CHEMISTRY CHANGES EVERYTHING

Coca-Cola Revealed…

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COCA-COLA REVEALED ......

-well partly, at least

Introduction

What is the secret of what is perhaps the most popular soft drink in the world? I'm not referring to water, but about Coca-Cola, otherwise known as Coke.
This beverage has existed for well over one hundred years and has undergone many changes in that period of time; changes in ingredients, changes in bottle shape – even changes in name.

When did this all begin?

Druggist John Stith Pemberton first produced and marketed the drink. In 1886, he sold it in Jacob's drugstore in a soda fountain. Initial sales did not look promising, as he sold just 9 drinks daily at the beginning. After one year, sales totalled just $50!
Prior to the marketing launch, it existed in an alcohol-based form. The original drink contained coca (from which cocaine-based drugs can be obtained), kola nuts (which contain caffeine) and damiana. This combination gave the drink stimulant and analgesic qualities.
(It has been suggested that the inclusion of coca was due to Pemberton's addiction to opiates, following his being wounded in the latter stages of the U.S. Civil War.)

Coca-Cola was sold in bottles from 1984 onwards and in cans from 1955.

From these humble beginnings, Coca-Cola has become what is probably the most popular soft drink of all time. It is now sold in over 200 countries, with over 1 billion drinks sold worldwide daily!

Is this really chemistry?

Well, we only have to look at the label to see what's in it. The ingredients are listed as: water, sugar, carbon dioxide, colour caramel E150d, phosphoric acid, flavours and caffeine.

The use of the word 'flavours' leaves a great deal to the imagination. The actual composition of this ingredient is still a mystery, sometimes called the "secret ingredient".

The phosphoric acid gives the drink a sour, biting taste. The caramel (E150) is there to provide the dark colour. Sugar and flavours help the drink to be more palatable. The carbon dioxide provides the refreshing fizz. Caffeine acts as a stimulant.

There have been many attempts over the years to copy the Coca-Cola taste, notably its closest rival Pepsi-Cola (now known simply as 'Pepsi'.) The true composition of Coca-Cola will probably never be known, unless industrial espionage can be encouraged!

So, do you want to try something out?

A very simple test which can be done at home is to show the acidic nature of Coca-Cola. All that is needed is a dirty 'copper' coin such as UK pennies, US cents or Euro cents. These can be immersed in Coca-Cola for a few minutes. The phosphoric acid reacts with the copper compounds which are responsible for causing the dull coating on the coin. These dissolve in the remainder of the drink leaving the coin bright and shiny.
[NOTE: do not drink the residual Coca-Cola, as it will now contain toxic copper salts!]

The acidity of the drink can also be shown by immersing a small strip of universal indicator paper into the drink. A red colour will be produced, suggesting a surprisingly low pH, perhaps pH2.

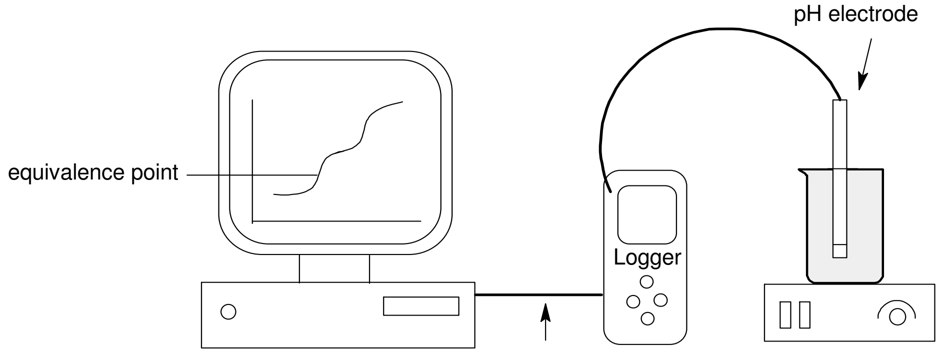
A somewhat more detailed investigation can be carried out in a chemistry laboratory:

How much carbon dioxide and phosphoric acid can be found in a cola drink?

Aim: To investigate the acid-base titration with cola drink straight from the bottle and compare with boiled cola drink and drink which has been left unstoppered for a short time. Describe the titration curve produced and find out/calculate approximate amount of carbon dioxide in fresh drink and phosphoric acid in both drinks.

