Notes On Making Cola

Issue 2

By

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1. Some Basic Chemistry

1.1. Molecules

*Molecule*s are one of the fundamental building blocks of chemical compounds and normally consist of groups of atoms held firmly together by *covalent bonds*. Molecules generally stay intact during physical processes, such as melting and boiling, but are broken apart and altered during chemical processes or reactions.

Roughly speaking covalently bonded molecules can be split into two basic types:

- Non-polar
- Polar

1.1.1. Non-polar Molecules

These include a group of *organic*[1] molecules called *hydrocarbons* that contain only hydrogen and carbon atoms. Examples of the simplest hydrocarbons are shown in Figure 1.1.

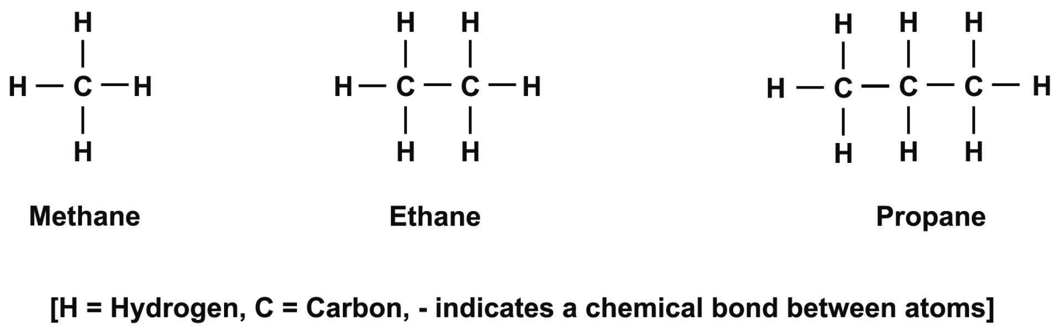

Figure 1.1: Simple hydrocarbon molecules.

More and more carbon atoms can be added to create large molecules. Such molecules can be found in petrol, kerosene, wax and other oils and plastics. Hydrocarbons need not be straight chain molecules (as those depicted in Figure 1.1) they can also be based on hexagon shapes (see Appendix A4 and Appendix A5).

Non-polar molecules have no permanent overall or localised electrical charges on them.

1.1.2. Polar Molecules

These molecules have no permanent overall electrical charge on them but do have small electrical charges at different points. For example water (H_20) consists of two hydrogen atoms and an oxygen atom; the hydrogen atoms have a small positive charge and the oxygen atom has a small negative charge (Figure 1.2). The small positive and negative charges attract each other in a similar way to which the north and south poles on a magnet will attract each other. This attraction causes weak bonds to be set up between molecules.

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[1] Organic molecules are based around carbon and hydrogen atoms but may contain other atoms such as nitrogen, oxygen and chlorine.

Ethanol (CH_3CH_2OH, the alcohol that gets you drunk) is another example of a polar molecule. It contains 2 carbon atoms 6 hydrogen atoms and 1 oxygen atom (Figure 1.3). Note that the ethanol molecule has a polar part (the alcohol group) and a non-polar part (the rest of the molecule). Whenever you see oxygen in an organic molecule you can assume it to be polar (or at least the part of it that contains the oxygen atoms). See Appendix A5 for other important oxygen containing groups. Ethanol is not the only alcohol. Any molecule that contains C and H atoms and one or more –OH groups is an alcohol. For example CH_3OH is called methanol and $CH_3CH_2CH_2CH_2OH$ is called butanol.

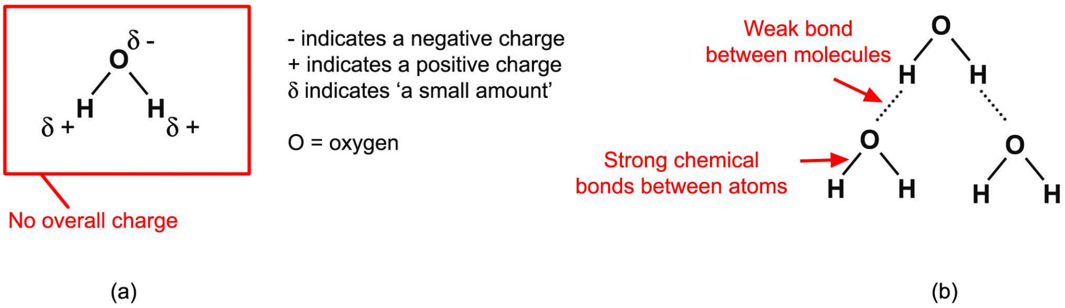

Figure 1.2: The water molecule.

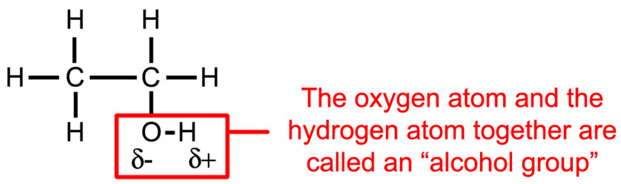

Figure 1.3: The ethanol (CH3CH2OH) molecules.

1.2. Solubility, Miscibility And Immiscibility

When one liquid dissolves in a second their molecules mix freely together and a solution is formed. Such liquids are said to be *miscible*. When two liquids will not mix (i.e. their molecules will not interact together freely) they are said to be *immiscible*; therefore engine oil and water are immiscible. When two immiscible liquids separate the one with the lowest density will rise to the top.

As a rule of thumb like dissolves like. That is to say that polar liquids will mix with other polar liquids but not non-polar liquids, also non-polar liquids will mix well with other non-polar liquids but not polar ones. Liquids that will not mix with water are said to be *hydrophobic* and those that will mix with water are said to be *hydrophilic*.

Substances are not necessarily soluble or insoluble, in many cases substances are slightly soluble. For example the solubility of alcohols in water is affected by the size of the hydrophobic portion of the molecule and the number of –OH groups present. Hence ethanol (CH_3CH_2-OH) is completely soluble in water and butanol ($CH_3CH_2CH_2CH_2OH$) is only partially soluble (7.9 g of butanol per 100 ml of water). Also Butanediol (HO-$CH_2CH_2CH_2CH_2$-OH) has two –OH groups and is completely soluble in water although it has the same number of carbon atoms as butanol.

1.3. Acidity And Dissociation

Some polar molecules lose their $H^{\delta+}$ atoms completely when they dissolve in water. The $H^{\delta+}$ atom then becomes a free H^+ *ion*[2]. Water molecules themselves are constantly *dissociating* to produces H^+ and OH^- ions and the ions in turn are *re-associating* to produce water molecules:

$$H_2O \rightleftharpoons H^+ + OH^-$$

Obviously when water molecules dissociate they produce equal numbers of H^+ and OH^- ions. Crudely speaking an *acid* is a substance that only produces H^+ ions when it is dissolved in water, thus forming a solution with more H^+ ions than OH^- ions. For example hydrochloric acid (HCl) dissolves in water to give:

$$HCl \rightleftharpoons H^+ + Cl^-$$

The acidity of a solution is measured using the *pH scale* which reflects the consecration of H^+ ions. A strongly acidic solution has a pH of 1 or 2, a *neutral* solution has a pH of 7 and a *basic* (or *alkali*) solution has a pH between 7 and 14. *Bases* form OH^- ions when dissolved in water (or put another way cause a deficit of H^+ ions).

HCl is a strong acid because each molecule will produce an H^+ ion. Alcohols on the other hand are very slightly acidic and when a volume of ethanol is dissolved in water a very small proportion of the molecules dissociate:

$$CH_3CH_2OH \rightarrow H^+ + CH_3CH_2O^-$$

Organic carboxylic acids, for example ethanoic acid (CH_3COOH, found in vinegar), have a COOH group (see Figure 1.4). When ethanoic acid disassociates in water it produces H^+ and CH_3COO^- ions.

Figure 1.4: The ethanoic acid molecule.

Alcohols and carboxylic acids are both found in essential oils, and while carboxylic groups are stronger acids than alcohols they are both relatively weak acids when compared to hydrochloric or sulphuric acids.

[2] As mentioned in Section 1.1.1 polar molecules have no overall charge. However, if a water molecule splits up it forms an H^+ ion , this is a hydrogen atom with a an electron missing and therefore it has a positive charge. An OH^- ion is also formed, which is an oxygen atom and a hydrogen atom joined together with the extra electron, it therefore has a negative charge.

1.4. Emulsions

1.4.1. Types Of Emulsion

When two liquids are immiscible but do not separate immediately they are said to form an *emulsion*. Some emulsions are quite stable and will take a long time to separate. For example milk is an emulsion of water and fat but is fairly stable. Other emulsions may separate quite quickly, for example a simple salad dressing of oil and vinegar will separate almost immediately (note that vinegar is water based).

The emulsion itself consists of small droplets of one liquid within the body of a second liquid. An emulsion containing droplets of oil in water is called an *oil-in-water* emulsion and the oil is called the dispersed phase while the water is called the continuous phase. An emulsion with droplets of water in oil is called a *water-in-oil* emulsion. A good oil-in-water emulsion will consist of very fine oil droplets homogeneously dispersed throughout the body of water.

