

Strong and Weak Acids

Vinegar has been made and used by people for thousands of years. Traces of it have been found in Egyptian urns from around 3000 BC.

Concentrated acetic acid and hydrochloric acid were discovered in the 8th century by the Persian alchemist Abu Musa Jabir ibn Hayyan (Geber). Among many he discovered the process of distillation. By distilling vinegar he produced acetic acid and by distilling a mixture of sulphuric acid and common salt he made hydrochloric acid (its historic name 'spirit of salt'). Both acids behave quite differently in an aqueous solution. For instance, to make for instance a solution of HCl as sour as vinegar you need very little of the compound HCl compared with the amount of acetic acid in vinegar.



A. Introduction ●●

The topic of acid-base reactions is a regular component of many chemistry curricula. This topic requires integrated understanding of many areas of introductory chemistry. Many students have considerable difficulties understanding concepts and processes involved in this topic (students often have difficulties to understand the pH scale).

This module offers activities in which acid-base reactions and differences in behaviour of strong and weak acids in solution are analysed. The following activities are available:

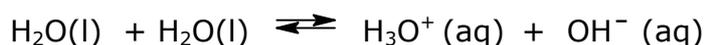
- 1. Data logging:** Two laboratory experiments:
 - To measure pH during the titration of strong and weak acids with a strong base.
 - To determine an unknown concentration of an acidic solution.
- 2. Modelling:** simulations based on mathematical models which describe the concentration of $[H_3O^+]$ and the change of pH during a titration. The simulations help to answer the questions raised in the data-logging activities..

All student activities are offered as Coach 6 Activities in the project Strong and Weak Acids.

1. Background theory

1. AUTO-IONISATION OF WATER

Water is an ionic substance: it ionises to a small but measurable extent. Water molecules react with each other, one molecule donates proton H^+ (acts as an acid) and the other molecule accepts proton H^+ (acts as a base).



In pure water at 25°C (298°K), the concentration of H_3O^+ ions is equal to the concentration of OH^- ions (each only 1×10^{-7} mol/L).

The equilibrium constant is:

$$K = \frac{[H_3O^+][OH^-]}{[H_2O]}$$

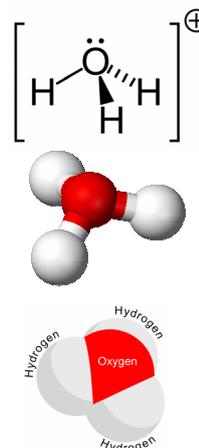


Figure. Hydronium ion (<http://en.wikipedia.org>)

where K is the equilibrium constant, $[H_3O^+]$ - concentration of H_3O^+ ions and $[OH^-]$ - concentration of OH^- ions.

Since the water concentration $[H_2O]$ is relatively constant (water in excess) multiplying both sides of the equation by $[H_2O]$ results a new constant – the ion product constant of water K_w :

$$K_w = [H_3O^+]\cdot[OH^-] \text{ and } K_w = 10^{-14} \text{ at } 25^\circ\text{C}$$

where K_w is constant for all dilute aqueous solutions.

Although the concentrations of H_3O^+ may change when substances are added to water, the product $[H_3O^+]$ and $[OH^-]$ remains the same. It means that if the concentration of ions $[H_3O^+]$ is 0.1 mol/L then the concentration of ions $[OH^-]$ is 10^{-13} mol/L.

2. THE PH SCALE

The pH scale was first used by the Danish biochemist Søren Sørensen in 1909 to create a more efficient notation for the enormous range of the H_3O^+ concentrations confronted within his experiments. He defined pH as the negative logarithm (with base 10) of the hydronium ion concentration and in that way reduced an inconvenient number to a simple number. Henceforth we will write log instead of \log_{10}

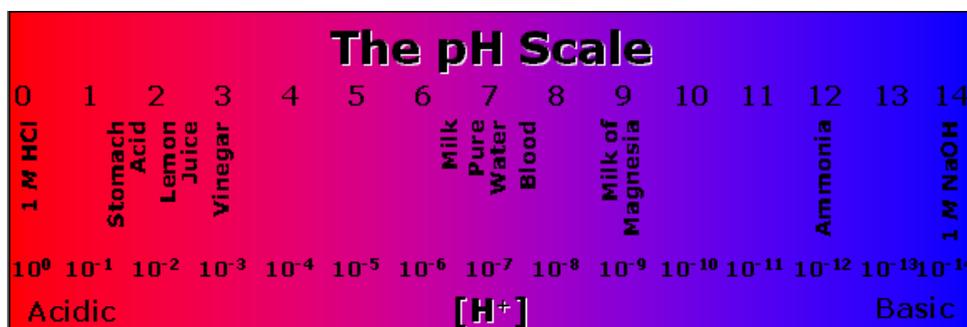
$$\text{pH} = -\log [H_3O^+]$$

$[H_3O^+]$ is expressed in powers of 10: $[H_3O^+] = 10^{-\text{pH}}$

In neutral solution: $[H_3O^+] = [OH^-] = 10^{-7}\text{mol/L}$ $\text{pH} = \text{pOH} = 7.$
(pure water at 25°C)

In acidic solution: $[H_3O^+] > [OH^-]$ $\text{pH} < 7.$

In basic solution: $[H_3O^+] < [OH^-]$ $\text{pH} > 7.$



origin: <http://library.thinkquest.org/3659/acidbase/ph.html>

In a definition similar to that of pH, the pOH scale is defined as the negative log of the hydroxide ion concentration.

$$\text{pOH} = -\log[\text{OH}^-]$$

At 25°C $K_w = 10^{-14}$ and $\text{p}K_w = \text{pH} + \text{pOH} = 14$

3. STRONG AND WEAK ACIDS

Acids are classified as strong or weak depending on the degree to which they ionize in water.

A **strong** acid, like hydrochloric acid HCl, ionizes completely in aqueous solution (no HCl exists in hydrochloric acid):

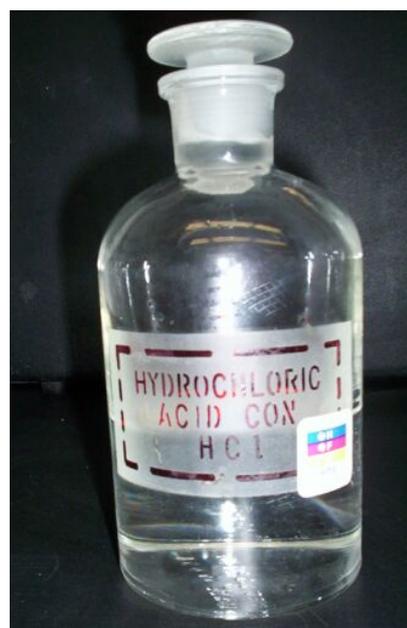


In 0.1 mol/L hydrochloric acid the concentration $\text{H}_3\text{O}^+(aq)$ is the same as the number of moles HCl used to make the solution $[\text{H}_3\text{O}^+] = 0.1 \text{ mol/L}$.

The pH of 0.1 mol/L hydrochloric acid will be

$$\text{pH} = -\log[\text{H}_3\text{O}^+] = -\log(0.1) = 1.$$

Of course, this reasoning only holds in case the hydrochloric acid solution is not too diluted. For example, a solution of 10^{-8} mol/L will not have a pH equal to 8: the pH must be less than 7 because after all it is still an acid solution.



A **weak** acid, like acetic acid CH_3COOH (from now on abbreviated as HAc) ionizes only slightly in aqueous solution. The following equilibrium exists in a HAc solution:



The equilibrium sign shows that a significant concentration of HAc is present along with Ac^- and H_3O^+ ions formed from it. The equilibrium acidity constant is:

$$K_a = \frac{[\text{Ac}^-][\text{H}_3\text{O}^+]}{[\text{HAc}]}$$

For acetic acid at 25°C this is approximately equal to $1.76 \times 10^{-5} \text{ mol/L}$.