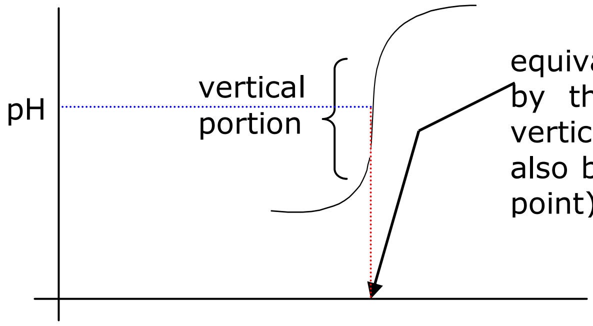
Materials and equipment: cola drink, NaOH (0.2 mol/l); beakers (250 ml, 50 ml), cylinder 100 ml; burner, tripod stand, stirrer, micropipette (0.3 ml), data logger*, pH electrode

Scheme:

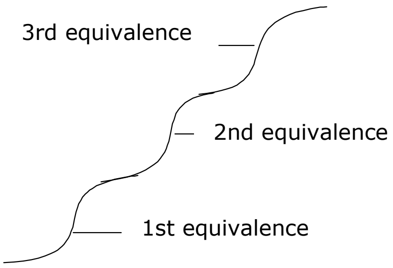


A data logger is an electronic device used in conjunction with a PC. It can be connected to various probes to measure a variety of quantities such as temperature, pH, light absorption, gas volume, mass etc.

Background: Titration is a method of quantitative analysis. It is often used to determine the unknown concentration of specific substance in a sample knowing the volume of the sample. Titration is a process when the known substance of known concentration (volumetric solution) is being added to a solution of unknown concentration until the equivalence point is somehow observed. The equivalence point represents when the given reaction is exactly in the ratio of stoichiometric coefficients. The equivalence point can be identified in many ways. The easiest is to use acid/base indicators which react at the equivalence point, accompanied by a colour change. Unfortunately, this change of colour is viewed differently depending on which person observes the change, because colour reception is unique to the individual. The accuracy also depends on the chosen indicator. These reasons lead us to use objective methods of detection, when the equivalence point is indicated by physico-chemical method. One of these methods is potentiometry, which uses the fact that the pH changes dramatically when close to the equivalence point. This point of maximum change is so called an inflexion point, where the titration curve changes its shape (from convex to concave and conversely). It is a point mid-way between the two bends on the titration curve (see figure below), therefore the titration is performed well beyond the equivalence point. The equivalence point can be determined by simply reading from a graph. A plot of pH (as ordinate) against volume of titrant (as abscissa), for a monohydric acid, produces the curve shown below:



In other cases, the curve shape depends on the number of available hydrogen ions. For example, the titration curve of phosphoric acid should be as follows:



As this is a triprotic acid, there should be three equivalence points, as shown.
In practice, we will see just two equivalence points, because the acid is only titrated to its first two stages, the third cannot easily be detected (it refers to very weak acid; furthermore the pH glass electrode won't be able to measure pH accurately in such a strongly basic solution).
The unknown concentration can be then found by knowing the volume at each equivalence point, the concentration of volumetric solution and the volume of sample used. To calculate the amount of phosphoric acid any of the points can be used, as long as we remember the reaction stoichiometry.
Another value can be read from the curve: pK_a - the negative logarithm of the dissociation constant K_a that describes the strength of acid. The value refers to the pH of the titration mixture half way to the equivalence point (i.e. between the start and the first eq. point and then between the first and second eq. point). pK_a is an important characteristic of a weak acid; it is used when calculating the pH of a weak acid or buffer preparation.
When there is more than one type of acid in the sample, the shape of titration curve produced changes. If the acids have a similar pK_a, the equivalence point is also in a similar range and so the influences of the acids are added together. Knowing the pK_a and pT helps in interpreting the mixed titration curves.
There are different acids in cola drinks: carbonic acid (coming from the CO_2 that is added to drinks to create sparkle - ca 3 g/l) and phosphoric acid to stabilize the pH (buffer).
The carbonic acid and phosphoric acid have following pK_a values:
(http://www.sanderkok.com/techniques/laboratory/pk$_a$_pk$_b$.html):