Since colas are oil-in-water emulsions this discussion of emulsions assumes that an oil phase is being dispersed within a water phase. In practice neither the water phase nor the oil phase of an emulsion are likely to be pure substances. For example in colas the continuous water phase is an acidic solution of citric or phosphoric acid together with other ingredients such as caramel and sugar, the oil phase is a complex mixture of organic molecules from the essential oil flavourings. In general the water soluble molecules all stay in the water phase and the oil phase will be a mixture of all the liquid molecules that are not soluble in water (i.e. a mixture of oils).

1.4.2. Surface Energy

All surfaces have a *surface energy*, this energy is responsible for phenomena such as surface tension. If you place a drop of oil into a glass of water a new surface at the interface between the oil and water is created and this surface will have an energy (Figure 1.5). This energy must be provided from somewhere, thus to create an emulsion from oil and water you must supply energy. For example you must shake salad dressing to create an emulsion from the oil and vinegar, if you do not shake it the two liquids stay in separate layers (Figure 1.6).

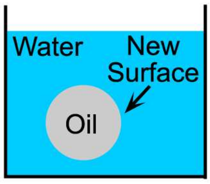

Figure 1.5: A drop of oil in water.

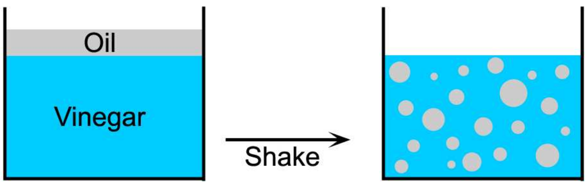

Figure 1.6: Making new surfaces in salad dressing emulsion.

Crudely speaking all systems try to reduce their energy to a minimum, thus our drop-of-oil-in-water system wants to reduce the area of the oil-water interface; less surface area equal less surface energy. For a given volume of oil the minimum surface area possible is obtained by forming a sphere; therefore oil drops in water and bubbles of gas in a liquid are always spherical.

1.4.3. Emulsion Failure

Emulsions can fail in four basic ways, each of which causes the homogenous dispersion of oil droplets to be lost (Figure 1.7):

i. *Coalescence* - Two small oil spheres have a combined surface area (and therefore surface energy) that is larger than a single big sphere containing the same volume of oil. Thus if salad dressing is left to stand the small bubbles will coalesce to form bigger and bigger spheres until the oils has completely separated from the water.

ii. *Flocculation* – The small spheres of oil stick together to form clumps or *flocs* which act as if they are larger drops. Therefore the oil is no longer evenly distributed through the water.

iii. *Creaming* – Most oils are less dense than water and will therefore float to the top. However, the drops will not necessarily coalesce.

iv. *Breaking* – Due to Coalescence and creaming combined, the oil separates completely from the water so that it floats at the top in a single, continuous layer.

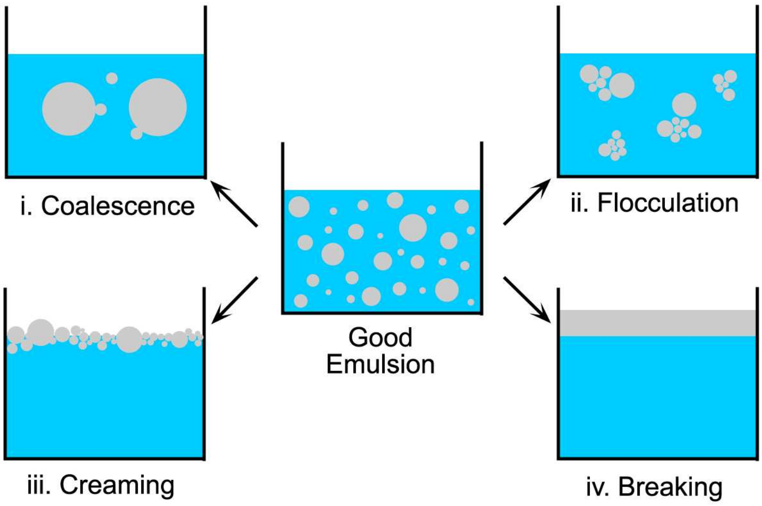

Figure 1.7: The failure of emulsions.

Figure 1.7 clearly shows that flocculation and creaming leave the fine oil droplets intact while making them less well distributed throughout the water. Therefore, these two processes can be reversed by putting in a small amount of energy (i.e. moderate stringing or shaking). Brownian motion, within the water phase, can provide enough energy to keep exceptionally small droplets agitated and hence creaming is less likely to happen with fine emulations. If the emulsion contains larger oil droplets, they will soon rise to the top.

Coalescence and breaking lead to large bodies of oil separating from the water and essentially result in the emulsion separating completely. To reverse this process the emulsion must be remade and this will require a lot of energy. Emulsions are all thermodynamically unstable, meaning that they will eventually separate however, they can be stabilised and in some cases they can remain intact indefinitely. Both coalescence and flocculation are more likely if the surface energy between the two phases is high and if the surface area to volume ratio is high (i.e. the oil droplets are very small). However, emulsions of small droplets are easier to stabilise because creaming is less likely.

1.4.4. The Origins Of Charged Droplets In Emulsions

In many emulsions the droplets of the dispersed phase have an *electrostatic charge*. In colas the droplets have a negative charge, this arises due to the dissociation of acidic groups at the surface of the droplets (Figure 1.8, also see Section 1.3). These acidic groups form part of some of the oxygen containing essential oil molecules.

The magnitude of the surface charge depends on the strength of the acid groups in the oil phase (for colas the carboxylic groups are quite weak acids and alcohols are very weak acids) and on the pH of the surrounding water phase (for coca-cola this is about 2.5). The more acidic a cola's water phase is, the less surface charge there will be on the droplets and as the pH is lowered a point is reached where the droplets no longer have a surface charge at all, this point is known as the *isoelectric point*.

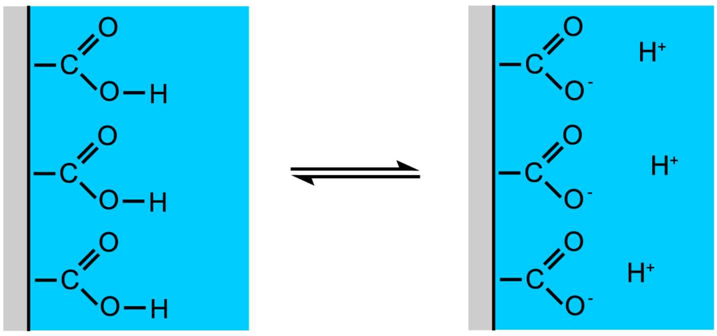

Figure 1.8: Carboxylic acid groups at an oil/water surface producing a surface charge by dissociation.

1.5. Stabilising Emulsions

Coalescence and creaming are constantly working to ruin emulsions however, there are several ways in which emulsions can be stabilised. These include electrostatic repulsion and the addition of additives called *emulsifiers* and *stabilisers*[3].

1.5.1. Electrostatic Stabilisation

As mentioned in Section 1.4.4 droplets in emulsions can carry electrostatic charges and these charges are dependent on acidic surface groups and the acidity of the surrounding water phase. Charged oil droplets will repel each other since alike charges repel, this prevents two droplets sticking together or coalescing.

1.5.2. Polymeric Stabilisation

Polymers[4], including natural polymers such as proteins and gums, can be used to stabilise emulsions. Some of these polymers contain certain polar chemical groups, for example alcohols, that can adsorb onto the surface of the oil droplet. Gum Arabic is an example of a *polysaccharide gum* that can adsorb to oil droplets.

[3] The terms emulsifier and stabiliser are often interchangeable however, emulsifiers are strictly additives that make the formation of emulsions easier and stabilisers are additives that prevent the failure of the emulsion once it has been mixed.

[4] Polymers are long molecules made up from a repeated pattern of smaller molecules stuck together.

The polymer molecules can either adsorb at a single point or at several points and the adsorbed layer prevents two droplets from coalescing by forming a barrier (Figure 1.9). Molecules that are attached at more than one point form a strong protective barrier around the droplets that can withstand vigorous agitation without becoming detached. These polymer barriers stabilise the emulsion once it has been formed but don't usually make formation easier.

Polymer molecules that can not adsorb onto the oil droplets but are soluble in water can stabilise emulsions by increasing the *viscosity*[5] of the water phase. Polysaccharide gums such as xanthan gum (but not gum Arabic) can be used to this end and are known as *hydrocolloids*. For coalescence and creaming to happen the water phase must easily flow around the oil droplets so that intimate contact between the droplets is possible. A more viscous water phase will flow less easily and sometimes cause water to be trapped between droplets that are trying to coalesce (Figure 1.10). Even small quantities of xanthan gum cause a large increase in the viscosity of the water phase.