To work out the pH, the concentration of hydronium ions should be found. We will assume that the concentration of hydronium ions is equal to the concentration of dissociated anions, i.e., $[H_3O^+] = [Ac^-]$, and that the HAc concentration is equal to the initial concentration c minus the concentration of hydronium ions, i.e., $[HAc] = c - [H_3O^+]$. This also means that we ignore the auto-ionisation of water. Thus:

$$K_a = \frac{[H_3O^+]^2}{c - [H_3O^+]}$$

You can compute the answer by finding the positive root of the following quadratic equation:

$$[H_3O^+]^2 + K_a \cdot [H_3O^+] - K_a \cdot c = 0.$$

Its positive solution is equal to

$$[H_3O^+] = \frac{-K_a + \sqrt{K_a^2 + 4K_a \cdot c}}{2}.$$

But, assuming that $[H_3O^+] \ll c$ you get the following approximate results

$$K_a = \frac{[H_3O^+]^2}{c}$$

and

$$[H_3O^+]^2 = \sqrt{K_a \cdot c}.$$

This is the formula that is used in most practical circumstances. Let us look at a concrete example to see how well the approximation works.

For 0.1 mol/L HAc we get with the approximative formule:

$$[H_3O^+]^2 = \sqrt{1.76 \times 10^{-6}} \approx 1.327 \times 10^{-3} \text{ mol / L}$$

$$pH = -\log(1.327 \times 10^{-3}) \approx 2.877.$$

Compare this with the result from the quadratic equation:

$$[H_3O^+]^2 \approx 1.335 \times 10^{-3} \text{ mol / L}$$

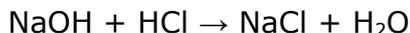
$$pH = -\log(1.335 \times 10^{-3}) \approx 2.874.$$

Indeed a negligible difference, which was expected because the condition $[H_3O^+] \ll c$ is met.

As we shall see in section 5, an exact formula for the hydronium concentration of any acid, weak or strong, strongly diluted or not, buffered by addition of a strong base or not, can also be derived. This will be needed for the computer models of titration curves. Approximations will hold only in certain regions of the titration curves.

4. REACTION OF A STRONG ACID WITH A STRONG BASE

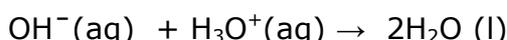
During the addition of a strong base to a strong acid a complete neutralization reaction occurs. The acid unites with the base to form a salt and water. Take for example the addition of a sodium hydroxide solution (NaOH) to a hydrochloric acid solution (HCl):



NaOH, HCl and NaCl are strong electrolytes and their solutions are therefore completely ionized:



Na^+ and Cl^- ions remain in the solution and actually play no part in the reaction; these ions can be eliminated to simplify the equation:



In essence, the chemical reaction is the neutralization.

During such titration the concentration of H_3O^+ ions decreases with the added OH^- . The following steps can be distinguished:

0. No NaOH added yet

In case the acid solution is not too diluted (and this is true under normal circumstances), the pH of the acidic solution can be calculated from initial concentration c_{HCl} of the acid:

$$\text{pH} = -\log(c_{\text{HCl}})$$

The easiest way to ensure that the pH is less than 7, even under strongly diluted conditions, is to adapt the formula to

$$\text{pH} = -\log(c_{\text{HCl}} + \sqrt{K_w})$$

For large enough concentrations, the term $\sqrt{K_w}$ can be ignored and we get the usual formula. For small concentrations, the formula can be approximated by $\text{pH} = \frac{1}{2} \text{p}K_w - \frac{c_{\text{HCl}}}{\sqrt{K_w}}$.

However, the exact formula is not much more difficult:

$$\text{pH} = -\log\left(\frac{c_{\text{HCl}} + \sqrt{c_{\text{HCl}}^2 + 4K_w}}{2}\right)$$

Note that if the effect of auto-ionisation can be ignored, i.e., if K_w can be taken as equal to 0, then this formula simplifies to the first given formula.

The exact formula can be derived as follows from three conditions:

1. Charge balance: $[H_3O^+] = [OH^-] + [Cl^-]$.
2. Mass balance: $[Cl^-] = c_{HCl}$ (we assume complete ionisation HCl).
3. Equilibrium: $[H_3O^+] \cdot [OH^-] = K_w$.

Substituting the 2nd and the 3rd equation into the 1st equation gives:

$$[H_3O^+] = \frac{K_w}{[H_3O^+]} + c_{HCl}$$

It can be rewritten as the following quadratic equation:

$$[H_3O^+]^2 - c_{HCl} \cdot [H_3O^+] - K_w = 0$$

the positive solution of which is equal to:

$$[H_3O^+] = \frac{c_{HCl} + \sqrt{c_{HCl}^2 + 4K_w}}{2}$$

1. Less added NaOH than HCl initially present in the solution, i.e., $[H_3O^+] > [OH^-]$

The solution is acidic and its $pH < 7$. The initial amount of HCl and the added amount of NaOH (in moles) are given by:

$$n_{HCl} = c_{HCl} \cdot V_{HCl} \text{ and } n_{NaOH} = c_{NaOH} \cdot V_{NaOH}$$

where n = number of moles of acid or base, c = initial concentration of acid or base, V = volume of acid or base.

The concentration of $[H_3O^+]$ at this point in the titration is approximately (when solutions are not too diluted):

$$[H_3O^+] = \frac{c_{HCl} \cdot V_{HCl} - c_{NaOH} \cdot V_{NaOH}}{V_{HCl} + V_{NaOH}}$$

Again, an exact formula can be derived as well:

1. Charge balance: $[H_3O^+] + [Na^+] = [OH^-] + [Cl^-]$.
2. Mass balance: $[Cl^-] = c_{HCl} \cdot \frac{V_{HCl}}{V_{HCl} + V_{NaOH}}$ (complete ionisation HCl).
 $[Na^+] = c_{NaOH} \cdot \frac{V_{NaOH}}{V_{HCl} + V_{NaOH}}$
3. Equilibrium: $\frac{[Cl^-] \cdot [H_3O^+]}{[HCl]} = K_a$
 $[H_3O^+] + [OH^-] = K_w$.

Substituting the 2nd and 3rd equation into the 1st equation gives:

$$[H_3O^+] = \frac{K_w}{[H_3O^+]} = \frac{c_{HCl} \cdot V_{HCl} - c_{NaOH} \cdot V_{NaOH}}{V_{HCl} + V_{NaOH}}$$

It can be rewritten as the following quadratic equation:

$$[H_3O^+]^2 - \left(\frac{c_{HCl} \cdot V_{HCl} - c_{NaOH} \cdot V_{NaOH}}{V_{HCl} + V_{NaOH}} \right) \cdot [H_3O^+] - K_w = 0,$$

the positive solution of which is equal to:

$$[H_3O^+] = \frac{c'_{HCl} + \sqrt{c'^2_{HCl} + 4K_w}}{2}$$

where

$$c'_{HCl} = \frac{c_{HCl} \cdot V_{HCl} - c_{NaOH} \cdot V_{NaOH}}{V_{HCl} + V_{NaOH}}.$$

Note that we have the same formula as in step 0 if we consider c'_{HCl} is the current concentration of the hydrochloric acid solution after reaction with the strong base using the current volume of the solution.

2. Equal amounts of added NaOH and initial HCl, i.e., $[H_3O^+] = [OH^-]$.

In such solution, all H_3O^+ ions of the acid are neutralized by the OH^- ions of the base, i.e., all hydrochloric acid has been neutralized by exactly the same amount of sodium hydroxide. At this so-called equivalence point a sodium chloride solution has been produced. Neither Na^+ ions nor Cl^- ions are acidic or a basic, so at this point the pH will only be influenced by the water equilibrium:



At the equivalence point:

$$K_w = [H_3O^+] \cdot [OH^-] = 10^{-14}$$

and

$$[H_3O^+] = [OH^-] = \sqrt{K_w} = 10^{-7} \text{ mol / L}$$

So: pH = 7.

