

Review Article

CHEMICAL FORMULATIONS FOR MOUTHWASHES

* Hebah Abdel-Wahab and Tamara Gund

Delaware County Community College, 901 Media Lane Rd, Media PA19063, New Jersey Institute of Technology, Newark, New Jersey, USA.

Email address: *dr.heathera@gmail.com, gund@njit.edu

Received 20th December 2021; Accepted 21th January 2022; Published online 28th February 2022

ABSTRACT

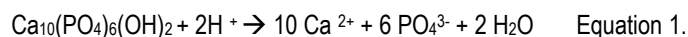
The chemical composition of the ingredients used in the making of the mouthwash were identified in table 1. The recommended preservative for the mouthwash is found to be sodium benzoate. The safe amount of hydrogenated castor oil is found to be below 5g/ kg. The recommended amounts of each chemical in the ingredient and available flavors that can be used in the mouthwash formulation were identified.

Keywords: formulation, ingredients, mouthwashes.

INTRODUCTION

An independent business owner in New Jersey is looking to produce small amount of homemade mouthwash to be sold and distributed locally. The ingredient included the following chemicals: distilled water, sodium chlorite, castor oil, peppermint extract, lemon juice directly from fruit, coconut oil, sodium benzoate, citric acid, and tetra sodium EDTA. The chemical compounds to be used in the formulation and the safe amounts of each chemical in the formulation are identified. Mouthwash can strengthen the teeth, prevent gum disease, and kill bacteria in the mouth that causes gingivitis and improve your oral health. If the mouthwash contains fluoride, it reduces cavity when used correctly. It is recommended by dentists to use mouthwash daily in addition to daily brushing and flossing. People with medical conditions, tooth sensitivity, dry socket, and Xerostomia find mouthwash essential in their daily routine. 1. Mouth wash is used to refresh and clean the oral cavity. To prevent the development of caries, formulation containing fluorides have been used, as it destroys and inhibits the oral microbial population that generates malodors or dental plaque. Mouthwash formulation mainly consists of ethanol, water, a humectant, a surfactant, flavor, color, and an active ingredient. Ethanol is used to enhance the flavor impact and adds freshness. The humectant such as glycerin, sorbitol or propylene glycol adds body to the formulation and improves the mouth feel when using the mouthwash. The surfactant is usually a nonionic such as poly oxy-propylene or poly oxyethylene co polymers, it produces foams, dissolves the flavor oil, and removes debris. The flavor is an oil used to make the mouthwash pleasant to use. The mouthwash may include an active ingredient, for example, anti-cares effect or antibacterial effect. 2. Dental Caries is a multi factorial disease produced within the dental plaque by microorganisms. It involves a process of enamel demineralization and remineralization due to the act of organic acids produced within the dental plaque by microorganisms. The enamel demineralization is the process of dissolution of hydroxyapatite by the act of extrinsic or intrinsic acids, according to equation 1, leading to erosion or dental cares. Dental Cares are caused by acetic or lactic acid that diffuses into the enamel pores through the plaque, decreasing the PH of the

fluid surrounding the enamel crystals. To prevent dental cares, fluorides, calcium and phosphates, and antimicrobials can be used as additives in the mouthwash formulation. The presence of fluorides in the microenvironment or around the teeth inhibits the demineralization and promotes the remineralization of the tooth surface. The incorporation of fluoride as fluorapatite into enamel decrease its solubility. Casein phospho-peptide amorphous calcium phosphate, CPP-ACP has been added to mouthwash, tropical pastes and chewing gums to increase remineralization and decrease demineralization. Antibacterial has some role in caries prevention, it helps with plaque and microbial control, Chloro-hexadiene and triclosan containing gels, toothpastes, and rinses has been used. 3.