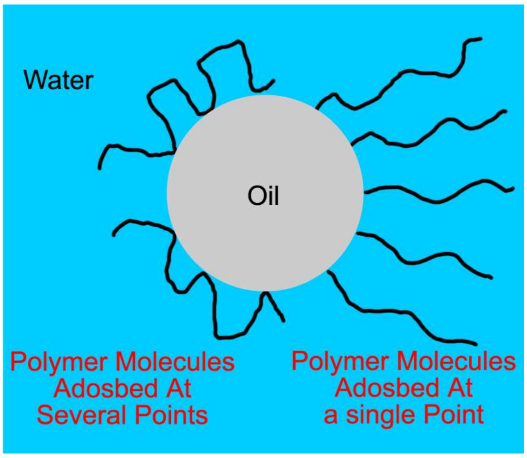

Figure 1.9: Adsorption of polymers at the oil/water interface.

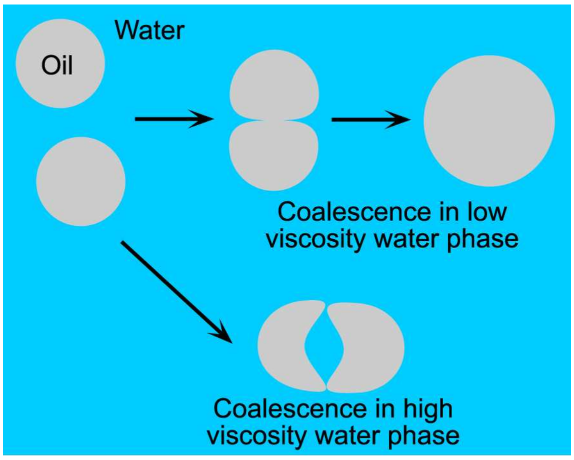

Figure 1.10: Coalescence of oil droplets in water phase.

1.5.3. Small Particles

Very small solid particles can be added to emulsions to act as a stabiliser. The effectiveness of these particles depends on how they interact with both liquids and the interface between them. Like polymeric stabilisation, the particles form a physical barriers around the oil droplets. While small particles can help stabilise an emulsion they probably will not make its initial formation easier.

1.5.4. Surfactants

The name *surfactant* is short for “surface active agents” and is given to molecules that have an effect on the surface energy of the oil/water interface. These chemicals not only increase the stability of emulsions but also make them substantially easier to form in the first place. Surfactants can achieve this because they act as a ‘bridge’ between the oil droplets and the water, reducing the surface energy of the interface and thus reducing the amount of energy needed to create new oil/water surfaces (see Section 1.4.2).

[5] Viscosity is a measure of the ability of a liquid to flow, therefore treacle has a higher viscosity than water.

Surfactants are molecules that are polar at one end and non-polar at the other, thus one end of the molecule dissolves in the oil droplet and the other end dissolves in the water phase (Figure 1.11).

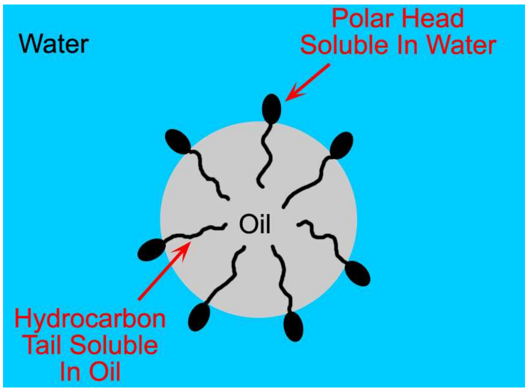

Figure 1.11: The action of surfactants bringing the oil/water interface.

Oil and water can be made to form a stable emulsion by adding soap as a surfactant. Soap often contains sodium stearate which has a long non-polar "tail" which dissolves in oil and a polar "head" which dissolves in the water (Figure 1.12). Any molecules with polar and non-polar parts will have some ability to act as an emulsifier. For example alcohol will stabilize an emulsion to some extent, although emulsifiers with longer "tails" and highly soluble polar "heads" tend to work best.

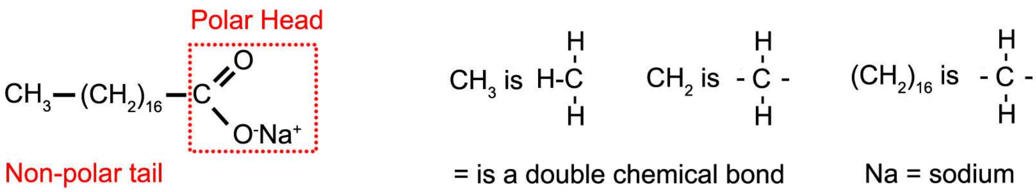

Figure 1.12: Sodium stearate.

1.5.5. Weighting Agents

Oil-in-water emulsions will eventually separate because most oils are less dense than water and will eventually float to the surface. This process is called creaming (see Section 1.4.3) and can be delayed if the oil droplets are very fine. Creaming will not happen if the oil phase has the same density as water.

Weighting agent are oils that, unusually, have a density greater than the density of water. Thus the overall density of the oil phase can be increased by add such a substances. The closer the density of the two phases, the more stable an emulsion will be.

2. A Few Cola Syrup Recipes

Note: All of the imperial measurements are US values and not UK values (see Appendix A2). The syrup is diluted by about 1:5 with carbonated water when bottled. More information about the ingredients can be found in Section 4.

2.1. The Original

The following recipe is supposedly the original coca-cola recipe that was unearthed in an old notebook that belonged to coca-cola inventor J. S. Pemberton. This recipe was largely substantiated by a second source who had been employed by coca-cola in the USSR during the 1940's. The recipe and account of how it was found is detailed in the book "For God, Country and Coca-Cola" by Mark Pendergrast (see Bibliography).

Ingredients:

1 oz Citrate Caffeine
1 oz Ext. Vanilla
2.5 oz Flavourings (see below)
4 oz F.E. Coco
Caramel – sufficient
3 oz Citric Acid
1 Qt. Lime Juice
30 lbs. Sugar
2.5 gal. Water

It seems that "F.E. Coco" refers to a fluid extract from coca leaves (the original recipe has the spelling mistake).

Flavourings (7X formula):

80 Oil Orange
120 Oil Lemon
40 Oil Nutmeg
1 Qt. Alcohol
40 Oil Cinnamon
20 Oil Coriander
40 Oil Neroli

There is no indication as to what the numbers preceding the flavour ingredients refer to. However, they may refer to the number of drops.

Directions:

Mix Caffeine Acid and Lime Juice 1Qt.
Boiling water add vanilla and flavourings when cool.
Let stand for 24 hours.

Source: www.sodamuseum.com, www.therisenrealm.com, en.wikipedia.org/wiki/Coca-Cola_formula, "For God, Country and Coca-Cola" by Mark Pendergrast (see the Bibliography).

It is suspected that most, if not all of the lime juice has been replaced by lime oil and that glycerine is now added as a preservative (emulsifier). Also, phosphoric acid is now used instead of citric acid. In the USA at least, some of the sugar has probably been replaced with high fructose corn syrup and artificial sweeteners.

It seems that the cocaine was removed in about 1901 by Asa Candler who commissioned a company to provide decocainized coca leaf. Because of the extraction method used (mulching the leaf in 20% alcohol) there was probably never more than 8.5 mg of cocaine in a 6 oz bottle. J S Pemberton insisted that the drink derived its invigorating properties from fourteen alkaloids[6] that are found in coca leaf and not just cocaine. There is no mention of Kola nuts. The kola nuts were used for their caffeine content and it is supposed that artificially produced caffeine citrate was used from an early date.

The original recipe was for a drink that was not bottled but sold out of “soda fountains” that where situated inside chemist’s shops. Therefore, the emulsion stability was not as critical as it is for drinks that are intended to be bottle and have a shelf life of several months.

2.2. Another Supposed Original

This version is from “Big Secrets” by William Poundstone NY:Quill (1983) (see Bibliography). This recipe is described by Mark Pendergrast as “a fairly accurate guesstimate” of the modern recipe. The recipe makes 1 gallon of syrup.

Ingredients:

2.4 kg Sugar, dissolved in the minimum of water
37 g Caramel
1.1 g Decocainized Coca Leaf
30 g Lime Juice
1.5 g Vanilla Extract
3.1 g Caffeine
11 g Phosphoric Acid
0.37 g Kola Nuts
19 g Glycerine (vegetarian)

Flavourings (7X formula):

0.88 g (1.032 ml) Lemon Oil
0.47 g (0.557 ml) Orange Oil
0.20 g (0.190 ml) Cassia Oil
0.07 g (0.077 ml) Nutmeg Oil
Trace Coriander Oil
Trace Lavender Oil
Trace Neroli Oil
4.9 g 95% Alcohol
2.7 g (2.7 ml) Water

Note: The millilitre (ml) values have been calculated from the weights in grams using the densities in Section 4.8.3 Cassia oil is also known as Chinese cinnamon oil.

