, potassium nitrate, strontium salts, and mixtures thereof.

[0038] The oral compositions of the present invention can optionally comprise other anti-plaque/plaque disrupting agents in addition to those set forth above, including without limitation: copper, magnesium, and strontium ion sources, typically provided in salt form; dimethicone copolyols such as cetyl dimethicone copolyol; urea; calcium lactate; calcium glycerophosphate; strontium polyacrylates; and mixtures thereof.

[0039] In certain embodiments, the active ingredient is an anti-inflammatory agent. Certain useful anti-inflammatory compounds include flavonoids, flavans, parthenolides, such as sesquiterpene lactone parthenolides, androstenediol (AED) and dehydroepiandrosterone (DHEA). Other useful anti-inflammatory agents are non-steroidal anti-inflammatory drugs (NSAIDs). Examples of useful NSAIDs include

indomethacin, flurbiprofen, ketoprofen, ibuprofen, naproxen, meclofenamic acid, and mixtures thereof. Other suitable anti-inflammatory agents useful for oral care active agents include oregano extract (for example, extracts from *Origanum vulgare* (commonly known as "oregano", "wild oregano", or "wild marjoram")) as disclosed in United States Patent Application Serial No. 11/256,788 to Worrell *et al.*, filed October 24, 2005, or magnolia extract, derived from plants in the *Magnoliaceae* family, such as *Magnolia Officinalis* as described in United States Patent Application Serial No. 11/285,809 to Gaffar *et al.*, filed November 23, 2005. Alternatively or in addition, a local or systemic analgesic such as aspirin, codeine, acetaminophen, sodium salicylate or triethanolamine salicylate can be used.

[0040] Further, a suitable anti-inflammatory active ingredient safe for oral care compositions comprises a combination of at least one flavonoid and at least one flavan, such an example is UNIVESTIN®, which is manufactured and sold by Unigen Pharmaceuticals, Inc., Superior, Colorado, United States of America. A full description of UNIVESTIN® can be found in United States Patent Application Publication No. 2003/0216481 to Jia.

[0041] Exemplary antioxidants useful as active ingredients include butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT), vitamin A, carotenoids, tocopherols (vitamin E), flavonoids, polyphenols, ascorbic acid (vitamin C), herbal antioxidants, chlorophyll, melatonin, chloride, calcium, calcium oxide, calcium chloride, disodium ubiquinone (coenzyme Q₁₀), ethylhexyl gallate, hydrogen peroxide (also useful as a whitening agent), iodine, lycopene, magnesium ascorbate, potassium sulfite, sodium bisulfite, thiolactic acid, and mixtures thereof. These active ingredients are also used in personal care and cleansing compositions.

[0042] In certain embodiments, the compositions comprise active ingredients that are antibiotics, such as augmentin, amoxicillin, tetracycline, doxycycline, minocycline, metronidazole, neomycin, kanamycin and clindamycin; and mixtures thereof.

[0043] Suitable nutrients include vitamins, minerals, amino acids, and mixtures

thereof. Vitamins include Vitamins C and D, thiamine, riboflavin, calcium pantothenate, niacin, folic acid, nicotinamide, pyridoxine, cyanocobalamin, para-aminobenzoic acid, bioflavonoids, and mixtures thereof. Nutritional supplements include amino acids (such as L-tryptophan, L-lysine, methionine, threonine, levocarnitine and L-carnitine), lipotropics (such as choline, inositol, betaine, and linoleic acid), fish oil (including components thereof such as omega-3 (N-3) polyunsaturated fatty acids, eicosapentaenoic acid and docosahexaenoic acid), and mixtures thereof.

[0044] The oral compositions are preferably provided in an orally acceptable carrier or vehicle. The carrier can be a liquid, semi-solid, or solid phase, in the form of a mouth rinse, dentifrice (including toothpastes, toothpowders, and prophylaxis pastes), confectionaries (including lozenges, and gum), medicament, film, or any other form known to one of skill in the art. Selection of specific carrier components is dependant on the desired product form.