	pK_{a1}	pK_{a2}	pK_{a3}
Phosphoric acid	2.12	7.21	12.67
Carbonic acid	6.37	10.25	

The pK_{a2} of phosphoric acid and pK_{a1} of carbonic acid are too close to each other, so the first eq. point of carbonic acid interferes with second eq. point of phosphoric acid. The second point of phosphoric acid is therefore influenced by the presence of carbonic acid. But if the carbonic acid is boiled off the solution, the curve produced now relates only to phosphoric acid. The difference in the volume of alkali used in the second equivalence points corresponds to the quantity of carbonic acid in the sample. From these curves therefore, we may calculate the content of phosphoric acid and carbonic acid, as well as the amount of carbon dioxide.

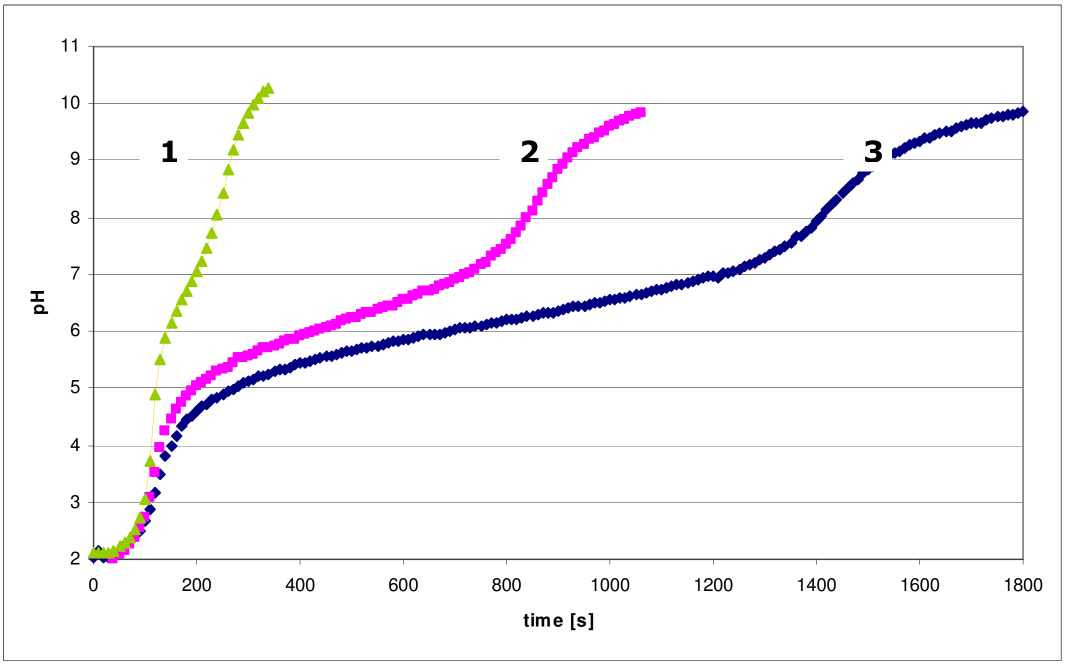
Computer set-up: sample/10sec, continuous measurement; micropipette: 0.3 ml

Procedure: 1. Set up the apparatus as shown above.
2. Pour 100 ml into a beaker, warm it until boiling, then let it cool.
3. Pour 100 ml of sample (cola drink) into another beaker, put it on mixer and mix for 2 minutes.
4. Pour the volumetric solution NaOH in a small beaker.
5. Set the measuring parameters in the computer software.
6. Measure the pH of the drink sample *before* any alkali is added. Start titrating: add a constant volume of volumetric solution (0.3 ml, by micropipette) to the sample solution at 10 second intervals. Keep adding the NaOH until the whole titration curve is measured; see the rising curve on the computer screen. Make sure that you go well past the equivalence point.
7. Titrate the sample of boiled and cooled cola drink the same way as the first sample.
8. Determine the equivalence points in both curves. Calculate the amount of phosphoric acid in the drink and from the difference of NaOH consumption calculate the amount of carbonic acid (carbon dioxide) in the cola drink.

Lab tasks:
1) Why do you boil the second sample of cola drink?
The boiling removes carbon dioxide from the sample. The only acid in the solution after boiling is the phosphoric acid. Therefore the second titration curve relates only to one acid.