Mouth wash can be classified into two main types, therapeutic and cosmetic. Therapeutic mouthwash reduce plaque, bad breath, tooth decay, and gingivitis. Children under the age of 6 shouldn't be using mouthwash as they may inadvertently swallow large amounts of liquids, unless directed by a dentist. Cosmetic mouthwash has no biological or chemical application beyond their temporary relief, they temporarily control bad breath and gives a pleasant taste and smell. 4. Active ingredients used in a therapeutic mouthwash are peroxides, fluorides, chlorhexidine, essential oils, and cetyl-pyridinium chlorides. Peroxides are used in whitening mouthwash. Fluorides are used to prevent tooth decay. 5. Chlorhexidine and essential oils are used to fight gingivitis and plaque. 6,7. Cetyl-pyridinium chlorides is used to prevent bad breath. 8. Antimicrobial, Fluoride, Anesthetic, and Chlorhexidine mouthwashes are examples for therapeutic mouthwashes. Antimicrobial mouthwashes are used in treatment of Oral Malodor, bad breath. Volatile sulfur compounds (VSC's) 9. is the major factor causing bad breath, they arise from breakdown of food, bacteria associated with dental disease and dental plaque. Cosmetic mouthwash can also temporarily mask bad breath, but it doesn't kill the bacteria that causes the bad breath and has no effect on volatile sulfur compounds causing bad breath. Therapeutic mouthwash containing an antimicrobial are more long term and can control bad breath. Antimicrobials in mouthwash formulations can include chlorhexidine, cetyl-pyridinium chloride, essential oils (e.g., methyl salicylate, eucalyptol, thymol, and menthol) and chlorine dioxide. Antimicrobial mouthwashes are also used in treatment of gingivitis and plaque. 10,11

*Corresponding Author: Hebah Abdel-Wahab,

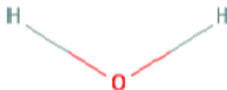
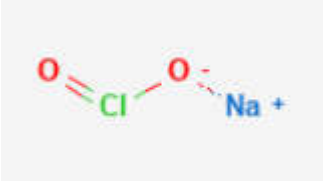
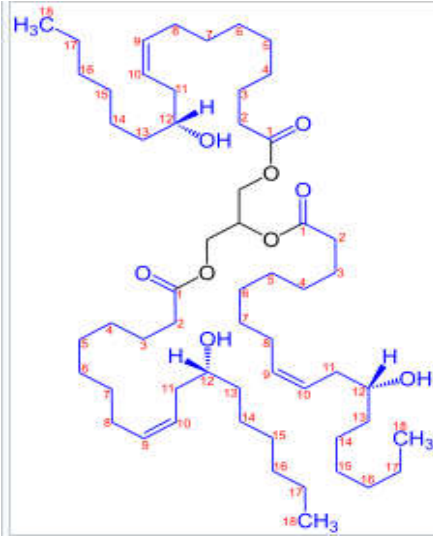
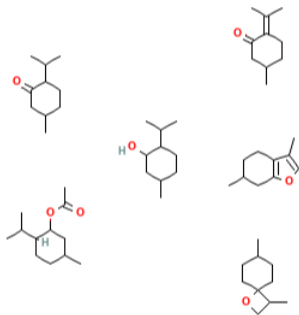
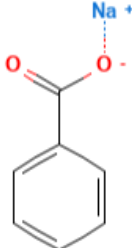
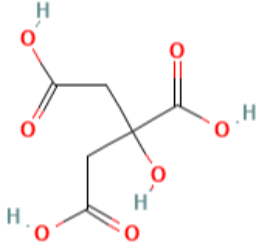
Delaware County Community College, 901 Media Lane Rd, Media PA19063, New Jersey Institute of Technology, Newark.