[0045] By way of example, the compositions comprising the siloxane active material can be provided in an oral care composition, which can be in the form of a dentifrice, such as toothpastes, toothpowders, and prophylaxis pastes, confectionaries, including gums, beads and chews, films, paint-on products, professional polishing formulations or any other form known to one of skill in the art.

[0046] In various embodiments, an orally acceptable dentifrice carrier used to prepare an oral composition comprises a water-phase. Conventional ingredients that can be used to form the carriers listed above are well known to the skilled artisan. As recognized by one of skill in the art, the oral compositions optionally include other materials in addition to those components previously described, including for example, surface active agents, such as surfactants, emulsifiers, and foam modulators, viscosity modifiers and thickeners, humectants, diluents, pH modifying agents, emollients, moisturizers, mouth feel agents, sweetening agents, flavor agents, colorants, preservatives, solvents, such as water and combinations thereof. It is understood that while general attributes of each of the above categories of materials may differ; there may be some common attributes and any given material may serve multiple purposes

within two or more of such categories of materials. Preferably, such carrier materials are selected for compatibility and stability with all of the constituents of the active ingredient, including siloxane polymer and any additional active compounds selected for the oral composition.

[0047] Typical useful surface active agents are disclosed in the patent references referenced and discussed above, including in United States Patent No. 4,894,220 and United States Patent Application No. 11/256,788 to Worrell. Surface active agents generally are an important aspect of the oral composition, as they can function as surfactants, emulsifiers foam modulators, and/or active ingredient dispersion agents. For example, in embodiments where the oral composition has an active ingredient comprising an anionic active ingredient, it is preferred that the carrier comprises surfactants that are not strongly cationic, as such anionic compounds can bind to the cationic active ingredient potentially reducing its bioavailability. Depending on the chemical composition of the siloxane polymer (for example, the identity of the R₁ and R₂ groups identified in Formula I above), the siloxane polymer may have anionic portions or characteristics. Thus, where the siloxane polymer has an anionic character in certain embodiments, it is preferred that the carrier is substantially free of non-compatible surfactants, such as strongly cationic surfactants.

[0048] Generally, suitable surface active agents for oral carriers are those which are reasonably stable and foam throughout a wide pH range. These compounds are well known in the art, and include non-soap anionic (*e.g.*, sodium lauryl sulfate (SLS), N-myristoyl, and N-palmitoyl sarcosine), nonionic (*e.g.*, Polysorbate 20 (polyoxyethylene 20 sorbitan monolaurate, TWEEN® 20) and Polysorbate 80 (polyoxyethylene 20 sorbitan mono-oleate, TWEEN® 80), Poloxamer 407, available under the trade name PLURONIC® F127 from BASF Corporation, Florham Park, New Jersey, United States of America, cationic, zwitterionic (*e.g.*, cocoamidopropyl betaine and lauramido propyl betaine), and amphoteric organic synthetic detergents. In embodiments where the active ingredient comprises an anionic compound, the surface active agent is preferably selected from the group consisting of: non-ionic surfactants,

anionic surfactants, amphoteric surfactants and mixtures thereof. In certain embodiments, one or more surface active agents are present in the oral composition in the range from about 0.001% to about 5%, preferably from about 0.5% to about 2.5%.

[0049] Any suitable flavoring or sweetening material may also be employed. Examples of suitable flavoring constituents are flavoring oils, *e.g.* oil of spearmint, peppermint, wintergreen, sassafras, clove, sage, eucalyptus, marjoram, cinnamon, lemon, lime, orange, grapefruit, and methyl salicylate. Also useful are such chemicals as menthol, carvone, and anethole. Suitable sweetening agents include sucrose, lactose, maltose, sorbitol, xylitol, sodium cyclamate, perillartine, AMP (aspartyl phenyl alanine, methyl ester), saccharine and the like. As discussed above, in certain embodiments, the oral compositions are substantially free of lipophilic agents, such as lipophilic flavorants. However, in certain embodiments, the flavor and sweetening agents may each or together be incorporated into the oral composition at a concentration of about 0.05 to about 5% and preferably about 0.5 to about 1.5%.