3. More NaOH added than initial HCl in the solution, i.e., $[H_3O^+] < [OH^-]$.

Beyond the equivalence point, the OH^- concentration can be found from the chemical amount of OH^- added after the equivalence point has been reached.

$$[OH^-] = \frac{c_{NaOH} \cdot V_{NaOH} - c_{HCl} \cdot V_{HCl}}{V_{HCl} + V_{NaOH}}$$

The pH follows from the mathematical equation $K_w = [H_3O^+] \cdot [OH^-]$:

$$[H_3O^+] = \frac{K_w}{[OH^-]} = \frac{K_w \cdot (V_{HCl} + V_{NaOH})}{c_{NaOH} \cdot V_{NaOH} - c_{HCl} \cdot V_{NaOH}}$$

The solution is basic and its $pH > 7$. In the above reasoning we have assumed that solutions are not too diluted. Otherwise the following formula must be used:

$$[OH^-] = \frac{c'_{NaOH} + \sqrt{c'^2_{NaOH} + 4K_w}}{2},$$

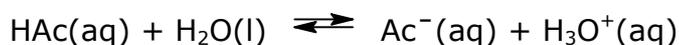
where

$$c'_{NaOH} = \frac{c_{NaOH} \cdot V_{NaOH} - c_{HCl} \cdot V_{HCl}}{V_{HCl} + V_{NaOH}}.$$

5. REACTION OF A WEAK ACID WITH A STRONG BASE

When adding a strong base to a weak acid, the base will react with the weak acid and form a solution that contains the weak acid and its conjugate base until the acid is completely gone. The difference with the strong acid-strong base case is that now equilibrium enters the picture.

As a prototypical example we will look at the addition of a sodium hydroxide solution (NaOH) to an acetic acid solution (recall that CH_3COOH is henceforth abbreviated as HAc):



We will use a systematic approach to this chemical equilibrium and we will show how approximative formulas follow.

The exact formula for the hydronium concentration at any moment during the titration can be derived as follows from three conditions:

1. Charge balance: $[H_3O^+] + [Na^+] = [OH^-] + [Ac^-]$.

2. Mass balance: $[HAc] = [Ac^-] = c_{HAc} \cdot \frac{V_{HAc}}{V_{HAc} + V_{NaOH}}$ (partly ionisation of weak acid).

$$[Na^+] = c_{NaOH} \cdot \frac{V_{NaOH}}{V_{HAc} + V_{NaOH}} \text{ (complete ionisation of strong base).}$$

3. Equilibrium: $\frac{[Ac^-][H_3O^+]}{[HAc]} = K_a$

$$[H_3O^+] \cdot [OH^-] = K_w.$$

To make coming formulas more readable it is convenient to introduce the following 'apparent initial concentrations' of acid and base:

$$a_{HAc} = c_{HAc} \cdot \frac{V_{HAc}}{V_{HAc} + V_{NaOH}} \text{ and } a_{NaOH} = c_{NaOH} \cdot \frac{V_{NaOH}}{V_{HAc} + V_{NaOH}}$$

First we express the concentration $[Ac^-]$ in terms of the equilibrium acidity constant K_a and the hydronium concentration by elimination $[HAc]$ from the first mass balance equation and the first equilibrium equation. We obtain the following formula:

$$[Ac^-] = \alpha_{Ac^-} \cdot a_{HAc}$$

Where α_{Ac^-} is

$$\alpha_{Ac^-} = \frac{K_a}{[H_3O^+] + K_a}.$$

Substitute this formula for $[Ac^-]$, $[OH^-] = \frac{K_w}{[H_3O^]}$, and $[Na^+] = a_{NaOH}$ into the charge balance equation to obtain

$$[H_3O^+] + a_{NaOH} = \frac{K_w}{[H_3O^+]} + \frac{K_a}{[H_3O^+] + K_a} \cdot a_{HAc}.$$

This can be rewritten as the cubic equation

$$[H_3O^+]^3 + (a_{NaOH} + K_a) \cdot [H_3O^+]^2 - ((a_{HAc} - a_{NaOH}) \cdot K_a + K_w) \cdot [H_3O^+] - K_a \cdot K_w = 0.$$

Henceforth we will assume that the auto-ionisation of water may be neglected prior to the equivalence point. Under this assumption, i.e., taking $K_w = 0$ in our formulas, the above cubic equation reduces to a quadratic equation:

$$[H_3O^+]^2 + (a_{NaOH} + K_a) \cdot [H_3O^+] - (a_{HAc} - a_{NaOH}) \cdot K_a = 0.$$

The positive solution of this quadratic equation is

$$[H_3O^+] = \frac{-(a_{NaOH} + K_a) + \sqrt{(a_{NaOH} + K_a)^2 + 4K_a \cdot (a_{HAc} - a_{NaOH})}}{2}.$$

We can consider a strong acid as a special case of a weak acid with a large value of K_a . Under this assumption, the cubic equation reduces to

$$[H_3O^+]^2 - (a_{HAc} - a_{NaOH}) \cdot [H_3O^+] - K_w = 0,$$

with the following positive solution

$$[H_3O^+] = \frac{(a_{HAc} - a_{NaOH}) + \sqrt{(a_{HAc} - a_{NaOH})^2 + 4K_w}}{2}.$$

This is also a formula that we found in the previous description of a strong acid – strong base reaction.

We will now continue the computation of the theoretic titration curve of the weak acid – strong base reaction. The following steps can be distinguished:

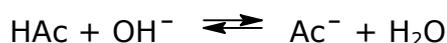
0. No NaOH added yet

We can use the above formula with $a_{NaOH} = 0$ and $a_{HAc} = 0$ to obtain the formulas that we already had found in the previous section for a weak acid:

$$[H_3O^+] = \frac{-K_a + \sqrt{K_a^2 + 4K_a \cdot c_{HAc}}}{2}$$

1. Prior to the equivalence point

The equilibrium is constantly disturbed by adding OH^- that reacts with H_3O^+ .



or



The equilibrium restores itself by dissociation of some HAc. After addition of OH^- it is [HAc] that almost linearly decreases. The concentration H_3O^+ does not change very little (constantly being replenished by dissociation of HAc). In the solution the base Ac^- conjugated with the acid HAc is formed (cf. Brønsted-Lowry theory).

The hydronium concentration can be computed by the following formula:

$$[H_3O^+] = \frac{-(a_{NaOH} + K_a) + \sqrt{(a_{NaOH} + K_a)^2 + 4K_a \cdot (a_{HAc} - a_{NaOH})}}{2}.$$

If $K_a \cdot (a_{HAc} - a_{NaOH}) \ll (a_{NaOH} + K_a)^2$, this formula can be approximated by

$$[H_3O^+] \approx \frac{(a_{HAc} - a_{NaOH}) \cdot K_a}{(a_{NaOH} + K_a)}$$

In other words, when K_a is small compared to the added amount of base:

$$pH \approx pK_a - \log\left(\frac{a_{HAc} - a_{NaOH}}{a_{NaOH}}\right)$$

This expression is called the Henderson-Hasselbalch equation and is usually written as

$$pH \approx pK_a - \log\left(\frac{[acid]}{[base]}\right),$$

where the logarithmic term contains the quotient of the acid concentration and the base concentration. Halfway to the equivalence point these concentrations are the same and the pH equals pK_a .

As was mentioned before, the pH of a solution of a weak acid and its conjugate base changes only little regardless of the addition of other ions (when acid and base concentrations change, but their quotient changes only a little bit). Such a solution is called a **buffer solution**.

A buffer solution is a solution that can absorb moderate amounts of acid or base without significant change in its pH. A buffer solution is usually a solution of a weak acid and its conjugate base or a solution of a weak base and its conjugate acid.

Buffer action has many important applications in chemistry and physiology. The human blood is a natural buffer, and so are other body fluids and plant fluids due to mixtures of weak acids and bases present in them.

2. At the equivalence point

This also called the stoichiometric point because at this point the amount of base added equals the initial amount of acid.

$$c_{HAc} \cdot V_{HAc} = c_{NaOH} \cdot V_{NaOH}$$

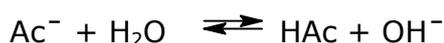
It follows from this formula that

$$[Na^+] = \frac{c_{NaOH} \cdot c_{HAc}}{c_{NaOH} + c_{HAc}}$$

At this point a sodium acetate solution has been produced. The Na^+ ions again do not influence the pH at the equivalence point but the Ac^- ions do. This is the weak base Ac^- .

To calculate the pH first the concentration of OH^- should be calculated. OH^-

ions are formed in the reaction of Ac^- with water.