Directions:

Mix the sugar with just enough water to dissolve it (high fructose corn syrup can be substituted for half the sugar). Add the caramel, caffeine and phosphoric acid. Then add the lime juice (or a solution of water with citric acid and sodium citrate at lime juice strength). Soak the coca leaf and kola nuts in 22 g of 20% alcohol, strain and add the liquid to the mix.

Mix together the essential oils and add the 95% alcohol. Shake. Add the water and let the mixture stand for 24 hours at about 15 °C. A cloudy layer will separate. Take off the clear part of the liquid only and add it to the sugar syrup.

Add the glycerine and vanilla extract. Add water (treated with chlorine) to make up to 1 gallon of syrup.

Source: A copy can be found at en.wikipedia.org/wiki/Coca-Cola_formula, **“**For God, Country and Coca-Cola” by Mark Pendergras (see the Bibliography)

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[6] Morphine, nicotine, caffeine, quinine and cocaine are all alkaloids – nitrogen containing organic molecules that occur in many plants.

Mark Pendergrast adds that this recipe tallies closely with a testimony by a coca-cola chemist at a Delaware court case in 1991: the differences are in the amounts – 13.2 g phosphoric acid (not 11 g), 1.86 g vanilla extract (not 1.5 g) and 91.99 g of single strength commercial caramel (not 37 g). This final difference may be due to a concentrated caramel being used, such products are widely marketed to the drinks industry.

2.3. The Supposed Pepsi-Cola Recipe

This is supposedly the original Pepsi-Cola recipe. It was submitted to a court in the USA when Pepsi-Cola filed for bankruptcy in 1923.

Ingredients:

7500 lbs. Sugar – standard confectioners
Up to 1200 gallons Water
58 lbs. Phosphoric Acid – S.G. 1.750
12 gal. Caramel – burnt sugar colour
12 gal. Lime Juice

Flavourings:

½ gal. Alcohol
6 fl oz. Lemon Oil
5 fl oz Orange Oil
1 fl oz Petit Grain
4 fl oz Cinnamon Oil
2 fl oz Nutmeg Oil
2 fl oz Coriander Oil

Note: Petit Grain is an essential oil extracted from the leaves and twigs of the lemon tree.

Pepsi-cola originally contained *pepsin*, an enzyme that aids digestion. Like coca-cola, pepsi-cola was first sold at soda fountains and it now probably contains gum Arabic as an emulsifier.

Source: www.sodamuseum.com

2.4. OpenSource Cola

The people who thought of open source software in the 1970's released this recipe.

Ingredients:

2 tsp. 7X Formula (see below)
3.50 tsp. 75% Phosphoric Acid or Citric Acid
2.28 l Water
2.36 kg Sugar – plain granulated
0.50 tsp. Caffeine (optional)
30 ml Caramel

Flavourings (7X formula):

3.50 ml Orange Oil
1.00 ml Lemon Oil
1.00 ml Nutmeg Oil
1.25 ml Cassia Oil
0.25 ml Coriander Oil
0.25 ml Neroli Oil
2.75 ml Lime Oil
0.25 ml Lavender Oil
10 g Gum Arabic
3 ml Water

Directions (quoted directly from the original source):

"Mix oils together in a cup. Add gum Arabic, mix with a spoon. Add water and mix well. I used my trusty Braun mixer for this step, mixing for 4-5 minutes. You can also transfer to a blender for this step. Can be kept in a sealed glass jar in the fridge or at room temperature. Please note that this mixture will separate. The Gum Arabic is essential to this part of the recipe, as you are mixing oil and water."

Note: no mention is made as to what you do once the mixture separates.

"In a one gallon container (I used the Rubbermaid Servin' Saver Dry Food Keeper, 1.3 US Gal/4.92 l), take 5 mls of the 7X formula, add the 75% phosphoric or citric acid. Add the water, then the sugar. While mixing, add the caffeine, if desired. Make sure the caffeine is completely dissolved. Then add the caramel color. Mix thoroughly."

Source: www.colawp.com/colas/400/cola467_recipe.html

2.5. Stevia Natural Sweetener Sugar Free Cola

This recipe is credited to Dr. Udo Kienle. It uses a sugar substitute but gives more details about the mixing process.

Ingredients (makes 1 litre of syrup):

0.07 kg/ l Stevia Natural Sweetener	6.0 ml/l Salt Solution
108.5 ml/l Cola Flavor Base (see below)	5.0 ml/l Citric Acid Solution, 50%
8.5 ml/l Phosphoric Acid, 85%	872.0 ml/l Processed water
0.007 kg/l Caramel, acid proof	

Flavour Base (makes 1 litre of flavour base):

1.32 g/l Vanilla Extract*	21.94 g/l Caffeine
4.29 g/l Solid Extract Kola nuts*	25.00 g/l Lime Oil Extract
41.74 g/l Cola Flavour Emulsion (see below)	75.56 g/l Phosphoric Acid, 85%
158.52 g/l Caramel, acid proof	671.63 g/l Processed Water

* A separate recipe is required for the extracts.

Cola Flavour Emulsion (makes 1 litre of flavour emulsion):

119.94 g/l Orange Oil Emulsion (see below)	2.64 g/l Oil of Lime, distilled
89.82 g/l Arabic Gum	2.64 g/l Oil of Orange, cold pressed
13.21 g/l Oil of Cinnamon	1.32 g/l Oil of Coriander
6.60 g/l Oil of Lemon, cold pressed	763.83 g/l Processed Water

Directions:

a) Combine the essential oils (except the orange oil), add magnesium carbonate and filter.
b) Prepare orange oil emulsion and Arabic gum by heating the orange oil up to 60 °C for ½ hour. Remove the oil from the heat and slowly add the Arabic gum. Stir for 15 minutes.
c) Add the essential oils to the orange oil mixture, then add the water and keep agitating for another 15 minutes.
d) Homogenize the mixture at 211 kg/cm^2.

Notes: There is no mention in the ingredients of magnesium carbonate. It probably refers to using very fine magnesium carbonate as a filtering aid. When filtering a 'slimy' substance a very fine inert powder can be used to prevent the filter from becoming clogged. 211 kg/cm^2 is the pressure to which a "homogenizer" is set (see Section 3.2.3.).

Source: www.uni-hohenheim.de/~www440/VTP/stevia/B0/B2

2.6. Another Recipe

This recipe is taken from "Food Flavourings" by Joseph Merory (see Bibliography).

Cola Flavourings Base Oils:

46.8 g Lemon Oil – California cold pressed	3.50 g Nutmeg Oil
14.20 g Lime Oil – distilled	0.01 g Neroli Oil
10.65 g Cassia or Cinnamon Oil	24.84 g Orange Oil

Note: The essential oils should be terpene free.

Dissolve in 11 fl. oz. of 95% alcohol. Agitate and add 5 fl. oz. water. Hold at 15°C. The mixture will separate and the clear portion is kept and filtered if necessary.

Phosphoric Acid Solution:
0.5 fl. oz. Phosphoric Acid USP 85% (liquid)
3.5 fl. oz. Water

Cola Nut Extract:
Mix 125 lbs Cola nut with 25 gal. warm water at 50°C. After 1 hour, mix with 25 gal. 95% alcohol. Stir the mulch twice daily. After 3 days take off 31 gals of the extract. Add 19 gals. of water and leave the remaining mulch for a further 2 days stirring twice daily before removing the final 19 gal. of extract and adding it to the previous extract.

Cola Flavour:

12 fl. oz. Cola Nut Extract (see above)	32 fl. oz. Lime Juice
2 fl. oz. Vanilla Extract*	32 fl. oz. Caramel – acid proof
2 fl. oz. Caffeine	12 fl. oz. Cola Flavour Base (see above)
100 fl. oz. Water	12 fl. oz. 95% Alcohol
16 fl. oz. Glycerine	

*The original source gives a long, detailed description of how to prepare the vanilla extract from vanilla beans. It has been left out for brevity.

4 fl. oz. of flavour and ½ fl. oz. phosphoric acid solution are added per gallon of syrup.

Note: The recipe does not say how much sugar is to be added per gallon of syrup.

3. General Notes On Cola Recipes

3.1. Rumours

Some people who have performed chemical analysis on Coca-Cola claim that it contains the following ingredients: cinnamon, nutmeg, vanilla, glycerine, lavender, fluid extract of guarana, lime juice and other citrus oils. Coca-Cola themselves admit that their drink contains at least 14 ingredients. There are some rumours that coca-cola had to announce to some Muslim countries (including Morocco) that the glycerine they used was produced from vegetable matter and not from pig fat.

3.2. Cola Emulsions And Emulsifiers

Cola is a water-based drink although it is flavoured with oil. This presents a problem since oil and water do not mix and an emulsifier is needed to create a stable beverage. If the cola has not been sufficiently stabilised the oil and water may separate during storage. Originally coca-cola was not intended to be bottled and stability was less of an issue. The original recipe (Section 2.1) does not contain an effective emulsifier, although alcohol and caramel will have some positive effect.