[0050] In embodiments where the oral composition is in the form of a mouthrinse an exemplary carrier is substantially liquid. The term "mouth rinse" includes mouth washes, sprays, rinses, and the like. In such a preparation, the orally acceptable carrier typically has an aqueous phase comprising either water, or a water and alcohol mixture. Further, in various embodiments, the oral carrier typically has a humectant, surfactant, and a pH buffering agent.

[0051] In embodiments where the oral composition is in the form of a confectionary, an exemplary carrier is substantially solid or semi-solid. Confectionary carriers are well known in the art. For a lozenge, the carrier typically comprises a lozenge base material (for example, comprising a non-cariogenic polyol and/or starch/sugar derivative), an emulsifier, a lubricant, a flavoring agent, a thickener, and optionally, a coating material. Chewing gum carriers generally have a chewing gum base, one or more plasticizing agents, a sweetening agent, and a flavoring agent.

[0052] In embodiments where the oral composition is in the form of a film, an exemplary carrier is substantially solid or semi-solid. Generally, such film carriers

comprise a water soluble or dispersible film forming agent, such as a hydrophilic polymer. Optionally, the film carrier may also comprise hydrophobic film forming polymers, either as a removable backing layer, or mixed with a hydrophilic film forming polymer. Film carriers optionally comprise plasticizers, surface active agents, fillers, bulking agents, and viscosity modifying agents.

[0053] In embodiments where an oral composition is in the form of a dentifrice, an exemplary carrier is substantially semi-solid or a solid. Dentifrices typically contain surface active agents, humectants, viscosity modifying agents and/or thickeners, abrasives, solvents, such as water, flavoring agents, and sweetening agents.

[0054] In various embodiments, an oral composition may be provided within a single component or phase. In other embodiments, the oral composition includes both a first and a second component that are separately maintained. Maintaining the components separately requires only that the components are maintained in such a way as to substantially prevent the interaction of one component of the oral composition with another component of the oral composition. Typically, a dual component oral composition is employed where there are one or more incompatible ingredients included in the oral composition. For example, if the active ingredient comprises a siloxane polymer ingredient that has an anionic nature, it is advantageous to separately maintain cationic compounds from strongly anionic components. The separation of components can be accomplished through any means known or to be discovered in the art and includes chemical, physical, and mechanical means of separation of any combination of these. For example, the first and second components may be combined but certain components are separately maintained by wrapping or encapsulating one or both in a film, coating, capsule, micelle, and the like.

[0055] Thus, any of the various embodiments of the oral care composition described above are contacted with or applied regularly to an oral surface, preferably at least one time a day, more preferably on multiple days in a week, and most preferably on a long-term daily basis.

[0056] The oral compositions may be prepared by suitably admixing the various ingredients. For instance, in the preparation of a mouthrinse, the siloxane polymer is dispersed in an aqueous solvent and/or alcohol and then added to a mixture of humectants, surfactants, and water. The resulting rinse product is then packaged.

[0057] Dentifrices are typically prepared by adding various salts (including fluoride salts, when included in the composition), and sweeteners (*e.g.*, saccharin), and any water-soluble oral care active ingredient compounds to water, where it is mixed. Into another container, all humectants, gums, and polymers, including the siloxane polymer ingredient, are added together. The water based mixture described above is added to the container with the humectants, gums, and polymers. The combined ingredients are optionally heated to a temperature of greater than about 40°C, for example from about 60°C to about 70°C, to disperse the gums and polymers. The heated mixture is then cooled to less than approximately 38°C (about 100°F). The mixture is then combined with abrasives, where it is mixed at high speed under a vacuum for about 15 to about 20 minutes. Any flavor oil and any lipophilic oral care active ingredients are admixed. This mixture is admixed to the water based mixture above, where it is mixed under high speed and vacuum until sufficiently dispersed. The surfactant(s) are added and the mixture is again mixed to disperse. The siloxane polymer may optionally be added with the surfactants, rather than into the polymer phase.