The equilibrium constant of this reaction is $K_b = \frac{[\text{HAc}] \cdot [\text{OH}^-]}{[\text{Ac}^-]}$.

$$K_b = \frac{K_w}{K_a} \text{ thus we have for acetic acid } K_b = \frac{10^{-14}}{1.76 \times 10^{-5}} \approx 5.68 \times 10^{-8}.$$

Using the same reasoning as for a solution of a weak acid: $K_b = \frac{[\text{OH}^-]^2}{c - [\text{OH}^-]}$,

where c is the initial concentration of the base in the solution. In our titration curve c is equal to $[\text{Na}^+]$. Thus:

$$[\text{OH}^-] = \frac{-K_b + \sqrt{K_b^2 + 4K_b \cdot c}}{2}$$

$$\text{where } c = \frac{C_{\text{NaOH}} \cdot C_{\text{HAc}}}{C_{\text{NaOH}} + C_{\text{HAc}}}.$$

$$\text{Then } [\text{H}_3\text{O}^+] = \frac{2K_w}{-K_b + \sqrt{K_b^2 + 4K_b \cdot c}}$$

Assuming that for a weak base $[\text{OH}^-] \ll c$ then $[\text{OH}^-] \approx \sqrt{K_b \cdot c}$

Thus at the equivalence point, approximative formulas are:

$$p\text{OH} = \frac{1}{2}pK_b + \frac{1}{2}\log c \text{ and } p\text{H} = \frac{1}{2}pK_w + \frac{1}{2}pK_a + \frac{1}{2}\log c$$

The pH value depends on the initial acid concentration and the concentration of the added base NaOH. For example when 10 mL 0.1 mol/L NaOH is added to 10 mL 0.1 mol/L HAc:

$$[\text{H}_3\text{O}^+] = \frac{2K_w}{-K_b + \sqrt{K_b^2 + 4K_b \cdot c}} = \frac{2 \times 10^{-14}}{-5.68 \times 10^{-8} + \sqrt{5.68^2 \times 10^{-16} + 4 \times 5.68 \times 10^{-8} \cdot 0.05}} \approx 1.88 \times 10^{-9}$$

then $p\text{H} = 8.73$

The above computation also shows that the approximate formula works as well:

$$p\text{H} = \frac{1}{2}pK_w + \frac{1}{2}pK_a + \frac{1}{2}\log c = \frac{1}{2} \times 14 + \frac{1}{2} \times 4.75 + \frac{1}{2}\log 0.05 \approx 8.72$$

The pH of the solution is larger than 7, the solution contains an excess of OH^- ions and is basic.

Reaction of ions with water is called hydrolysis. Water always react with these ions a weak electrolyte (acid or base) is re-established. In general salts formed from weak acids and strong bases hydrolyse in water to form basic solutions and salts formed from strong acids and weak bases, e.g., NH_4Cl hydrolyse in water, form acidic solutions.

3. Beyond the equivalence point

After the equilibrium point the pH results from the excess of base NaOH. In the solution the weak base Ac^- is still present, but its dissociation constant is much smaller compared to the strong base and its influence on the pH value can be neglected. The concentration of H_3O^+ ions is found in the similar way to the titration of a strong acid with a strong base.

$$[\text{OH}^-] = \frac{c'_{\text{NaOH}} + \sqrt{c'_{\text{NaOH}}{}^2 + 4K_w}}{2}$$

where

$$c'_{\text{NaOH}} = \frac{c_{\text{NaOH}} \cdot V_{\text{NaOH}} - c_{\text{HCl}} \cdot V_{\text{HCl}}}{V_{\text{HCl}} + V_{\text{NaOH}}}$$

6. TITRATION

Titration is an analytical method in which a standard solution with the known concentration is used to determine the concentration of another solution.

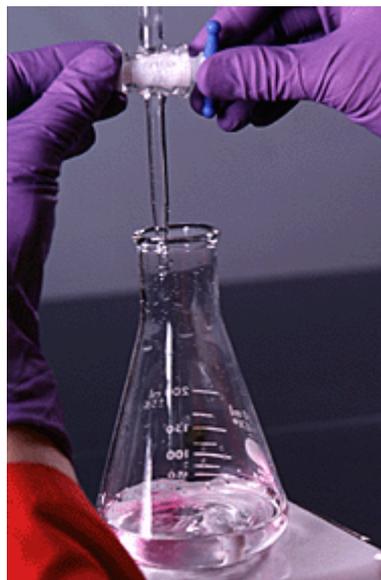
During titration the standard solution (also known as titrant) is slowly added to the solution of unknown concentration by means of a burette. The endpoint of the reaction can be observed by the colour change when using an indicator (for example phenolphthalein) or detected by pH measurement. At the end point an amount of standard solution has been added that just completely reacts with the solution titrated.

The moles of standard solution can be calculated by multiplying the volume of standard solution used by its molarity.

$$n_{\text{standard solution}} = V_{\text{standard solution}} \times c_{\text{standard solution}}$$

The moles in the titrated solution of unknown concentration are then found using the coefficient in the chemical equation. Then, dividing the moles of the titrated solution by the volume of that solution gives the concentration of the titrated solution.

$$c_{\text{titrated solution}} = n_{\text{titrated solution}} / V_{\text{titrated solution}}$$



2. Pre-requisite knowledge required

- Chemical calculations using the mole
- Chemical equilibriums
- Brønsted-Lowry acid-base model
- Acid/base equilibriums (equilibrium constant K_a , K_b and K_w)
- Definition of pH and the pH scale

3. Science concepts developed in the module

- pH and the concentration H_3O^+ resulting from the dissociation of strong and weak acids in water
- Acid-base reactions
- Neutralization of an acidic solution
- Chemical equilibrium
- Buffer solutions

4. Other useful information

Helping you to understand Chemistry
<http://www.chemguide.co.uk>

Drechsler M. and Schmidt H.J., (2005), Textbooks' and teachers' understanding of acid-base models used in chemistry teaching., *Chemistry Education Research and Practice*, **6** (1), 19-35.

Furió-Mas C., Calatayud M.L., Guisasola J. and Furió-Gómez C., (2005), How are the Concepts and Theories of Acid-Base Reactions Presented? Chemistry in Textbooks and as Presented by Teachers., *International Journal of Science Education*, **27** (11), 1337-1358

Mary B. Nakhleh, Joseph S. Krajcik, (1994). Influence of levels of information as presented by different technologies on students' understanding of acid, base, and ph concepts, *Journal of Research in Science Teaching*, 31 (10), 1077-1096.

Juan Quílez-Pardo and Joan Josep Solaz-Portolés, (1995). Students' and teachers' misapplication of le chatelier's principle: Implications for the teaching of chemical equilibrium, *Journal of Research in Science Teaching*, 32 (9), 939-957.

B. Didactical approach ●●

1. Pedagogical context

The proposed module can be used as an application module. Students use concepts that were already introduced and apply them to new situations (titrations). The goal is to

have students generalize the application of their knowledge. This application of the principles leads to further understanding of the theories and models.

2. Common student difficulties

Students have difficulties in:

- Distinguishing between different acid-base models (Arrhenius, Brønsted-Lowry models) [1]
- Classifying water as an acid or a base [1]
- Qualitative understanding of pH (problems with understanding the inverse and logarithmic nature of the pH scale) [4]
- Understanding the difference between “strong” and “concentrated” [5]
- Understanding what is happening to the value of pH during a titration [4]
- understanding the concept of neutralisation; neutralisation does not mean neutral solution of pH = 7; [2] [3]

REFERENCES:

1. Drechsler M. and Schmidt H.J., (2005), Textbooks’ and teachers’ understanding of acid-base models used in chemistry teaching., *Chemistry Education Research and Practice*, **6** (1), 19-35.
2. Kousathana M., Demerouti M. and Tsaparlis G., (2005), Instructional Misconceptions in Acid-Base Equilibria: An analysis from a history and philosophy of Science perspective., *Science and Education*, **14**, 173-193.
3. Schmidt H.J., (2000), Should Chemistry lessons be more intellectually challenging?, *Chemistry Education: Research and Practice in Europe*, **1** (1), 17-26.
4. Sheppard K., High school students’ understanding of titrations and related acid-base phenomena, *Chemistry Education Research and Practice*, 2006, **7** (1), 32-45.