3.2.1. Alcohol Flavour Extraction

The method from the original recipe (Section 2.1) instructs that the oils should be mixed with ethanol (alcohol) before a little water is added. Essential oils are a complex blend of hydrocarbons and oxygenated organic compounds (see Sections 1.1.1, 1.1.2 and 4.8). The hydrocarbons have no polarity, will not interact with the alcohol and will separate once the water is added. The compounds that contain oxygen will interact with the alcohol and form a more stable emulsion with the water. Thus this process creates two phases, a flavour extract (clear part) and a washed oil (cloudy part); the flavour extract is used in the cola.

Treating the oils with alcohol will affect the flavour slightly since some of the molecules in the oils are removed. However, the hydrocarbon molecules that are removed (such as limonene and other terpenes, see Appendix A5) do not contribute much to the characteristic flavour of citrus oils. The alcohol extraction has a marked affect on the emulsion stability because the molecules that are removed are the most hydrophobic, and therefore the ones that are most likely cause the emulsion to breakdown. Also the hydrocarbon molecules will not contribute to the surface charge on the oil droplets reducing the effects of electrostatic stabilisation.

The recipe in Section 2.6 specifies that the essential oils are “terpene free”. Alcohol extraction will remove these compounds however, there are other extraction methods that do not require alcohol (see Section 4.8.1 and 4.8.2 for details). It seems unlikely that coca-cola sold in Muslim countries would be with prepared using alcohol.

3.2.2. Emulsifiers

Several ingredients can be added to give the cola a longer term stability. Coca-cola seems certain to contain glycerine however, pepsi-cola’s website does not list glycerine as an ingredient in any of their beverages. Gum Arabic is commonly used as an emulsifier in colas and is included on Pepsi’s ingredient list. New gum Arabic substitutes made from starches are available for use in soft drinks and may be easier to mix.

Caramel, added to cola primarily for its flavour and colour, can also act as an emulsifier. However, it can only stabilise an emulsion of very fine oil droplets.

Weighting agents can also be added to help prevent the oil and water phases separating (see Section 1.5.5). These substances are oils with unusually high densities (greater than the density of water). They are mixed with the flavouring oils so that the overall density of the oil phase is the same as the density of water (1 g/ml). Weighting agents therefore stop the oil droplets, contained within the emulsion, migrating to the surface under the influence of gravity. A common weighting agent is brominated vegetable oil (BVO), however this appears to be banned in Europe and only contained within beverages manufactured in the USA. Even in the USA the amount of BVO that can be added to a beverage is strictly limited.

Glycerol ester of wood rosin (E445, extracted from the stumps of pine trees) is another weighting agent that is sometimes used in citrus flavoured drinks. There are some concerns about the affects that it has on several organs within the human body, it is therefore limited to less than 100 ppm within soft drinks. Other weighting agents suitable for citrus based drinks, such as sucrose acetate isobutyrate, are available from chemical companies.

The densities of various flavouring oils are shown in Section 4.8.3, most are in the range 0.85 g/ml to 0.90 g/ml. An exception is cassia oil, which has a density slightly greater than the density of water; therefore adding more cassia oil will increase the density of the oil phase and increase the stability of the emulsion.

3.2.3. Mixing

Several industrial machines are widely used to mix food emulsion. Normally these use a *shearing* action to break large droplets up, rather than a simple stirring action (Figure 3.1).

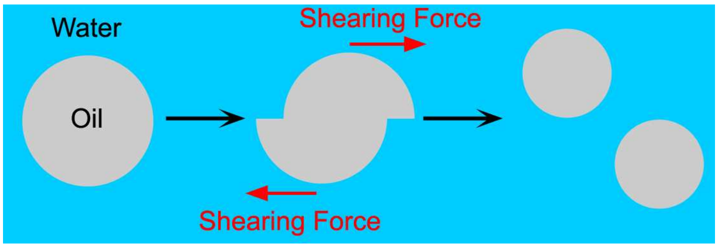

Figure 3.1: The shearing of large oil droplets.

Pressure homogenisers force liquid through a valve at high velocities (50 - 200 ms^{-1}) and pressures up to 10 000 psi (69 MNm^{-2}). The valve gap is about 15 - 300 microns and oil drops in the size 0.1 - 0.2 microns[7] are formed. Two-stage homogenisers force the liquid through a second valve at a lower pressure (400 - 500 psi, 2.8 - 3.4 MNm^{-2}) to break up any droplet flocs that form exiting the first value. These machines tend to be quite large and use several pistons to provide the pressure.

Colloid mills consist of two concentric discs separated by a gap of 50 – 150 microns. One disc remains stationary while the other spins at 3000 – 10 000 rpm. The emulsion

[7] 1 micron = one 1000^{th} of a millimetre.

is sheared between the discs producing droplets that are 1 – 2 microns in size. Colloid mills tend to be much smaller than pressure homogenisers.

The mixing of the emulsifier with the other ingredients is critical. Often the gum Arabic is first mixed with a small amount of water before it is added to the flavouring oils. Other ingredients, such as caramel and citric acid are usually added as solutions to insure that they mix in easily. For stable emulsions it is usually estimated that the oil droplets should be no bigger that 3 microns, however if a good emulsifier is not used the droplets should not exceed 1 micron.

3.2.4. Acidulants

The sugar/acid balance in colas is very important for “mouth feel” and taste. Phosphoric acid or citric acid are added to create acidity (see Sections 4.6 and 4.12). Citric acid is said to have a light and fruity character, whereas phosphoric acid is said to have a flat, drier flavour. In addition to these acids the carbon dioxide (CO_2) in carbonated drinks also acts as an important acidulant; creating carbonic acid in water (see Section 4.5).

3.2.5. Antioxidants

Oil based flavourings are vulnerable to deterioration by oxidation because air becomes trapped in the emulsion during the mixing process. Colas don’t seem to have antioxidants routinely added however, other soft drinks contain various chemicals to prevent oxidation. These include compounds that contain tocopherols[8].

3.2.6. Preservatives

Carbonated soft drinks can support the limited growth of micro-organisms. Acidulants provide some protection since a lot of micro-organisms are not tolerant to acidic conditions, however such substances are considered to be a safe guard and not a primary barrier to microbial growth. Other substances such as sulphur dioxide (SO_2) and benzoic acid can be added as preservatives (see Sections 4.2 and 4.14). These two substances are normally added together because they have a synergistic effect; SO_2 acts against micro-organisms and benzoic acid guards against yeasts.

3.2.7. Foaming Agents

Foaming agents are added to soft drinks so that a good head is formed on pouring. *Saponins* from bark of Quillaia or yucca trees are often included to fulfil this purpose.

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[8] Tocopherol is the chemical name for vitamin E. Tecopherols are molecules derived from tocopherol.

4. A Review Of Ingredients

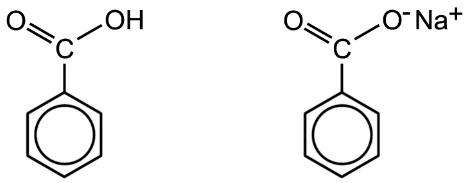
4.1. Alcohol

Alcohol refers to ethanol that has the formula CH_3CH_2OH, (C_2H_6O) and has a density of 0.79 g/ml. It is used in some of the recipes to remove the more hydrophobic molecules (terpenes) from the essential oils thus creating a more stable oil/water flavouring emulsion. The alcohol is not later removed from the mixture but once the syrup is completed and subsequently diluted it is present in very small quantities.

The concentration of alcohol in a solution is normally increased by distillation however, it is not possible to get above 95.6% alcohol using this method. For this reason most "pure" alcohol is sold as *95% alcohol*. Higher purities of alcohol can be obtained using chemical processes and 100% alcohol is sold as *absolute alcohol*.

4.2. Benzoic Acid (E210) & Benzoates (E211)

Both of these compounds are added to soft drinks as preservatives. The sodium (Na) salt of benzoic acid is more soluble than the acid (Figure 4.1) itself and is more commonly used. Un-dissociated acid molecules (formed from the salt in solution) are responsible for the anti-microbial action and this is optimum in the pH range 2.5 – 4. These preservatives are effective against yeast but not bacteria and so are usually used in conjunction with sulphur dioxide (see Section 4.14).



(a) (b)

Figure 4.1: Molecules of (a) benzoic acid and (b) sodium benzoate.

4.3. Caffeine

Caffeine is an alkaloid (Figure 4.2) found in cola nuts and numerous other plant matter. It has limited solubility in water and is often added to drinks as the more soluble citrate of caffeine. There is between 70 - 100 mg of caffeine in a cup of coffee and 10g of neat caffeine is enough to kill a person.

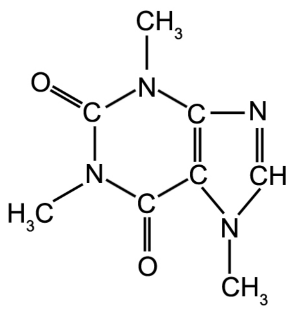


Figure 4.2: The caffeine molecule.

Source: "Coffee Vol 1: Chemistry", edited R J Clarke & R Macrae (see Bibliography).