2) Write down the equation of carbon dioxide dissolving in water.
Knowing the equation, try to interpret what happens during the addition the strong base to the sample solution.
$CO_2 + H_2O \rightarrow H_2CO_3$
$H_2CO_3 \rightarrow H^+ + HCO_3^-$
The hydroxide ion gradually neutralizes carbonic acid in the sample: neutralizing H^+ causes the equilibrium of the reaction to shift to the right: to restore the equilibrium, another CO_2 molecule dissolves in the solution, which shifts the equilibrium to products until all the CO_2 is titrated from solution.

3) Describe the following graph of three titration curves for three measurements of cola drink. The samples differ according to their conditions or state, i.e. whether it is the fresh drink, open drink or boiled drink. Which acids were in each drink? Mark in the graph the equivalence points and pKa for all three curves and comment on the consumption of volumetric solution that you will use in determination of carbonic acid (and then carbon dioxide).



1) The titration curve of boiled cola drink: there is only H_3PO_4 in the solution and therefore the consumption up to the second equivalence point (HPO_4^{2-}) will be twice the consumption of titrant compared to the first the equivalence point ($H_2PO_4^-$).
2) The titration curve of boiled cola drink: the second equivalence point is influenced by the presence of H_2CO_3 (CO_2 resp.), therefore it shifts in the *x* axis direction (NaOH consumption = time).
3) The titration curve of fresh cola: the second equivalence point is influenced by the presence of H_2CO_3 (CO_2 resp.), therefore it shifts in the *x* axis direction (NaOH consumption = time). There is much more H_2CO_3 in fresh drink than in the open drink, so the consumption of volumetric solution is higher than in the two previous samples.
The first equivalence point is for the three samples the same, which means that it is not influenced by the presence of H_2CO_3, the first equivalence point is therefore caused only by H_3PO_4 (causing $H_2PO_4^-$ ions), because pKa_1 of phosphoric acid is 2.12, while pKa_1 carbonic acid is 6.37. In the pH range from 7 both of the acids are being titrated together – H_3PO_4 to its second equivalence point and H_2CO_3 to its first equivalence point. That is why only the second point in the titration curve is influenced and it depends on the amount of other acids that are present besides the phosphoric acid in the solution.

4) Find out now, what is the content of carbonic acid and carbon dioxide in the opened drink.
c(NaOH) = 0.201 mol/l
V(NaOH) for 2. eq. point during the titration of open drink: 820s/10s= 82 addition X 0.3 ml = 24.6 ml
V(NaOH) for 2. eq. point during the titration of cooked drink: 230s/10s= 23 adition X 0.3 ml = 6.9 ml
V(NaOH) corresponding to H_2CO_3 (see 3.): 24.6 ml – 6.9 ml = 17.7 ml NaOH

Determine the mass of carbonic acid in open cola drink sample from the ratio of reaction. Do not forget that the carbonic acid is titrated only into its **first** equivalence point:

$$H_2CO_3 + NaOH \rightarrow Na^+ + HCO_3^- + H_2O$$

1. eq. point: $n(H_2CO_3) = n(NaOH)$
$m(H_2CO_3)/M(H_2CO_3) = c(NaOH) \times V(NaOH)$
$m(H_2CO_3) = c(NaOH) \times V(NaOH) \times M(H_2CO_3)$
$m(H_2CO_3)$ = 0.201 mol/l x 0.0177 l x 62.024 g/mol = **0.2207 g H_2CO_3** (in 100 ml sample)

Determine the content of carbon dioxide in the sample from the mass of carbonic acid in the sample. Give the final answer in **g/l**:
$M_r(H_2CO_3)$ = 62.024 g/mol
$M_r(CO_2)$ = 44 g/mol
m (H_2CO_3) = 0,22066 g ….. $M_r(H_2CO_3)$ = 62.024 g/mol
m (CO_2) = ? g ………………. $M_r(CO_2)$ = 44 g/mol

$m_r(CO_2)$ = 44 g/mol x 0.22066 g / 62.024 g/mol = 0.1565 g CO_2 ….in 100 ml sample