Fluoride mouthwashes are used to prevent tooth decay in children. 12 and can also be used in treatment of xerostomia, a condition where the amount of saliva bathing the oral mucous membrane is reduced. It is found that rinsing weekly with 0.2% NaF mouthwash or daily with a 0.02% NaF would reduce dental caries by 20-40% in children. 13 Anesthetic mouthwashes are used to relieve pain and they contain anesthetics, dyclonine hydrochloride, phenol, lidocaine, benzocaine, tetracaine hydrochloride, or butamin. 14 Whitening mouthwash mostly contain 1.5-2% hydrogen peroxide 15 or 10% carbamide peroxide. 16. Chlorhexidine mouthwash, without the use of antibiotics is found to be effective for AO prevention following extractions. 7 Dry socket, alveolar osteitis, which is a condition that might follow an extraction procedure, intense pain 2-3 days after procedure. 17. Additives that make a therapeutic mouthwash can be classified into either antibacterial agents or compounds that effect VSC formation. Antibacterial agents help reduce the number of anaerobic bacteria in the mouth. Examples of antibacterial agents that are used in mouthwash formulation are cetyl pyridinium chloride, essential oils/antiseptic formulations, triclosan, and Chlorhexidine gluconate. It is found that the use of 0.75% Cetyl pyridinium chloride (CPC) mouth rinse reduces plaque by 35% over a 6 month period, the use of a 0.2% chlorhexidine gluconate oral rinse solution cause reduction in VSC level (It shows some side effects, it alters sense of taste and causes staining of mouth and tongue). Compounds that effect VSC formation, neutralizes VSC's to improve quality of breath. Examples of ingredients that effect VSC's are zinc compounds and chlorine dioxide (sodium chlorite, is an oxidizing agent and is able to degrade sulfur containing amino acids, which the building block of VSC's, making fewer of them available to bacteria, leading to fewer VSC's formed). It's found that using mouthwash containing 1% sodium chlorite, reduces VSC for a period of 8h. Some metal ions have the ability to oxidize the thiol, sulfur-based molecules found on VSC's. Example of metal ions are zinc, copper, magnesium, tin, and sodium, zinc also has an antibacterial property, doesn't cause tooth staining like other metal ions, and has low toxicity. A 1% zinc acetate mouthwash has a significant effect on VSC levels, even 3 hours after use. A typical formulation for essential oils / antiseptic mouthwash is: 0.092% eucalyptol, 0.042% menthol, 0.06% methyl salicylate and 0.064% thymol in a solution containing 21.6% to 26.9% alcohol, high concentration of alcohol in the formulation (25% ethanol) may cause drying effect on oral tissue, increasing breath malodor. The most effective mouthwash for bad breath is found to use a multifaceted approach, using a combination of formulations. Other products are used for breath control may include gum, toothpaste, mints, drops, lozenges, and sprays. It is found that six compounds are mainly used in the formulation of mouthwash designed to fight bad breath (halitosis); zinc chloride, triclosan, essential oils/antiseptic formulations, chlorhexidine gluconate, cetyl-pyridinium, and chlorine dioxide. 18. Studies show that using a 0.09% zinc chloride mouth rinse is effective in reducing the formation of calculus in people. 43 Sodium chlorite is the main the ingredient used in the newer classes of mouthwashes such as Pro Fresh, CloSYS, Thera Breath, and Oxyfresh, it's sometimes used as a water purifier. These mouthwashes are said to freshen breath up to six hours. Smart Mouth uses sodium chlorite as a main ingredient, but it must be mixed with zinc chloride right before use. The zinc ions block receptor sites of amino acids, after eating food containing amino acids, so the bacteria can't produce rancid gases, and it lasts for up to twelve hours before another rinse is needed. 44 Flavors are one of the main ingredients that make a mouthwash, as it gives flavor to the formulation and makes the mouthwash pleasant to use. The different known flavors that can used in a mouthwash ingredient are: Clove Leaf Oil, Cubeb

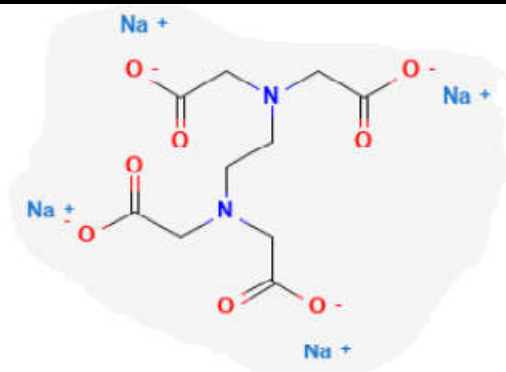
Oil, Cedarwood Oil, Eucalyptus Oil, Lemon Oil, Italian Type, Cold pressed, Myrrh Oil, Mentha Arvensis Oil, sweet Orange Oil, Peppermint Oil, Sucralose, Saccharin Sodium, Dihydrate, Granular, Spearmint Oil, Camphor, Methyl Salicylate, and Cinnamon Extract. 45.