[0058] The oral composition can be incorporated into confectionary and tropes. Such methods of forming confectionary (*e.g.*, gum) or tropes (*e.g.*, lozenges) are well known by one of skill in the art, and can be prepared by stirring the other oral care active compound(s) into a warm gum base or coating the outer surface of a gum base (for example, jelutone, rubber latex, vinylite resins, *inter alia*), desirably with conventional plasticizers or softeners, sugar or other sweeteners or carbohydrates such as glucose, sorbitol and the like. Preferably, the siloxane polymer is added to the gum base.

[0059] Where the oral composition is in the form of a film, it can be formed by any number of conventional film forming processes, such as conventional extrusion or solvent casting processes. For example, to prepare a film by solvent casting, a film forming polymer is dissolved in a sufficient amount of a solvent which is compatible with the polymer. After a solution has been formed, a plasticizer can be added with stirring, and heat can be applied, if necessary, to aid dissolution, until a clear and homogeneous solution has been formed, followed by the addition of the active ingredients, including the siloxane polymer, surface active agents, bulking agents, and any other ingredients such as flavors and sweeteners. For ease of use, the dry film can be cut into pieces of suitable size and shape and packed into a suitable container.

[0060] The following examples further describe and demonstrate various embodiments contemplated by the disclosure.

Example I

[0061] Three oral compositions are prepared in accordance with various embodiments of the disclosure, with each containing a distinct siloxane polymer having a hydrophilic portion. Two compositions designated "Composition A" and "Composition B" contain siloxane polymer having phosphorus-containing moieties, namely the PECOSIL®WDS-200 and PECOSIL® PS-100, respectively. "Composition C" contains a siloxane polymer comprising a hydrophilic portion having polyethylene and polypropylene oxide, namely DC-190. Each of these polymers was fully described above. Compositions A, B, and C are prepared using the ingredients listed in Table I. Additional active ingredients included in the composition are tetrasodium pyrophosphate (an anti-calculus active ingredient) and sodium fluoride (an anticaries active ingredient).

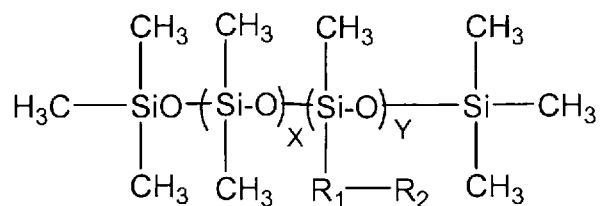
TABLE I			
Toothpaste formula with silicone (Weight %)			
Composition	A	B	C
Polyethylene glycol	3.0	3.0	3.0
Sodium CMC	0.6	0.6	0.6
Tetrasodium pyrophosphate	0.5	0.5	0.5
Purified water	q.s.	q.s.	q.s.
Sodium fluoride	0.243	0.243	0.243
Sorbitol	53.9	53.9	53.9
Sodium saccharin	0.3	0.3	0.3
ZEODENT® 115	25.5	25.5	25.5
Sodium lauryl sulfate	1.2	1.2	1.2
WDS-200	1.0	0	0
PS-100	0	1.00	0
DC-190	0	0	1.00
FD&C Blue #1 1% solution	0.16	0.16	0.16
Flavor	0.72	0.72	0.72
Total	100	100	100

[0062] Dentifrice compositions containing the siloxane polymers having at least one hydrophilic region have good antiplaque activity. The oral compositions are applied to one or more oral surfaces in the oral cavity, and promote overall oral health, including inhibition of plaque formation, gingivitis, periodontitis, caries, and the like. For example, where an oral care composition comprises a siloxane polymer having at least one hydrophilic region, the oral composition effectively inhibits plaque formation and growth of various oral bacteria on an oral surface. In certain embodiments, the oral composition further provides at least one of: antitartar, anti-caries, biofilm disruption and/or anti-inflammatory activity. Thus, certain oral compositions provide multiple oral care benefits simultaneously.