$c_m(CO_2)$= 1.565 g/l

5) What is the mass concentration of phosphoric acid in the cola drink?
1. equivalence point: $H_3PO_4 + NaOH \rightarrow Na^+ + H_2PO_4^- + H_2O$
c(NaOH) = 0.201 mol/l
V(NaOH) for 1. eq. point: 130s/10s= 13 addition X 0.3 ml = 3.9 ml
$M(H_3PO_4)$ = 98 g/mol
$n(H_3PO_4) = n(NaOH)$
$m(H_3PO_4)/M(H_3PO_4) = c(NaOH) \times V(NaOH)$
$m(H_3PO_4) = c(NaOH) \times V(NaOH) \times M(H_3PO_4)$
$m(H_3PO_4)$ = 0.201 mol/l x 0.0039 l x 98 g/mol = 0.0768 g / 100 ml
$m(H_3PO_4)$ = 0.768 g/l

Conclusion: The opened cola drink contains 0.22 grams of carbonic acid (in 100 ml sample). The concentration of CO_2 in open sample was 1.565 g/l. The concentration of phosphoric acid was 0.768 g/l.

How is it made?

Now that Coca-Cola is sold worldwide, it is essential that the bulk is reduced for ease of transport. Consequently, the water, sugar and carbon dioxide are added in the county of production. The remainder of the ingredients are shipped abroad by the Coca-Cola Company as a syrup concentrate, which is blended with the remaining ingredients before bottling or canning. This also helps to protect the composition of the "secret ingredient".

Steps must be taken to ensure that the water is always of the same composition to that specified by the Coca-Cola Company. If this was not done, the finished article would be different, depending on where it was produced. This could include filtration, sterilization of the water by chlorine and/or ozone, addition of certain minerals, such as magnesium sulfate, potassium chloride etc. and deodorizing.

What are the benefits/risks?

Over the years there will have been millions of satisfied customers. Each one of these persons would claim that there have been many advantages to a regular intake of Coca-Cola. These may range from curative effects, pain relief, refreshment or just simply a passion for the taste. None of these claims can easily be proven scientifically. Without doubt, there have been millions- if not billions of people who have enjoyed the drink.

In its early years, the fact that it was associated with cocaine featured as one of its selling points, although from 1903 this did not remain as an ingredient.

One of the major problems with Coca-Cola is the very high sugar content. Typically, a 330ml can of the drink contains 35 grams of sugar. This can lead to obesity, tooth decay and even diabetes. The phosphoric acid in the drink can cause erosion of tooth enamel as well as kidney problems or osteoporosis.

Future developments?

Since Coca-Cola was introduced over 100 years ago, there have already been numerous developments. One major development was the introduction of diet coke. This contains no sugar at all. It relies on artificial sweeteners, such as aspartame.
There may be further breakthroughs in the introduction of new sweeteners, which could be used in colas.
Over the years, there have been many variations on the basic cola. These include:

Cherry coke
Coke with lemon
Coke with lime
Coke with vanilla
Coke zero (no sugar and zero calories!)
Who is to say where the urge to create new variations to the basic Coca-Cola taste will end? Will it follow the same path as potato chips e.g. chilli flavoured Coke? What about chocolate/coffee variants? There is no end to the suggestions.
Ultimately, it will be the customers who decide whether any new versions will have any future or not.

Interested in what you've read?

If so, you can find a great deal more to interest you at:

www.coca-cola.com

http://en.wikipedia.org/wiki/Coca-cola

http://www.youtube.com/watch?v=hKoB0MHVBvM

Sugar in coke: http://www.youtube.com/watch?v=yKZ2ZqBYlrI

http://www.youtube.com/watch?v=BkrLoQj71Kc (Chinese variant)

http://recipes.howstuffworks.com/coca-cola.htm

http://www.medindia.net/news/Sugar-sweetened-Drinks-Boost-Type-2-Diabetes-Risk-39912-1.htm

http://en.wikipedia.org/wiki/Diabetes
http://www.naturalnews.com/004416.html,

http://www.cspinet.org/liquidcandy/

http://www.beverageinstitute.org/ingredients/glossary.shtml

http://en.wikipedia.org/wiki/Osteoporosis

http://yourtotalhealth.ivillage.com/soft-drinks-hazardous-your-health.html

http://www.webmd.com/osteoporosis/features/soda-osteoporosis).

http://joshmadison.com/article/will-coke-dissolve-a-nail-experiment/

Mentos: http://www.youtube.com/watch?v=hKoB0MHVBvM