Experimental

Distilled water (purified water) with formula of H₂O and molecular weight of 18.015g/mol is used as solvent in which the ingredients are soluble in, it's a cooled boiling water steam returned to its liquid state after removing 99.9% of the minerals dissolved in water. 19. Sodium Chlorite with formula of NaClO₂ and molecular weight of 90.44 g/mol is used as an antimicrobial agent in mouthwash, it reduces bacteria living in the mouth and causing bad breath, it also degrades building blocks of the volatile sulfur compounds causing bad breath, it degrades sulfur based amino acids, causing fewer of them being available to bacteria, fewer volatile sulfur compounds are formed. It is found that one time use of mouthwash containing 1% sodium chlorite is effective in reducing the RVS level for eight hours and beyond. 20. Castor oil with formula of C₅₇H₁₀₄O₉ and molecular weight of 933.4 g/mol 21 has the ability to break bio film, a protective coating created by detrimental bacteria in the microbiome. (22-24). It makes the environment more hospitable to the healthy bacteria and eradicates the bad bacteria. It also reduces inflammation of the gums. 25. Castor oil is slightly toxic chemical and safe amount of Castor oil is found to be below 5g/kg, below mass percent (m/m) of 0.099%. 26. Pepper extract with formula of C₆₂H₁₀₈O₇ and molecular weight of 965.5g/mol is used as flavoring agent, antiseptic and anti-viral agent. There is no evidence that it has the ability to treat any medical condition. However high concentration of menthol in the extract causes side effects in children and infants when inhaled. 27. Sodium Benzoate with formula of C₇H₅NaO₂ and molecular weight of 144.11 g/mol is used as a preservative in food, medicine, and cosmetics. It's converted to benzoic acid under these conditions, which is fungi static and bacterio static. Due to the insolubility of benzoic acid in water, it isn't used directly as a preservative. It's concentration as a preservative is determined by the FDA to be 0.1%. 28. Lemon juice is a good source of citric acid, containing 1.44g/oz citric acid, which is 4.83 percent by mass citric acid in lemon juice. 29. Citric acid with formula of CHO and molecular weight of 192.124g/mol 30 is known to cause tooth enamel to dissolve quickly. More dentin is exposed as enamel dissolves, causing teeth cracks and chips and the edges of the teeth become more irregular. 31. Tetra sodium EDTA with formula of C₁₀H₁₂N₂Na₄O₈ and molecular weight of 380.171g/mol 32 is a water-soluble acid with chelating properties and is an emulsion stabilizer. It bonds with metal ions in solution causing them to be inactive and is used as a preservative for cosmetic formulation and skin care products, creams, and lotions ...etc. It prevents the change in PH, texture, and color of skincare products. And is used as a co-preservative in skincare formulations. Also, it can enhance foaming and cleaning ability when binding to iron, calcium or magnesium. 33. Coconut oil contains 80-90% unsaturated fat, is 100% fat, and contains traces amounts of minerals and vitamins. Is used for cooking in food, as fuel source in industry and as base ingredient for the manufacture of soap. 34. Lemongrass oil with formula of C₅₁H₈₄O₅ and molecular weight of 777.2 g/mol is known to be used as an herbal alternative (0.25%) to chlorhexidine (0.2%) in mouthwash. It prevents and treats periodontal diseases. 35.

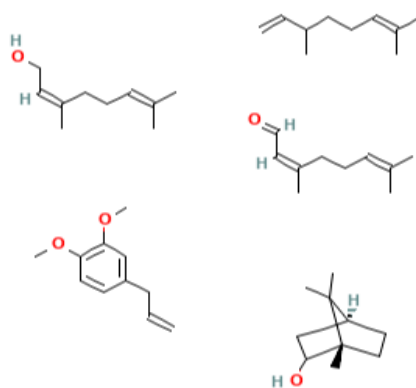
Household and Chemical Name	Chemical	Chemical structure	Molecular Formula	Molecular Weight (g/mol)
Distilled water .36.			H ₂ O	18.015
Sodium chlorite .37.			NaClO ₂	90.44
Castor oil.38.			C ₅₇ H ₁₀₄ O ₉	933.4
Major component of castor oil, triester of glycerol and ricinoleic acid.				
Peppermint Oil.39.	extract/		C ₆₂ H ₁₀₈ O ₇	965.5
<u>(Menthol)</u> , <u>(3,7-Dimethyl-1-oxaspiro[3.5]nonane)</u> , <u>(Menthyl acetate)</u> , <u>(p-Menth-4(8)-en-3-one)</u> , <u>(p-Menthan-3-one)</u> and <u>(Menthofuran)</u> .				
sodium benzoate.40.			C ₇ H ₅ NaO ₂	144.11
Lemon Juice (citric acid). 41.			C ₆ H ₈ O ₇	192.124

tetrasodium edta

C₁₀H₁₂N₂Na₄O₈

380.171

Lemongrass oil.42.