5. Vanessa Kind, *Beyond Appearances: Students' misconceptions about basic chemical ideas* available via <http://www.chemsoc.org/networks/learnnet/miscon.htm>
6. <http://www.daisley.net/hellevator/misconceptions/misconceptions.pdf>

3. Evaluation of ICT

The specific qualities of ICT which benefit student learning are specified below per a type of activity.

DATA LOGGING

In the data-logging activities real-time titrations of strong and weak acid are performed. The pH changes are monitored using the pH sensor. The adding of the titrant is done by using the glass burette (a titration curve is a function of time) or by using the CMA step-motor burette (a titration is a function of volume).

The data-logging technique makes the graph of pH against volume visible immediately and when the reaction is finished the pH changes can be analyzed. By differentiation on the graph the equivalence point is easily found.

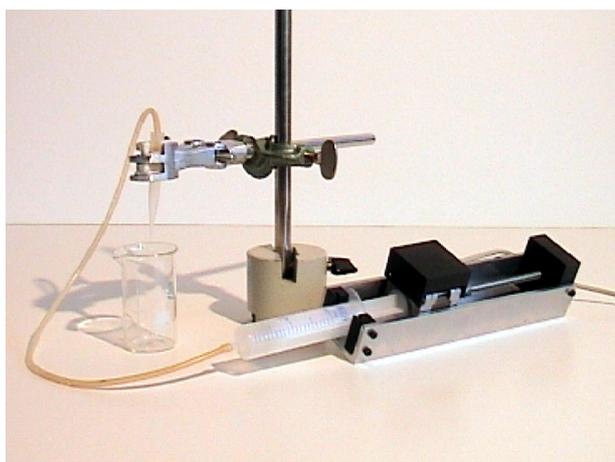
The experiment can be easily repeated, in the given activities strong and weak acids are used but also strong and weak bases may be used. In this way, the characteristic shapes of these graphs may be compared.

Activity 0. Calibration of the CMA step-motor burette

Step motor burette is a cheap, accurate, dosage device that can be used to control a process of adding a titrant in titration experiments. The burette is equipped with four 4mm plugs and is connected to control outputs of the CoachLab II interfaces.

Before the step-motor burette can be used in titration experiments a calibration factor of the burette has to be determined. This calibration factor is the number of steps the motor has to turn to add 1.00 mL of titrant solution. This calibration factor is used in the control program to calculate the volume added by the burette.

In this experiment students realise that well calibrated apparatus is a necessity for obtaining quantitative reliable results. Using a computer is no exception.



The activity is also used to understand the functioning of the step-motor burette and to test it.

Activity 1A. Neutralization of strong and weak acids

**Activity 1B. Neutralization of strong and weak acids
(with the step-motor burette)**

During these activities students record titrations. They analyse the changes of the pH that occur during titrations. They calculate and plot the changes of the H_3O^+ ion concentration. They observe and interpret differences in shapes of titration curves when strong and weak acids are combined with strong base.

In activity 1A an acid solution (titrant) drips from a burette into the base solution at a constant rate. Based on the dripping rate the volume of acid added for any time during the titration can be calculated (volume (mL) = time (s) * dripping rate (mL/s)) and a graph of pH versus volume can be created.

In activity 1B the step-motor burette is used to add titrant. A Coach control program controls the movement of the step motor of the burette.

Correctly executed titrations are directly distinguished from bad ones. The effect of stirring for instance is immediately visible.

It is also important that each pH system (pH amplifier and pH electrode) be well calibrated. The two-point calibration is sufficient.

It can be valuable to discuss with students the effect of response time of the pH electrode. The pH system needs some time for its pH to stabilize. Near the equivalence point, the curve may not be as steep as in actual titrations. This may result in a time difference between the time you see the indicator change colour and the large jump in pH.

2A. Acid-base titration.cma

2B. Acid-base titration with the step-motor burette.cma

In these activities students use the titration method to determine unknown concentrations of acid solutions.

MODELING

The Modeling activities enable numerical models of continuous changing systems to be created and used. In such models the dynamic change of the system is described step-by-step.

Modeling allows creating models of complex phenomena and solving realistic problems which are quite difficult to solve analytically at the school level. The formulation of such numerical models is often rather simple and conceptually easy to understand.

Modeling can also be used as simulation program, with the difference that the model is visible, and can be changed. By changing a model parameter different situations can be investigated.

The model results can be then compared with experimental data (from measurement or video measurement). The model can be easily modified or a parameter can be changed so students can test their hypothesis and make links between the real experiment and the theoretical model.

Activity 3A. Titration curve of strong acid

Activity 3B. Titration curve of weak acid

Graphical computer models aim to calculate the $[H_3O^+]$, $[OH^-]$ and pH changes during the titrations. Ready-made models are available in the activities and students can use them as simulations. By using the *Simulate* option available in the Tool menu of the Model window students have the possibility to experiment with different parameters for investigating different conditions.

Computer model of a titration of a strong acid with a strong base

The model describes the process of adding a NaOH solution (a strong base) to a HCl solution (a strong acid). HCl dissociates completely, i.e., no HCL remains in the solution; the amount of moles of H^+ ions is equal to the amount of moles of HCl put initially into solution.

The initial volume in a beaker is equal to the initial volume of HCl solution and the increase of volume during the titration process is equal to the incremental NaOH volume ($V_{NaOH} = 0.001L$, which is the volume added per time unit).

$$\text{Volume}(t) = \text{Volume}(t-dt) + (\text{increase_volume}) * dt$$

$$\text{increase_volume} = V_{NaOH}$$

The initial amount of acid solution HCl is $c_{HCl} * V_{HCl}$ moles and this amount decreases because the acid reacts instantly and completely with the base added to form the salt NaCl:

$$n_{HCl}(t) = n_{HCl}(t-dt) + (-\text{removal_speed_HCL}) * dt$$

$$\text{removal_speed_HCL} = \text{removal_speed_NaOH}$$

The initial amount of NaOH is 0 moles. The total amount of NaOH results from the amount of added NaOH moles minus the amount of reacted moles.

$$n_{NaOH}(t) = n_{NaOH}(t-dt) + (\text{addition_speed_NaOH} - \text{removal_speed_NaOH}) * dt$$

$$\text{addition_speed_NaOH} = c_{NaOH} * V_{NaOH}$$

The amount of reacted NaOH moles is equal to the amount of added NaOH moles as long as there is more HCl present in the solution than NaOH added to the solution. Once the amount of HCl is less than the amount of NaOH added, a basic solution remains and the removal speed of NaOH becomes zero after one further time step in the simulation.

```

If nHCl >= addition_speed_NaOH*dt
Then removal_speed_NaOH = addition_speed_NaOH
Else removal_speed_NaOH = nHCl/dt
EndIf

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The concentration of H_3O^+ ions is calculated with the following mathematical formula:

$$[\text{H}_3\text{O}^+] = (\text{nHCl}/\text{Volume} + \sqrt{(\text{nHCl}/\text{Volume})^2 + 4 \cdot 10^{-(\text{pKw})}})/2$$

The concentration of OH^- ions is calculated as follows:

$$[\text{OH}^-] = (\text{nNaOH}/\text{Volume} + \sqrt{(\text{nNaOH}/\text{Volume})^2 + 4 \cdot 10^{-(\text{pKw})}})/2$$

The pH value is calculated in the following way:

```

If nHCl > 0
Then pH = -Log([H3O+])
Else pH = 14 + log([OH-])
EndIf

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For the theoretical underpinning of the above formulas we refer to *1. Background Theory, 4. Reaction of a strong acid with a strong base.*