4.4. Caramel (E150d)

Caramel colours are amorphous, brown to brownish materials resulting from the carefully controlled heat treatment of food grade carbohydrates in the presence of small amounts of food grade acids, alkalis or salts. They are often liquids with very fine particles suspended in them (*colloid suspensions*) and have a density of between 1.25 and 1.36 g/ml. Caramel is added primarily for its colouring properties however it will also act as an emulsifier. If caramel is to be the only emulsifier the drops of oil in the emulsion need to be exceptionally small (about 1 micron).

Caramels have a range of pH values and the one that you use should have a low pH (2.5 - 3.5) that is matched to the acidic environment of the cola itself. You should also check that the isoelectric point is lower than pH 1.5 (see Section 1.4.4). Caramels that are appropriate to colas are often called "negative", "acid proof", "class IV" or "ammonium sulphate type" caramels. These caramels are made by heating carbohydrates in the presence of ammonium sulphate and they have negatively charged particles that match the negatively charged droplets in the cola emulsion. Failure to choose an appropriate caramel may cause caramel particles being attracted to the negatively charged oil droplets in the cola emulsion, resulting in a sediment forming at the bottom of the cola. Since the caramels are so acidic care should be taken when handling them.

Source: **www.caramelworld.com/solution_center/basics_of_caramel_colors.asp**, "Beverages" by Alan H Varnam and Jane P Sutheralnd (see Bibliography).

4.5. Carbon Dioxide (E290)

Carbon dioxide (CO_2) is the only gas suitable for creating fizzy drinks and 2 – 3 volumes are added to the water used to dilute the syrup. Water containing CO_2 is acidic and has an odour due to the formation of carbonic acid (H_2CO_3):

$$H_2O + CO_2 \rightleftharpoons H_2CO_3$$

The carbonic acid is an important acidulant (see Section 3.2.4).

Source: "Beverages" by Alan H Varnam and Jane P Sutheralnd (see Bibliography).

4.6. Citric Acid (E330)

A carboxylic acid (see Appendix A4) that is abundant in lemons and limes, making up about 8% of their dried weight. It is used extensively in foods and drinks as a preservative and as flavouring. It has a chemical formula of $COOHCH_2C(COOH)(OH)CH_2COOH$ (Figure 4.3), ($C_6H_8O_7$) and has a density of 1.665 g/cm^3. Normally 1 ½ times the amount of phosphoric acid is added for the same feeling of acidity on the palate. Citric acid is also said to be lighter and fruitier than phosphoric acid.

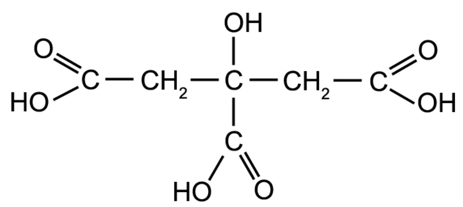


Figure 4.3: The citric acid molecule.

Source: "Beverages" by Alan H Varnam and Jane P Sutheralnd (see Bibliography).

4.7. Cola Nut

Also known as guru, goora or bissey nuts. They have a caffeine content of 2.16% which can be extracted by soaking the nuts in alcohol.

Source: "Food Chemistry" by H-D Berlitz & W Grosch (see Bibliography).

4.8. Essential Oils

These oils are a complex mixture of molecules, some of which dissolve more readily in alcohol than others. The exact composition of each oil will vary depending on the source and extraction method. The constituent molecules can be broken down into three categories:

- *Hydrocarbons compounds* – These are made up from atoms of carbon and hydrogen only. They do not readily dissolve in water but can form an emulsion if an emulsifier is used. Common molecule types include terpenes and monoterpenes (see Appendix A5).
- *Oxygenated Compounds* – These are organic molecules that contain oxygen. Examples are esters, aldehydes, ketones, alcohols, phenols and oxides. Because they contain polarising oxygen atoms they will be less hydrophobic than the hydrocarbon molecules (see Appendix A4).
- *Miscellaneous Compounds* – Including acids, lactones, sulphur compounds and nitrogen compounds.

It is the oxygenated compounds that contribute most to the oil's flavour. Different oils will have different proportions of hydrocarbons and oxygenated molecules, therefore different oils will have different solubilities in alcohol. Citrus oils have large amounts of terpenes and are not very soluble in alcohol. However other oils have much larger quantities of alcohols and esters, and are soluble in much smaller volumes of alcohol. Section 4.8.3 summarises the compositions and solubility of the essential oils used in colas.

4.8.1. Flavour Extraction

Extraction processes can be used to remove the hydrocarbon molecules, particularly the terpenes, which have little contribution the flavour and are very hydrophobic. *Terpene free* essential oils are marketed for use in beverages. As mentioned above (Section 2 and 3.2.1) some cola recipes suggest that the essential oils are mixed in alcohol to remove terpenes, resulting in a mixture that will form a more stable emulsion with water.

Other commercial extraction methods are available including distillation and *counter-current extraction*. This latter method involves using methanol and hexane; the methanol dissolves the oxygen containing compounds and the hexane dissolves the hydrocarbon molecules, the methanol is easily removed after extraction. Distillation may result in the loss of some of the more volatile flavour components.

Source: "Beverages" by Alan H Varnam and Jane P Sutheralnd."Common Fragrances and Flavor Materials" By Kurt Bauer and Dorothea Garbe (see Bibliography)

4.8.2. Oil Extraction

There are several ways to extract essential oils from plants and the molecular composition of the final oil will depend to some extent on the method used, although many oils can only be extracted by one method:

- *Cold Pressing (Expression)* – This is probably the most desirable method for flavouring oils but is normally only used for citrus oils. Terpenes are extracted from the plant material by this methods and a subsequent process, such as distillation or counter-current extraction, is needed to make a terpene free oil.
- *Liquid CO_2* – Liquid CO_2 at 10 °C and a very high pressure is used as a solvent to remove the essential oils from plant material. Once at atmospheric pressure the CO_2 easily escapes leaving no residue. This process does not remove terpenes and can therefore create a terpene free oil.
- *Steam distillation* – This is probably the most common extraction method. Steam is used to break down the plant material and the essential oils are released as vapour which is then condensed. This method is not recommended if there is an alternative because insoluble terpenes are extracted and additional terpenes may be created when the plant material is heated. Also some of the more volatile flavour molecules may be lost. Terpenes may be removed from the oil by a subsequent distillation process, however even more of the volatile components may be lost.
- *Solvent Extraction* – Solvents are used to remove the oils from the plants. This method is not suitable for flavouring oils because solvent residues will taint their flavour.

Source: “Common Fragrances and Flavor Materials” By Kurt Bauer and Dorothea Garbe, “Development In Food Flavours” Ed. G G Birch and M G Lindley (see Bibliography).

4.8.3. The Properties Of Essential Oils

Note: Alcohol in the ‘solubility’ Section refers to ethanol. For more detail about the constituent molecules see Appendix A5. Exact compositions, solubility and densities depend on the country of origin and the extraction method.

Cassia Oil

Source:	Steam distillation of leaves and young twigs from *Cinnamomum cassia* (both cinnamon bark and leaf oils are obtained from *Cinnamomum zeylanicum*).
Composition:	Contains up to 90% cinnamaldehyde with lesser amounts of eugenol and other compounds. The composition is similar to that of cinnamon bark oil but cinnamon leaf oil has about 70-90% eugenol and about 7% cinnamaldehyde.
Solubility:	1 part in 2, in 80% alcohol. Will form a clear solution in 3 parts 70% alcohol.
Density:	1.045-1.065 g/ml @ 25°C

Coriander Oil

Source: Steam distillation of partially dried, fully ripe fruits of *Coriandrum stivum.*

Composition: Main component is linalool (60-80%). The remainder is mainly terpene hydrocarbons including α-pinene and γ-terpinene (about 5% each).

Solubility: 1 part in 8 in 65% alcohol. 2 parts in 1 in absolute alcohol and 1 part in 3 70% alcohol forming a clear solution in the absence of terpenes.

Density: 0.863-0.878 g/ml @ 25°C

Lavender Oil

Source: Steam distillation of freshly cut flower tops from *Lavandula angustifolia* (French lavender oil), *Lavandula spica* (Spanish spike lavender oil) or a hybrid of the two (lavindin oil).

Composition: Chief components are alcohols and esters. The composition varies considerably depending on the source. French is up to 60% linalyl acetate (ester). Spanish spike has far more linalool. Lavindin is between the other two.

Solubility: Between 1 part in 5, to 1 part in 3 in 70% alcohol, with Spanish spike oil being the most soluble.

Density: 0.880-0.895 g/ml @ 25°C

Lemon Oil

Source: Pressed peel of *Citrus Limon* (lemon petitgrain is from steam distillation of leaves).

Composition: Depends on variety of lemon. Contains mainly terpenes – limonene (about 65%), β-pinene and γ-terpinene (8-10% each). The lemon flavour is chiefly from citral (aldehydes) (3-10%).