CLAIMS

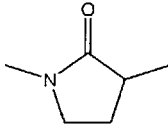
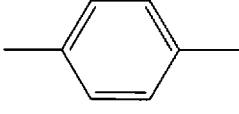
We claim:

1. An oral care composition comprising a siloxane polymer having a phosphorus-containing moiety.
2. A composition according to claim 1, wherein at least one of the moieties comprising phosphorus is selected from the group consisting of: phosphate, phosphonate, phospholipids, a phosphate-containing group, and combinations thereof.
3. A composition according to claim 1, wherein the siloxane polymer comprises a compound having the formula:



wherein R_1 is selected from the group consisting of: alkyl, aryl, amide, ester, pyrrolidone, vinyl, acrylate, siloxane, urethane, carbonate, vinyl alcohol, alkylene oxide, and combinations thereof; and R_2 comprises a moiety selected from the group consisting of: phosphate, phosphonate, phospholipids, a phosphate-containing group, and combinations thereof, "x" is 0 to 100 and "y" is 1 to 100.

4. A composition according to claim 3, wherein R_1 has the formula: $-(\text{CH}_2)_v-(\text{Q})_z$, where Q is at least one group selected from: $\text{C}_2\text{H}_2\text{O}$, $\text{C}_3\text{H}_6\text{O}$; $\text{CH}_2\text{CH}(\text{OH})$;

CONH, CO_2 , NH, CONH,  and , wherein "v" and "z" are 1 to 16.

5. An oral care composition according to claim 1 comprising about 0.001 to about 3% by weight of the siloxane polymer.

6. A composition according to claim 1, wherein the composition comprises an ingredient selected from the group consisting of: surface active agents, viscosity modifiers, thickeners, humectants, diluents, fillers, pH modifying agents, plasticizers, fillers, waxes, texture modifiers, flavoring agents, sweetening agents, coloring agents, preservatives, solvents, and mixtures thereof.

7. A composition according to claim 1, further comprising an active ingredient selected from the group consisting of an antimicrobial agent, an antitartar agent, an anti-plaque, an anticaries agent, a biofilm disruption agent, an antioxidant, an anti-inflammatory agent, a tooth whitening agent, an anti-adhesion agent, a desensitizing agent, a malodor control agent, a flavoring agent, a coloring agent, an anti-aging agent, a salivary stimulant, a periodontal active, a conditioning agent, a natural extract, an essential oil, a nutrient, an enzyme, a protein, an amino acid, a vitamin, an analgesic, and mixtures thereof.

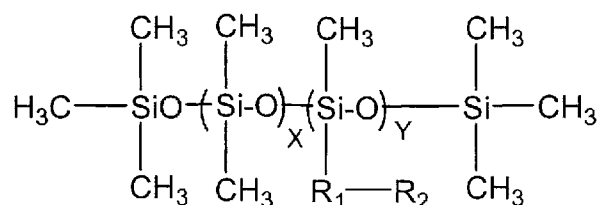
8. An oral care composition comprising a siloxane polymer having a phosphorus-containing moiety, wherein the siloxane polymer is an anti-attachment agent that substantially inhibits bacteria from forming a biofilm on a tooth surface.

9. An oral care composition according to claim 8, wherein the moiety containing phosphorus is selected from the group consisting of: phosphate, phosphonate, phospholipids, a phosphate-containing group, and combinations thereof.

10. An oral care composition according to claim 9, wherein the siloxane polymer comprises an alkyl phosphate siloxane.

11. An oral care composition according to claim 9, wherein the siloxane polymer comprises a polydimethylsiloxane phosphate.