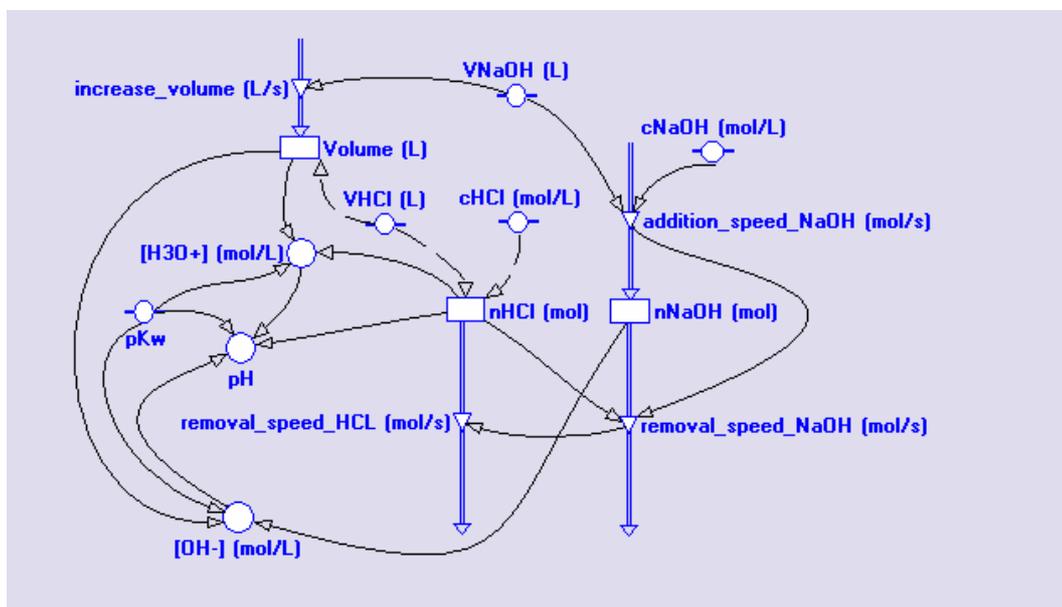


Figure. Computer model of a titration of a strong acid with a strong base

Computer model of a titration of a weak acid with a strong base

The computer model describes the process of adding a NaOH solution (a strong base) to a HAc solution (a weak acid). The reaction of acetic acid (HAc) with water is not complete: a significant concentration of HAc is present along with the A^- and H_3O^+ ions because of incomplete dissociation of acetic acid.

The initial volume in a beaker is equal to the initial volume of HAc solution and the volume increase during the titration process is equal to the incremental NaOH volume ($V_{NaOH} = 0.001L$, which is the volume added per time unit).

$$\text{Volume}(t) = \text{Volume}(t-dt) + (\text{increase_volume}) * dt$$

$$\text{increase_volume} = V_{NaOH}$$

In the computer model, the concentration of H_3O^+ at equilibrium is at every step in the simulation computed from an 'apparent initial concentration' of acid and base, the two substances that react with each other and lead to a new equilibrium. It is assumed that the neutralization reaction generates one Ac^- ion for every OH^- ion added. In other words, the variable n_{Acmin} in the computer model can be used at any moment to determine the apparent initial concentration of the base. This is why this variable can be used in the computation of the concentration of H_3O^+ ions.

The apparent initial amount of acid solution (n_{HAc}) is equal to $c_{HAc} * V_{HAc}$ moles and this amount decreases because of reaction with the base:

$$n_{HAc}(t) = n_{HAc}(t-dt) + (-\text{removal_speed_HAc}) * dt$$

$$\text{removal_speed_HAc} = \text{removal_speed_NaOH}$$

The initial amount of NaOH is 0 moles. The total amount of NaOH results from the amount of added NaOH moles minus the amount of reacted moles.

$$n_{NaOH}(t) = n_{NaOH}(t-dt) + (\text{addition_speed_NaOH} - \text{removal_speed_NaOH}) * dt$$

$$\text{addition_speed_NaOH} = c_{NaOH} * V_{NaOH}$$

The apparent initial amount of Ac^- ions is 0 moles and this amount increases because of neutralization of the acid with the base.

$$n_{Acmin}(t) = n_{Acmin}(t-dt) + (\text{removal_speed_HAc}) * dt \text{ (mol) mol}$$

The amount of reacted NaOH moles is equal to the amount of added NaOH moles as long as there is more HAc present in the solution than NaOH added to the solution. Once the apparent initial amount of HAc is less than the amount of NaOH added, a basic solution remains and the removal speed of NaOH becomes zero after one further time step in the simulation.

$$\text{If } n_{HAc} \geq \text{addition_speed_NaOH} * dt$$

$$\text{Then } \text{removal_speed_NaOH} = \text{addition_speed_NaOH}$$

$$\text{Else } \text{removal_speed_NaOH} = n_{HAc} / dt$$

EndIf

The concentration of H_3O^+ ions is calculated from:

If $n\text{HAc} > 10^{-12}$

$$\text{Then } [\text{H}_3\text{O}^+] = \frac{-\left(\text{Ka} + \frac{n\text{Acmin}}{\text{Volume}}\right) + \sqrt{\left(\text{Ka} + \frac{n\text{Acmin}}{\text{Volume}}\right)^2 + 4 \cdot \text{Ka} \cdot \frac{n\text{HAc}}{\text{Volume}}}}{2}$$

$$\text{Else } [\text{H}_3\text{O}^+] = \frac{2 \cdot \text{Kw}}{-\text{Kb} + \sqrt{\text{Kb}^2 + 4 \cdot \text{Kb} \cdot \frac{n\text{Acmin}}{\text{Volume}}}}$$

EndIf

Concentration of OH^- ions is calculated with the following mathematical formula:

$$[\text{OH}^-] = \frac{\left(\frac{n\text{NaOH}}{\text{Volume}} + \sqrt{\left(\frac{n\text{NaOH}}{\text{Volume}}\right)^2 + 4 \cdot \text{Kw}}\right)}{2} \text{ (mol/L)}$$

The pH is calculated as follows:

If $n\text{NaOH} = 0$

$$\text{Then } \text{pH} = -\text{Log}([\text{H}_3\text{O}^+])$$

$$\text{Else } \text{pH} = 14 + \text{log}([\text{OH}^-])$$

EndIf

For the theoretical underpinning of the above formulas we refer to *1. Background Theory, 5. Reaction of a weak acid with a strong base*.

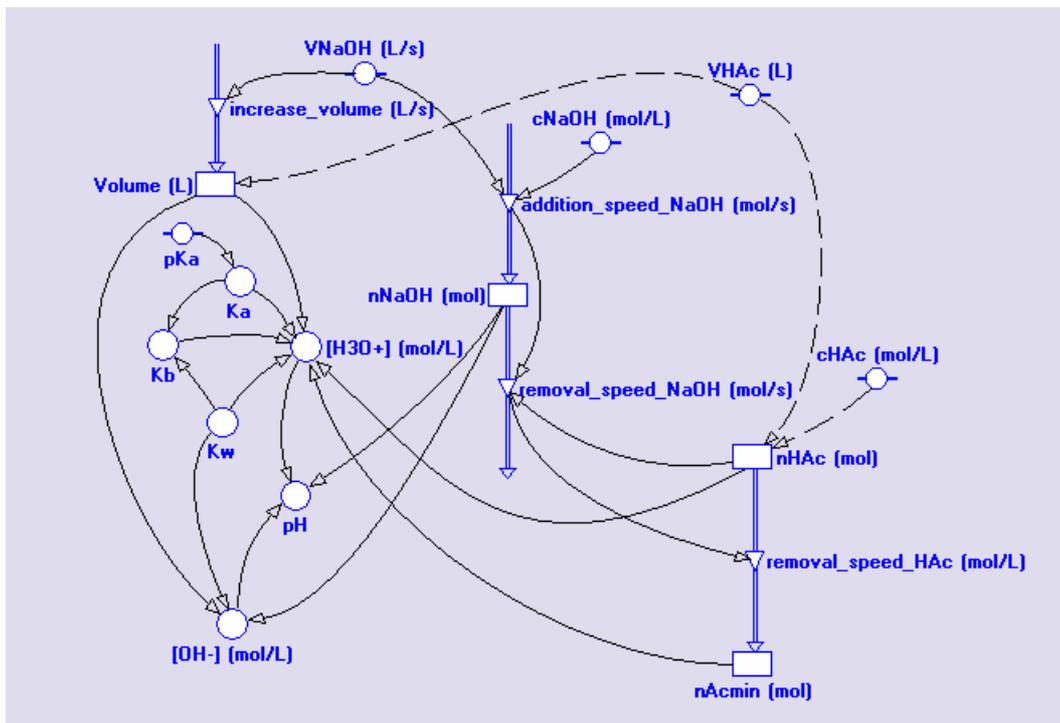


Figure. Computer model of a titration of a weak acid with a strong base

4. Teaching approaches

The three activities presented here offer distinctive but complementary insights into the science involved in this topic. The first activity (1A or 1B) concentrates on the observing titrations, recording pH curves and interpreting the changes of the pH (or H_3O^+ ion concentrations) during the reactions. The second activity applies the titration method, in similar way to chemistry laboratories, to find an unknown concentration of an acidic solution. The Modelling activities offer graphical models describing process of titrations. These models are proposed to be used as simulations.