Solubility: Soluble 1 part in 12 absolute alcohol. Probably will not form a clear solution due to wax-like constituents.

Density: 0.851-0.855 g/ml @ 25°C

Lime Oil

Source: From whole cold pressed fruit or steam distilled fruit from *Citrus aurantifolia.*

Composition: Cold pressed: 50-60% limonene and 10% each of β-pinene and γ-terpinene. The lime flavour come from citral (4.5-9%). The steam distilled oil has 0.5-2.5% citral.

Solubility: Cold pressed: 1 part in 0.5 part 95% alcohol. Steam distilled: 1 part in 5 90% alcohol.

Density: 0.910-0.915 g/ml @ 25°C

Neroli Oil

Source: Steam distillation of the flowers of *Citrus aurantium* (bitter orange tree).

Composition: Depends on the flower source and distillation method but has about 30% linalool.

Solubility: 1 part in 2 80% alcohol.

Density: 0.868-0.880 g/ml @ 25°C

<u>Nutmeg Oil</u>

Source: Steam distilled from nutmeg, the dried fruit of *Myristica fragrans*.
Composition: About 90% terpene hydrocarbons. Very similar to mace oil.
Solubility: 1 part in 3-4 parts 90% alcohol.
Density: 0.862-0.882 (West Indian), 0.883-0.917 (Indonesian) g/ml @ 25°C

<u>Orange Oil (Sweet)</u>

Source: Pressed peels of *Citrus sinensis*.
Composition: Limonene over 90%. Aldehydes include citral, octanal, decanal. Esters include octyl and neryl acetate. The exact composition depends on the source.
Solubility: Soluble 1 part in 7 parts alcohol. A clear solution will not always form because of the presence of waxy non-volatile substances.
Density: 0.842-0.849 g/ml @ 25°C

<u>Orange Oil (bitter)</u>

Source: Pressed peels of *Citrus aurantium*.
Composition: Limonene over 90%. Less aldehydes and more esters than sweet orange.
Solubility: Soluble 1 part in 7 parts alcohol. A clear solution will not always form because of the presence of waxy non-volatile substances.
Density: 0.845-0.851 g/ml @ 25°C

Source: www.ibiblio.org, “Common Fragrance and Flavor Materials” by Kurt Bauer and Dorothea Garbe, “Analysis Of Essential Oils By Gas Chromatography And Mass Spectrometry” By Yoshiro Masada (see Bibliography).

4.9. Glycerine (E442)

Glycerine, also known as glycerin and glycerol, has the chemical formula $HOCH_2CH(OH)CH_2OH$ and has a density of 1.26 g/ml. It can be obtained from either animal fat or vegetable matter, therefore you should check if you intent to make a vegetarian cola.

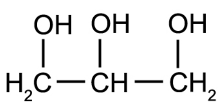


Figure 4.4: The glycerine molecule.

Glycerine is added to the cola flavour emulsions as an emulsifier and because it has the combined solvent effects of alcohol and water. It may also act as an anti-oxidant.

Source: “Food Flavourings” by Joseph Merory (see Bibliography).

4.10. Guar Gum (E412)

A polysaccharide gum that can be used to stabilise emulsion .

4.11. Gum Arabic (E414)

Gum arabic is a polysaccharide prepared from the stems and branches of sub-Saharan *Acacia senegal* and *Acacia seyal* trees. Unlike other polysaccharide gums molecules of gum Arabic can adsorb to oil droplets in flavour emulsions (see Section 1.5) but has little effect on the viscosity of the water phase in solutions below a 50% concentration. Gum Arabic is soluble in water up to a 50% solution.

In colas it is used as an emulsifier because of its ability to form a protective barrier around oil droplets. Care must be taken to use a gum appropriate for foodstuffs, also there are "emulsion grade" gums that are specially prepared to be used as emulsifiers in beverages. Significant amounts of gum are needed to stabilise cola emulsions; somewhere between 18 and 22% weight/volume. Gum substitutes made from starch are now available.

Source: www.lsbu.ac.uk/water/, http://www.foodproductdesign.com/ (articles entitled "Pop Art" and "Beverage Stabilizers"), "Food Chemistry" by H-D Belitz & E Grosch, "Polysaccharides In Food" by J M U Blanshard & J R Mitchell. (see Bibliography).

4.12. Phosphoric Acid (E388)

A mineral acid with the formula H_3PO_4 (Figure 4.5). It is used as an alternative to citric acid and is substantially cheaper to produce in bulk. It has been linked with osteoporosis. It is a liquid with a density of 1.834 g/ml (at 18 °C). Normally considered to be flatter and dryer in flavour than citric acid. Phosphoric acid is added at about two thirds of the amount of citric acid to give the same feeling of acidity on the palate.

Phosphoric acid is sold as 50, 75 and 80% strengths.

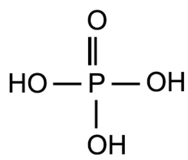


Figure 4.5: The phorsphoric acid molecule.

Source: "Beverages" by Alan H Varnam and Jane P Sutheralnd (see Bibliography).

4.13. Sugar

Sugars are carbohydrates, therefore they contain carbon, hydrogen and oxygen atoms. Normal granulated sugar is sucrose; a sucrose molecule is made from a glucose molecule and a fructose molecule joined together.

Often some of the sugar is replaced with high-fructose corn syrup (HFCS) and artificial sweeteners. There is a small risk that using HFCS will cause the cola to be contaminated with yeast.

4.14. Sulphur Dioxide (E 220)

Sulphur dioxide (SO_2) is added to soft drinks as a preservative and forms sulphurous acid and thus bisulphate and sulphite ions when mixed with water:

$$SO_2 + H_2O \rightleftharpoons H_2SO_3$$
$$2H_2SO_4 \rightleftharpoons H^+ HSO_3^- + 2H^+ SO_3^{2-}$$

Anti-microbial action depends on undisolved sulphurous acid molecules being present, this occurs at low pHs. Sulphur dioxide is effective against all micro-organisms but not some yeasts, it is therefore used in conjunction with Benzoic acid (see Section 4.2).

Source: "Beverages" by Alan H Varnam and Jane P Sutheralnd (see Bibliography).

4.15. Water

The mineral content of water is important. High levels of minerals such as iron and copper can have an adverse effect on flavour. The stability of emulsions can be reduced if alkaline water (i.e. hard water with a pH greater than 7) is used, therefore calcium and magnesium carbonates should be kept to a minimum. Bottled water is sold with a chemical analysis printed on the label; you should choose the one with the lowest concentrations of Ca^{+} and Mg^{2+} ions.

Parameter	Maximum Permitted Level (mg/l)
Total Dissolved Solids	500 – 850
Alkalinity (as $CaCO_3$)	50
Chloride	250 – 300
Sulphate	250 – 300
Iron	0 – 0.3
Aluminium	0 – 0.2

Table 4.1: Chemical standards for water for soft drink manufacturers.

In addition to the specifications in Table 4.1 the nitrate level should be kept below 10 mg/l if the cola is to be canned. Also if the water is to be carbonated the level of dissolved oxygen should be below 1 mg/l. Chlorine can be removed from water by passing it through a granulated activated carbon filter or by reverse osmosis.

Source: http://www.foodproductdesign.com/ (articles entitled "Pop Art" and "Beverage Stabilizers"), "Beverages" by Alan H Varnam and Jane P Sutheralnd (see Bibliography).

4.16. Xanthan Gum (E415)

Produced by the fermentation of the *Xathamonas campestris* micro-organism on a glucose medium. Like gum Arabic, xanthan gum is a polysaccharide and it can be used to stabilize emulsions. It acts as a hydrocolloid increasing the viscosity of the water phase and does not act as a surfactant or adsorb to the surface of the oil droplets oil (see Section 1.5.4). About 1% Xanthan gum can produce a surprisingly large increase in viscosity. Xanthan gum is also very stable across a wide range of temperatures and pH.

Source: Polysaccharides In Food edited J M U Blanshard & J R Mitchell (see Bibliography).

Appendix A1. Abbreviations

b.p.	Boiling Point
BVO	Brominated Vegetable Oil.
deg. C	Degrees Centigrade.
Ext.	Extract
F.E.	Fluid Extract.
fl. oz.	Fluid Ounce.
g	Gram.
g/cm^3	Grams Per Centimetre Squared, a measure of density (1g/ g/cm^3=1g/ml).
g/l	Grams per litre.
g/ml	Grams Per Millilitre, a measure of liquid density (1g/ g/cm^3=1g/ml).
g/l	Grams Per Litre.
gal.	Gallon.
HFCS	High-Fructose Corn Syrup.
kg	Kilogram.
Kg/cm^2	Kilograms Per Centimetre Squared, a measure of pressure.
Kg/l	Kilograms per litre.
l	Litre.
lbs.	Pound.
mg.	Milligram.
ml	Millilitre.
MNm^{-2}	Mega Newtons Per Metre Squared, a measure of pressure.
ms^{-1}	Metres Per Second.
oz.	Ounce.
pH	The measurement of acid/base strength .
ppm	Parts per million
psi	Pounds Per Square Inch, a measure of pressure.
Qt.	Quart.
rpm	Revs. Per Minute
s.g. & S.G.	Specific Gravity.
tsp.	Teaspoon.