C₅H₈O₅

777.2

(Methyleugenol), (L-Borneol), (Nerol), (Dihydromyrcene) and (Neral).

Summery and Conclusion

The therapeutic mouthwash formulation shouldn't include the following chemical compounds: citric acid, lemon juice, EDTA, and coconut oil. Citric acid/lemon juice is known to weaken and dissolve tooth enamel, both EDTA and coconut oil are known neither to be used in the pharmaceutical industry nor in mouthwash formulations. EDTA is commonly used in skin products as a chelating agent and coconut oil is a fat that is known to be used in cooking, fuel, and in the making of soaps. The therapeutic mouth wash formulation may include 1.0% Sodium chlorite as an active ingredient, 0.1% sodium benzoate as a preservative, water as the solvent and less than 0.09% percent by mass castor oil. To improve the quality of the mouthwash formulation, other chemical compounds may be used, glycerin as a humectants and poly oxy-propylene co polymer as a surfactant. Color and flavor may be used to improve the quality of the mouthwash. Some other additives such as zinc chloride may also be used, it's known to freshen breath up to twelve times higher when combined with sodium chlorite.

Acknowledgement

We would like to sincerely thank the Association of Consulting Chemist and Chemical Engineers for their efforts in making our profiles available on the web for clients in the USA and Worldwide.

REFERENCES

- <https://www.westenddental.com/blog/is-mouthwash-necessary/>
- Johansson I, Somasundaran P, Handbook for Cleaning/Decontamination of Surface, Elsevier, Kidlington, Oxford OX5, 2007. Pp 382-383.
- Manton David J., Hayes-Cameron L., Handbook of Pediatric Dentistry 4th edition, 2013, Dental Caries, Mosby Elsevier, Canberra Australia. pp-49-78.
- <https://www.ada.org/resources/research/science-and-research-institute/oral-health-topics/mouthrinse-mouthwash>
- Torres CR, Perote LC, Gutierrez NC, Pucci CR, Borges AB. Efficacy of mouth rinses and toothpaste on tooth whitening. Oper Dent 2013;38(1):57-62.
- Marinho VC, Higgins JP, Logan S, Sheiham A. Topical fluoride (toothpastes, mouthrinses, gels or varnishes) for preventing dental caries in children and adolescents. Cochrane Database Syst Rev 2003(4):CD002782.
- Hasson H, Ismail AI, Neiva G. Home-based chemically-induced whitening of teeth in adults. Cochrane Database Syst Rev 2006(4):CD006202.
- Sharma N, Charles CH, Lynch MC, et al. Adjunctive benefit of an essential oil-containing mouthrinse in reducing plaque and gingivitis in patients who brush and floss regularly: a six-month study. J Am Dent Assoc 2004;135(4):496-504
- Blom T, Slot DE, Quirynen M, Van der Weijden GA. The effect of mouthrinses on oral malodor: a systematic review. Int J Dent Hyg 2012;10(3):209-22.
- Araujo MW, Charles CA, Weinstein RB, et al. Meta-analysis of the effect of an essential oil-containing mouthrinse on gingivitis and plaque. J Am Dent Assoc 2015;146(8):610-22.
- Sharma N, Charles CH, Lynch MC, et al. Adjunctive benefit of an essential oil-containing mouthrinse in reducing plaque and gingivitis in patients who brush and floss regularly: a six-month study. J Am Dent Assoc 2004;135(4):496-504
- Fedorowicz Z, Aljufairi H, Nasser M, Outhouse TL, Pedrazzi V. Mouthrinses for the treatment of halitosis. Cochrane Database Syst Rev 2008(4):CD006701.
- Leary, Kecia S., Nowak, Arthur J., Pediatric dentistry: infancy through adolescence, Prevention of Dental Disease, P455-460; 2019.