For the activities to be effective for teaching and learning, it is helpful for teachers to consider two types of skills in using the software tools:

- **Operational skills** which concern the manipulation of the computer hardware and knowledge of the features in the software.
- **Procedural skills** which concern the manner in which the software tools are employed in the lesson context for the purpose of achieving learning benefits. A dominant aspect of these skills is the development of an inquiring approach to the analysis and interpretation of data and to making links with previous knowledge.

Such skills are important for the preparation of pupils for the activities, and the activity sheets below each contain indications of the skills needed for the particular activity.

For the teacher, there are further **pedagogical skills** which contribute to the effectiveness of the activities:

1. Clarity of learning objectives for each activity.
2. Understanding of the special value of the ICT method and exploiting its full potential in purposeful ways.
3. To manage the activity in a way which promotes 'appropriate' rather than 'indiscriminate' use of ICT.
4. To integrate the learning from each activity to develop pupils' understanding of the topic.

The development of the last of these is a particular aim of the IT for US Project, and the activities presented have been specially selected to illustrate how integration might be achieved. Comparisons of the observations and results of each activity form a central role in this integration process. For example:

- Use the results from the titration of a strong acid with a strong base and a model (activity 4) to contribute to a discussion about reactions of a strong acid with a strong base;
- Use the results from the titration of a weak acid with a strong base and a model (activity 4) to contribute to a discussion about reactions of a weak acid with a strong base.

In these, the graph is a key tool in facilitating comparisons and interpretations and skills with graphs generally provide a common thread in exploiting IT for US activities.

The management of the classroom setting also has an important influence on the successful integration of activities. When access to computer equipment is scarce it is likely that the teacher will wish to present the activity as a demonstration in a didactic manner. In this mode, the teacher can give strong guidance to pupils' thinking about the comparisons between the activities.

Alternatively, pupils could perform the activities in small groups of three or four pupils, each group engaged on a different activity.

Integration might be achieved by each group making a presentation of their results to the whole class. In chairing these presentations the teacher can prompt discussion of the significant findings of each group.

It is worth considering that all the activities may be used in a variety of learning contexts.

Although the activities have been designed to provide complementary experiences, it is not essential to use all of them; two or three activities might be chosen according to how well they suit the needs of teachers and pupils in a particular context. In varying conditions between schools and within schools at different times of the year or different stages in the curriculum, needs and appropriateness are likely to change; for example, data-logging equipment might not be available at the time of need, an individual pupil might need a revision or extension activity, an enrichment activity might be required to occupy some spare time, a quick activity might be needed if time is scarce. The overlapping features, such as graphical presentation, between the activities allows them to be used to a certain extent as alternatives, but their distinctive features also allow them to be used as complements to each other. The table below summarises the distinctive potential learning benefits of each. It is a useful guide to the special value of each ICT activity.

Activity	Potential learning benefits, 'ICT value'
Data logging	<p>Graph of pH versus volume is displayed during the experiment.</p> <p>Graph analysis tools facilitate detailed investigation of data.</p> <p>Processing tools allow calculation of H_3O^+ ions concentrations.</p>
Modelling	<p>The models calculate the $[\text{H}_3\text{O}^+]$, $[\text{OH}^-]$ and pH changes.</p> <p>Models are used as simulations.</p> <p>The model data can be compared with the experimental data.</p>

5. Resources for Student Activities

USING COACH 6 SOFTWARE

Activity	Software program	Files available in Coach 6 Project Strong and weak acids
0. Control (optional)	Coach 6	0. Calibration of CMA step-motor burette.cma (activity file)
1. Data-logging	Coach 6	1A. Neutralization of strong and weak acids.cma (activity file) 1B. Neutralization of strong and weak acids with the step-motor burette.cma (activity file)
2. Data-logging	Coach 6	2A. Acid-base titration.cma (activity file) 2B. Acid-base titration with the step-motor burette.cma (activity file)
3. Modelling	Coach 6	3A. Titration curve of a strong acid.cma (activity file) 3B. Titration curve of a weak acid.cma (activity file)

EQUIPMENT AND MATERIALS FOR ACTIVITY 1 AND ACTIVITY 2 (DATA-LOGGING)

- Computer
- Software – See table above
- Interface (CoachLab II/II⁺ interface)
- pH sensor
- 25-mL burette (method A) or CMA step-motor burette (method B)
- several 100-mL beakers, magnetic stirrer or stirring bar, distilled water

FOR ACTIVITY 1

- 0.1 mol/dm³ (M) sodium hydroxide NaOH (strong base)
- 0.1 mol/dm³ (M) hydrochloric acid HCl (strong acid)

- 0.1 mol/dm³ (M) acetic acid HC₂H₃O₂ (called also HAc) (weak acid)

FOR ACTIVITY 2

- hydrochloric acid HCl of an unknown concentration

C. Student Activities ●●

ACTIVITY 0. CALIBRATION OF CMA STEP-MOTOR BURETTE

Learning Objectives:

1. To make a measuring device from a simple mechanical construction connected to a computer
2. To calibrate a step-motor burette

Operational Skills:

- Connecting an interface and step-motor burette
- Calibrating the step-motor burette

Procedural Skills:

- Analysing data using a table
- Reading values
- Calculating the calibration factor
- Evaluating measurement quality

Materials:

- Interface (CoachLab II/II⁺)
- CMA step-motor burette (art. nr 061) including syringe, plastic tube and micro-pipette
- 100-mL beaker and water

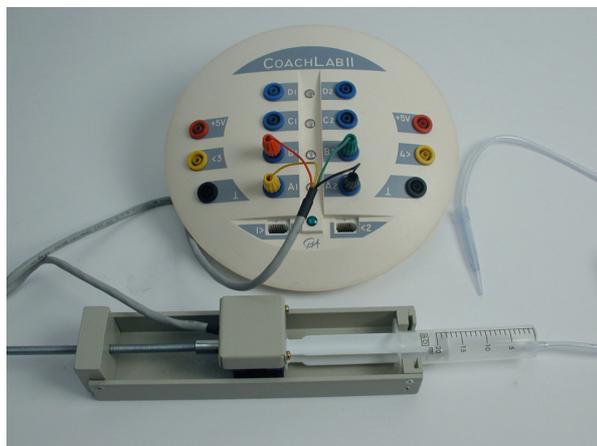
APPLIED ICT TECHNOLOGY:
DATA LOGGING (CONTROL)

STUDENT LEVEL:
AGE 17

RECOMMENDED SETTINGS:
STUDENT ACTIVITY IF
ENOUGH EQUIPMENT IS
AVAILABLE OTHERWISE
TEACHER DEMONSTRATION

Activity method:

1. Connect the step-motor burette to the four lower outputs of CoachLab II/II⁺. The correct connections are given on the bottom side of the burette.
2. Test the connection by starting the motor with the green *Start* button. The burette should move forward and press the syringe. When necessary change the connection order of the wires.
3. Bring the motor in a suitable initial position by manually turning the screw.
4. Fill the syringe with water. Control the presence of a droplet on the pipette. Remove the droplet.
5. Place a syringe filled with water and turn the screw until the syringe is fixed.
6. Weight an empty beaker (100-mL) and place it under the pipette.
7. Start the step-motor burette with the *Start* button. The step motor keeps turning until <Esc>-key is pressed.
8. Stop the burette when 6500 steps are made.
9. Determine the mass of the water in the glass. This determines the water volume (V).
10. Read the exact number of steps (S) from the table.
11. The calibration factor is S/V (in steps/mL). Calculate and write down this value.
12. Repeat this calibration few times and determine an average calibration factor. A typical value for the delivered syringe is $660 [\pm 2]$ steps/mL.