Appendix A2. Metric/Imperial Conversions

Note: The name 'imperial' normally refers to the UK values and the US values are usually referred to as 'US customary units'.

Volume:
1 UK gallon = 4.546 litres
1 US gallon = 3.785 litres

1 UK fluid ounce = 28.41 millilitres
1 US fluid ounce = 29.57 millilitres

1 UK tablespoon = 15 millilitres (*Note:* in Australia 1 tablespoon= 20 ml)
1 US tablespoon = 14.8 millilitres

1 UK teaspoon = 5 millilitres
1 US teaspoon = 4.93 millilitres

1 UK quart = 1.101 litres (1/4 US gallon = 2 pints)
1 US quart = 0.946 litres (1/4 US gallon)

Note:
1 litre = 1000 millilitre = 1000 cubic centimetres (cc or cm^3) = 100 centilitres (cl)

Mass:
1 grain = 0.065 grams
1 ounce = 28.349 grams
1 pound = 0.454 kilograms

Note:
1 kg = 1000 grams

Appendix A3. Volume/Mass Conversions

Volume and mass are linked to density by the following simple equation:

density = mass/volume

Therefore to convert from a mass (in grams) to a volume (in millilitres) you must divide the mass by the density. To convert from a volume to a mass you must multiply the volume by the density.

Note: It is essential that you keep the mass, volume and density in the correct units. For example mass in grams, volume in millilitres and density in grams per millilitre.

The density of water is 1 g/ml or 1 kg/l, therefore 1 ml of water has a mass of 1g and 1 l of water has a mass of 1 kg.

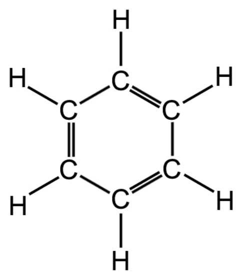
Note: That the overall density of the oil phase will depend on the proportion of each constituent oil.

Appendix A4. Important Organic Functional Groups

Functional groups are important because they dictate the chemical nature of a molecule. For example all simple alcohols will undergo similar reactions. In representing these groups ‘R’ indicates a simple hydrocarbon group. Therefore writing R-OH indicates any simple alcohol, for example CH3OH (methanol) and CH_3CH_2OH (ethanol).

<u>Benzene Ring</u>

The benzene molecule (C_6H_6) consists of six carbon atoms arranged in a closed hexagon with alternate single and double bonds, each carbon atom is bonded to a single hydrogen atom. Benzene rings can form part of larger molecules.



The benzene ring

The simplified representation of the benzene ring.

<u>Alcohol</u>

Group: R — OH

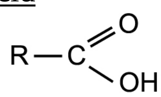
An -OH group attached to a hydrocarbon.

Example: CH_3CH_2 — OH

Ethanol

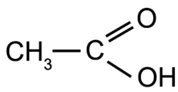
<u>Carboxylic Acid</u>

Group:



A double bonded oxygen atom and an –OH group bonded to the same carbon atom which is also bonded to a hydrocarbon group.

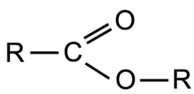
Example:



Acetic Acid – found in vinegar

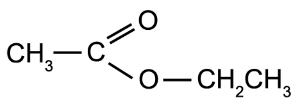
<u>Ester & Ether</u>

Group:



A double bonded oxygen atom and an oxygen atom linking a hydrocarbon group are both attached to the same carbon, which is also bonded to a second hydrocarbon group. Ethers have the linking oxygen but not the double bonded oxygen.

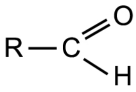
Example:



Ethyl Acetate (an ester)

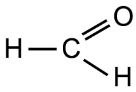
Aldehyde

Group:



A double bonded oxygen atom and a hydrogen atom bonded to the same carbon atom which is also bonded to a hydrocarbon group.

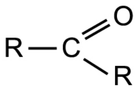
Example:



Formaldehyde

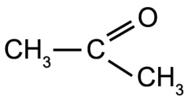
Ketone

Group:



A double bonded oxygen atom and two hydrocarbon groups bonded to the same carbon atom.

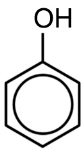
Example:



Acetone

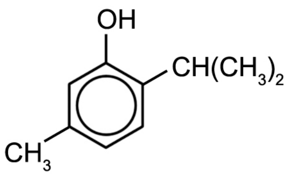
Phenol

Group:



An –OH group bonded directly to a benzene ring.

Example:



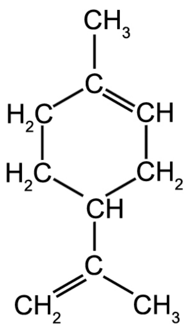
Thymol

Appendix A5. Molecules Commonly Found In Essential Oils

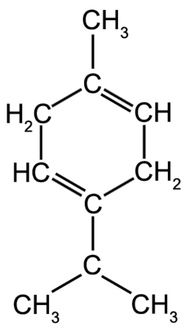
A5.1. Terpenes

Terpenes are hydrocarbon molecules which are based around the formula $C_{10}H_{16}$. They make up a substantial part of several oils, especially citrus oils. There are two main types of terpene: cyclic and acyclic terpenes.

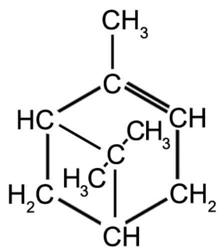
<u>Cyclic Terpenes</u>



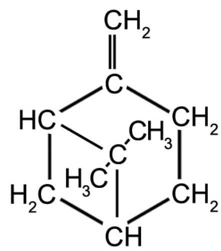
Limonene
b.p. 178 °C



γ-Terpinene
b.p. 183 °C

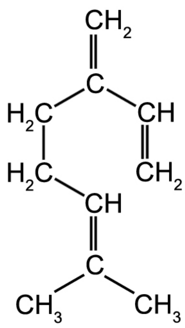


α-Pinene
b.p. 156 °C

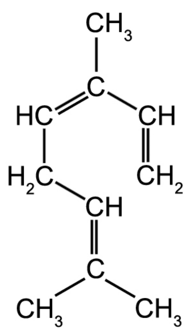


β-Pinene
b.p. 164 °C

<u>Acyclic Terpenes</u>



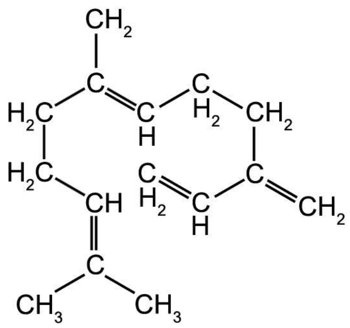
Myrcene



Ocimene

A5.2. Sesquiterpenes

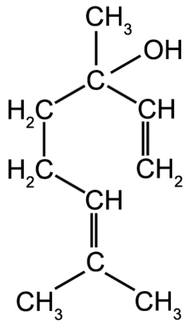
Sesquiterpenes hydrocarbon molecules which are based around the formula $C_{15}H_{24}$.



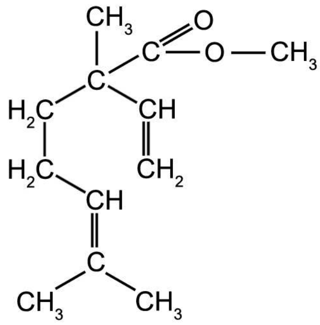
β-Farnesene

A5.3. Oxygen Containing Molecules Derived From Terpenes

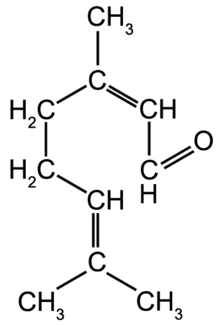
Many oxygen containing molecules are derived from terpenes including acids, alcohols, esters, aldehydes and ketones.



Linalool (an alcohol)
b.p. 198 °C

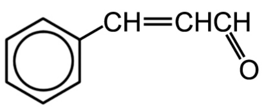


Linalyl Acetate (an ester)
b.p. 220 °C

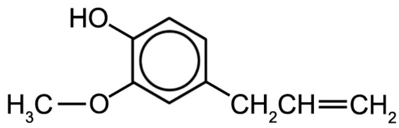


Citral (an aldehyde)
b.p. 118 °C

A5.4. Oxygen Containing Molecules Derived From Benzene



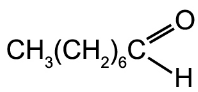
Cinnamaldehyde (aldehyde)
b.p. 253 °C



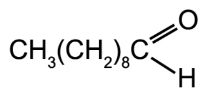
Eugenol (phenyl ether)
b.p. 121 °C

A5.5. Aliphatic Aldehydes

Aliphatic is the name given to any organic molecule that has all its carbon atoms in a straight line.



n-Octanal
b.p. 171 °C



n-Decanal
b.p. 208 °C

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