14. Mariotti AJ, Burrell, K.H. Mouthrinses and Dentifrices. 5th ed. Chicago: American Dental Association and Physician's Desk Reference, Inc.; 2009.
15. Mariotti AJ, Burrell, K.H. Mouthrinses and Dentifrices. 5th ed. Chicago: American Dental Association and Physician's Desk Reference, Inc.; 2009.
16. Hasson H, Ismail AI, Neiva G. Home-based chemically-induced whitening of teeth in adults. *Cochrane Database Syst Rev* 2006(4):CD006202.
17. Kerr AR, Corby PM, Kalliontzis K, McGuire JA, Charles CA. Comparison of two mouthrinses in relation to salivary flow and perceived dryness. *Oral Surg Oral Med Oral Pathol Oral Radiol* 2015;119(1):59-64.
18. https://www animated-teeth.com/bad_breath/t5_halitosis_cures.htm
19. <https://www.webmd.com/diet/distilled-water-overview#1>
20. https://www animated-teeth.com/bad_breath/t5_halitosis_cures.htm
21. <https://pubchem.ncbi.nlm.nih.gov/compound/Castor-oil>
22. Andrade IM, Andrade KM, Pisani MX, et al. Trial of an experimental castor oil solution for cleaning dentures. *Braz Dent J.* 2014;25(1):43-47.
23. Badaró MM, Salles MM, Leite VMF, et al. Clinical trial for evaluation of *Ricinus communis* and sodium hypochlorite as denture cleanser. *J Appl Oral Sci.* 2017;25(3):324-334.
24. Salles MM, Badaró MM, Arruda CN, et al. Antimicrobial activity of complete denture cleanser solutions based on sodium hypochlorite and *Ricinus communis* – a randomized clinical study. *J Appl Oral Sci.* 2015;23(6):637-642.
25. Vieira C, Evangelista S, Cirillo R, et al. Effect of ricinoleic acid in acute and subchronic experimental models of inflammation. *Mediators Inflamm.* 2000;9(5):223-228.
26. Gosselin, R.E., H.C. Hodge, R.P. Smith, and M.N. Gleason. *Clinical Toxicology of Commercial Products*. 4th ed. Baltimore: Williams and Wilkins, 1976., p. II-152
27. https://en.wikipedia.org/wiki/Peppermint_extract
28. https://en.wikipedia.org/wiki/Sodium_benzoate
29. Penniston K.L., Nakada S.Y., Holmes R.P., Assimos D.G., Quantitative Assessment of Citric Acid in Lemon Juice, Lime Juice, and Commercially-Available Fruit Juice Products, National Library of Medicine, *Journal of Endourology*, 2008;22(3):567-70.
30. <https://pubchem.ncbi.nlm.nih.gov/compound/Citric-acid>
31. <https://www.glowdental.co.uk/how-citric-acid-affects-your-teeth/>
32. https://en.wikipedia.org/wiki/Tetrasodium_EDTA
33. <https://www.lorealparisusa.com/ingredient-library/disodium-edta>
34. <https://www.hsph.harvard.edu/nutritionsource/food-features/coconut-oil/>
35. <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4625327/>
36. <https://pubchem.ncbi.nlm.nih.gov/compound/Water>
37. https://en.wikipedia.org/wiki/Sodium_chlorite
38. https://en.wikipedia.org/wiki/Castor_oil
39. <https://pubchem.ncbi.nlm.nih.gov/compound/Peppermint-oil>
40. <https://pubchem.ncbi.nlm.nih.gov/compound/Sodium-benzoate>
41. <https://pubchem.ncbi.nlm.nih.gov/compound/Castor-oil>
42. <https://pubchem.ncbi.nlm.nih.gov/compound/Lemongrass-oil>
43. Charles C.H, Cronin M. J., Dembling W. Z., Petrone D. M., McGuire J. A., Anticalculus efficacy of an antiseptic mouthrinse containing zinc chloride, *Journal of American Dental Association*, 2001;132(1):94-8, doi: 10.14219/jada.archive.2001.0033.
44. https://usatoday30.usatoday.com/news/health/2008-05-13-bad-breath_N.htm
45. <http://dentalingredients.spectrumchemical.com/products/oral-care-flavorants>