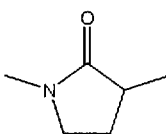
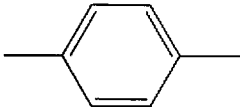
12. An oral care composition according to claim 8, wherein the siloxane polymer comprises a compound having the formula:



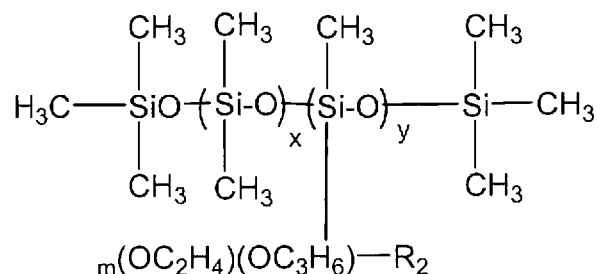
wherein R₁ is selected from the group consisting of: alkyl, aryl, amide, ester, pyrrolidone, vinyl, acrylate, siloxane, urethane, carbonate, vinyl alcohol, alkylene oxide, and combinations thereof; and R₂ comprises a moiety selected from the group consisting of: phosphate, phosphonate, phospholipids, a phosphate-containing group, and combinations thereof, "x" is 0 to 100 and "y" is 1 to 100.

13. An oral care composition according to claim 12, wherein R₁ has the formula:

-(CH₂)_v-(Q)_z, where Q is at least one group selected from: C₂H₂O, C₃H₆O; CH₂CH(OH);

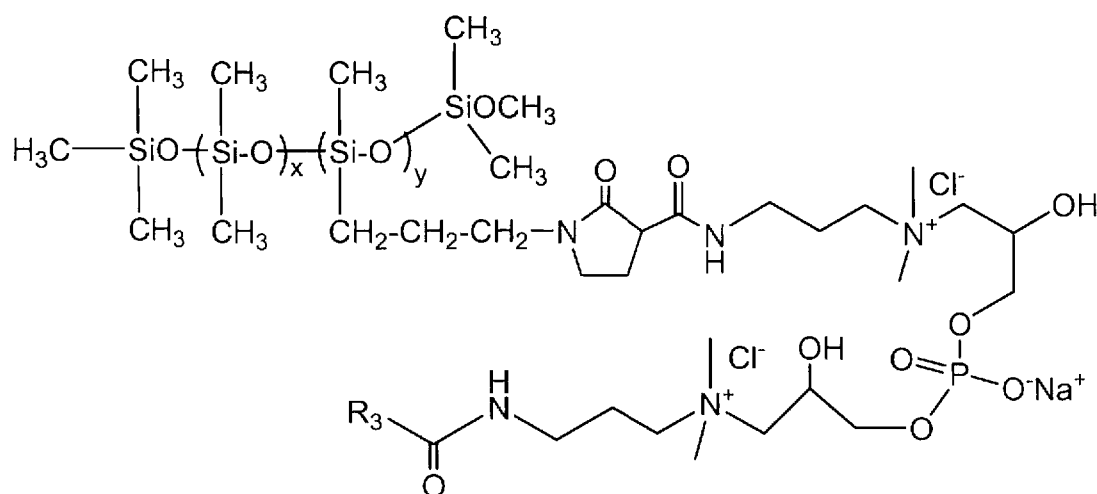
CONH, CO₂, NH, CONH,  and , wherein "v" and "z" are 1 to 16.

14. An oral care composition according to claim 8, wherein the siloxane polymer comprises a compound having the formula:



wherein R₂ is -PO₃H₂ or -(CH₃CH₂H₃O)_nPO₃H₂, "x" is 0 to 100, "y" is 1 to 100, and "m" is 0 to 15.

15. An oral care composition according to claim 8, wherein the siloxane polymer comprises a compound having the formula:



wherein R₃ is an alkyl group, "x" is 0 to 100, and "y" is 1 to 100.

16. An oral care composition according to claim 15, wherein R₃ is a C₁₈ alkyl group.

17. An oral care composition according to claim 8 comprising about 0.001 to about 3% by weight of the siloxane polymer.

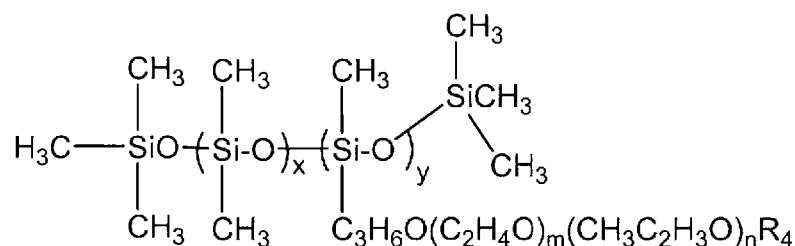
18. An oral care composition according to claim 8, further comprising an active ingredient selected from the group consisting of an antimicrobial agent, an antitartar agent, an anti-plaque, an anticaries agent, a biofilm disruption agent, an antioxidant, an anti-inflammatory agent, a tooth whitening agent, an anti-adhesion agent, a desensitizing agent, a malodor control agent, a flavoring agent, a coloring agent, an anti-aging agent, a salivary stimulant, a periodontal active, a conditioning agent, a natural extract, an essential oil, a nutrient, an enzyme, a protein, an amino acid, a vitamin, an analgesic, and mixtures thereof.

19. An oral care composition according to claim 8, further comprising a carrier ingredient selected from the group consisting of surface active agents, viscosity modifiers, thickeners, humectants, diluents, pH modifying agents, emollients, moisturizers, mouth feel agents, sweetening agents, flavoring agents, solvent, water, colorants, preservatives, and mixtures thereof.

20. An oral composition comprising an anti-plaque and/or antitartar active ingredient comprising a siloxane polymer having at least one hydrophilic region, wherein the siloxane polymer is an anti-attachment agent that substantially inhibits bacteria from forming a biofilm on a tooth surface, and wherein the composition is substantially free of lipophilic active ingredients.

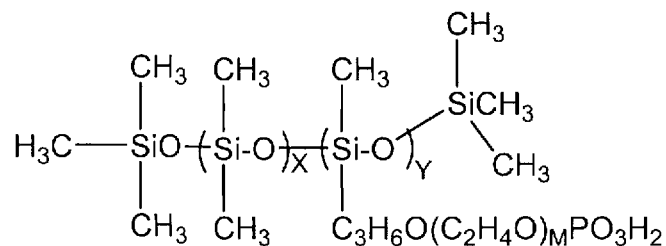
21. An oral composition according to claim 20, wherein the hydrophilic region comprises a moiety selected from the group consisting of: alkylene oxides, phosphates, phosphonates, phospholipids, amines, and combinations thereof.

22. An oral composition according to claim 20, wherein the siloxane polymer comprises a compound having the formula:



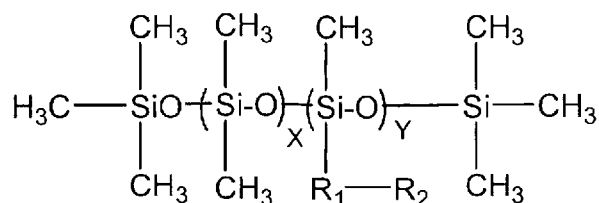
wherein R_4 is selected from H or $-\text{PO}_3\text{H}_2$, "x" is 0 to 100, "y" is 1 to 100, "m" is 0 to 15, and "n" is 0 to 15.

23. An oral composition according to claim 20, wherein the siloxane polymer comprises a compound having the formula:



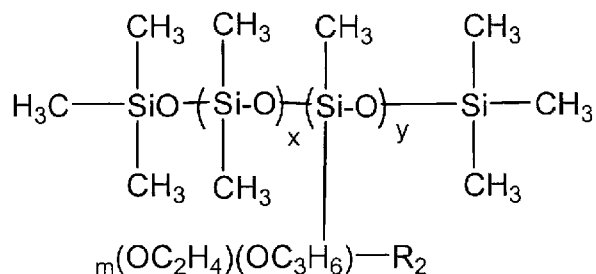
wherein "x" is 0 to 100, "y" is 1 to 100, and "m" is 0 to 15.

24. An oral composition according to claim 20, wherein the siloxane polymer comprises a compound having the formula:



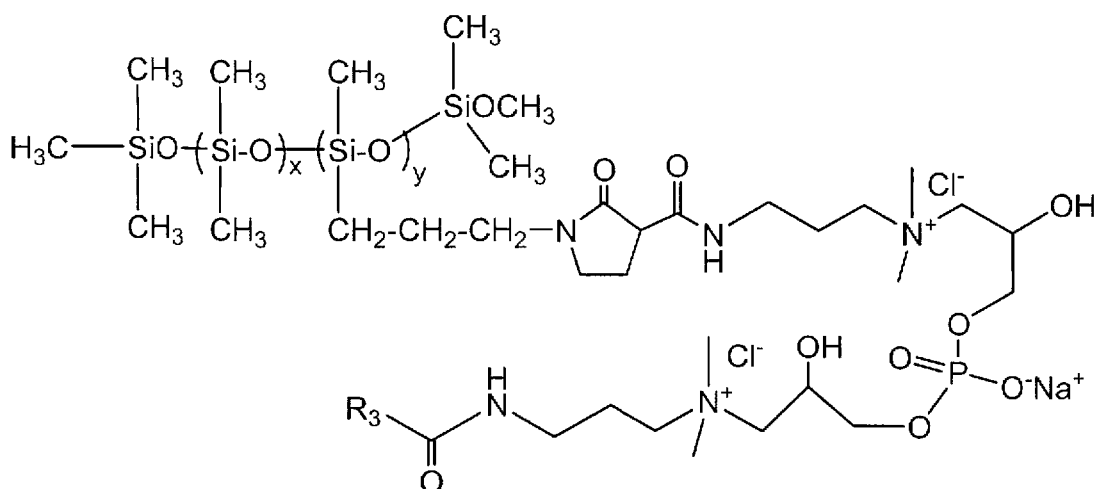
wherein R_1 is selected from the group consisting of: alkyl, aryl, amide, ester, pyrrolidone, vinyl, acrylate, siloxane, urethane, carbonate, vinyl alcohol, alkylene oxide, and combinations thereof; and R_2 comprises a moiety selected from the group consisting of: phosphate, phosphonate, phospholipids, a phosphate-containing group, and combinations thereof, "x" is 0 to 100 and "y" is 1 to 100.

25. An oral composition according to claim 20, wherein the siloxane polymer comprises a compound having the formula:



wherein R_2 is $-\text{PO}_3\text{H}_2$ or $-(\text{CH}_3\text{CH}_2\text{H}_3\text{O})_N\text{PO}_3\text{H}_2$, "x" is 0 to 100, "y" is 1 to 100, and "m" is 0 to 15.

26. An oral composition according to Claim 20, wherein the siloxane polymer comprises a compound having the formula:



wherein R_3 is a C_{18} alkyl group, "x" is 0 to 100, and "y" is 1 to 100.

27. An oral composition according to claim 20 comprising about 0.001 to about 3% by weight of the siloxane polymer.

28. An oral composition according to claim 20, further comprising a non-lipophilic active ingredient selected from the group consisting of an anticaries agent, a biofilm disruption agent, an antioxidant, an anti-inflammatory agent, a tooth whitening agent, an anti-adhesion agent, a desensitizing agent, a malodor control agent, a flavoring agent, a coloring agent, an anti-aging agent, a salivary stimulant, a periodontal active, a conditioning agent, a natural extract, an essential oil, a nutrient, an enzyme, a protein, an amino acid, a vitamin, an analgesic, and mixtures thereof.