Coach 6 Activity:

0. Calibration of CMA step-motor burette

ACTIVITY 1.

NEUTRALIZATION OF STRONG AND WEAK ACIDS

Learning Objectives:

1. To interpret pH-curves and the processes that influence it
2. To interpret the shapes of titration curves for strong and weak acid
3. To understand the neutralization process

APPLIED ICT TECHNOLOGY:
DATA LOGGING

STUDENT LEVEL:
AGE 17

RECOMMENDED SETTINGS:
STUDENT ACTIVITY IF
ENOUGH EQUIPMENT IS
AVAILABLE OTHERWISE
TEACHER DEMONSTRATION

Operational Skills:

- Connecting an interface and sensors/actuators
- Cleaning and preparation of a titration setup
- Starting and finishing real-time logging
- Defining formulae

Procedural Skills:

- Active observation during the experiment
- Analysing data using a graph
- Evaluating measurement quality
- Processing data

Materials:

- Interface (CoachLab II/II⁺)
- pH sensor
- 25-mL burette (method A) or CMA step-motor burette (art. nr 061) (method B)
- 0.1 mol/dm³ (M) sodium hydroxide NaOH (strong base)
- 0.1 mol/dm³ (M) hydrochloric acid HCl (strong acid)
- 0.1 mol/dm³ (M) acetic acid HC₂H₃O₂ (called also HAc) (weak acid)
- several 100-mL beakers
- magnetic stirrer or stirring bar
- distilled water

Activity method:

A. Activity method - without the step-motor burette

1. Prepare the experiment.
CAUTION: Avoid contact of all chemicals with eyes or skin
 - Rinse the proper parts of the experimental setup with the correct solution.
 - Fill the burette with 0.1 mol/dm^3 sodium hydroxide NaOH solution and clamp the burette above the reaction beaker.
 - Pipette 0.1 mol/dm^3 hydrochloric acid HCl into a beaker.
 - Place the beaker on a magnetic stirrer and add a stirring bar. If no magnetic stirrer is available you can stir with the stirring rod.
 - Connect the pH sensor to input 1 of the CoachLab II/II⁺ interface.
 - Clamp the pH sensor and place its electrode in the beaker so that it is not in the way of the stirring bar. The solution must be well stirred during the titration. During the titration the salt bridge of the pH-sensor must be submerged in the solution.
2. Start the measurement by clicking the green Start button. First start stirring then carefully open the burette stopcock to provide a dripping rate of about 1 drop per second. Be sure to make measurements that will allow you to calculate the added volume for any time during the titration.
3. Repeat the experiment using again 0.1 mol/dm^3 sodium hydroxide NaOH solution as titrant and 0.1 mol/dm^3 acetic acid solution $\text{HC}_2\text{H}_3\text{O}_2$ (weak acid). Remember to wash the reaction beaker and pH electrode with distilled water before repeating the experiment.

B. Activity method - with the step-motor burette

1. Before you start the titration with CMA step-motor burette you need to enter a calibration factor in the control program. The calibration factor is the number of steps the motor has to turn to add 1 mL of titrant. The calibration factor can be determined in the Activity 0. Calibration of CMA step-motor burette.
2. Click the *Program Window* button to open the Program window. In this window an exemplary control program is already prepared.
 - Enter the calibration factor of your step-motor burette in the program.

- Test this program by pressing the green *Start* button.
- If needed erase a program and create a new one by selecting commands from the command list. The following commands are available:

[steps/mL] = calibration factor

Titrate(a;b) where a = number of mL and b = speed (fast, medium, slow, very slow)

MotorBack(a) where a = number of mL

Note:

By a high step speed (speed = fast) the motor deliver less power. Then steps can be skipped. Use this speed only when motor doesn't have to push a syringe. The absolute speed (mL/s) depends on the computer type.

3. Prepare the experiment.

CAUTION: Avoid contact of all chemicals with eyes or skin

- Rinse the proper parts of the experimental setup with the correct solution.
 - Fill the syringe with 0.1 mol/dm³ sodium hydroxide NaOH solution and place it in the burette.
 - Pipette 0.1 mol/dm³ hydrochloric acid HCl into a beaker.
 - Place the beaker on a magnetic stirrer and add a stirring bar. If no magnetic stirrer is available you can steer with the stirring rod.
 - Connect the pH sensor to input 1 of the CoachLab II/II⁺ interface.
 - Connect the step-motor burette to four lower outputs of CoachLab II/II⁺. The connections are given on the bottom side of the burette
 - Clamp the pH sensor and place its electrode in the beaker so that it is not in the way of the stirring bar. The solution must be well stirred during the titration. During the titration the salt bridge of the pH-sensor must be submersed in the solution. Push a syringe so it fills the burette tip.
4. Start the measurement by clicking the green *Start* button. First start stirring then start the addition of 0.1 mol/dm³ NaOH solution.
5. Repeat the procedure using again 0.1 mol/dm³ sodium hydroxide NaOH solution as titrant and 0.1 mol/dm³ acetic acid HC₂H₃O₂ (weak acid). Remember to wash the reaction beaker and pH electrode with distilled water before repeating the experiment.

Questions/Assignments

for titration of HCl (strong acid) with NaOH (strong base):

1. Explain the starting value of the pH of the hydrochloric acid solution
2. Determine how much the pH has increased after addition of 5.0 mL sodium hydroxide solution.
3. At the sharp rising of the pH-curve the acid solution has been neutralized. Describe what it means to neutralize an acid solution.
4. Explain the sharp rising of the pH-curve.
5. Sketch a graph to predict the change of the H_3O^+ concentration during this titration (ignore the change in volume during the titration). Sketch the change of the OH^- concentration in the same graph.
6. Why does the rise of the pH quit suddenly diminish?
7. Sketch a graph to predict the change of the H_3O^+ ion concentration during this titration (ignore the change in volume during the titration). To check your prediction add a $[\text{H}_3\text{O}^+]$ graph to your measuring results. In Coach 6:
 - Click an arrow next to the yellow *Diagram* button and select *Add new*.
 - Name your new diagram *H3O+ during titration*
 - Set as a connection for C1: variable *Volume*. Select the horizontal axis and enter proper unit and range.
 - Set as a connection for C2: *Analog in 1: pH-sensor*. Make this connection invisible.
 - Set as a connection for C3: *Formula*. Type in, or click the *Edit Formula* button to use Formula editor, and create the formula to calculate H_3O^+ .
 - As the Quantity use $[\text{H}_3\text{O}^+]$. Enter proper unit and range.
 - Click *OK* and place the diagram in a pane below the titration curve.
8. Repeat instructions from the point 7 but now for the change of the OH^- ion concentration
9. At the equivalence point just enough base has been added to the acid to offer the solution of a salt. Which ions are mainly present at the equivalence point?
10. Describe a method to make the same neutralized solution starting from a solid salt and water.

11. Do the ions present in the salt influence the pH? Explain why or why not.
12. The titration mixture at the equivalence point has a certain pH. This means that H_3O^+ ions and OH^- ions are present. Explain the presents of these ions by invoking a chemical equilibrium
13. Does the concentration of H_3O^+ ions at the equivalence point offer a serious error in the determination of the acid concentration by means of a titration? Explain your answer.

Questions/Assignments

for titration of HAc (weak acid) with NaOH (strong base):

1. Determine the starting pH of the acetic acid solution.
2. The volume of a drop 0.1 mol/dm^3 NaOH solution is about 0.05 mL. Show by calculation that one drop of this solution is enough to remove all H_3O^+ from 10.0 mL acetic acid solution if no equilibrium should establish itself again.
3. Write down the equation of the equilibrium that maintains the H_3O^+ concentration.
Also give the equilibrium condition for this equilibrium and find a value for K_a .
4. Calculate the fraction acetic acid dissociated at the starting point.
5. During the whole titration the addition of a drop NaOH solution should have a much large pH effect than actually measured
 - Explain what this means for the concentration of the acetate ion..
 - Calculate the concentration of the acetate ion after adding 6.00 mL.
 - Calculate the amount of NaOH solution needed to obtain $\text{pH} = \text{p}K_a$.
6. At the equivalence point enough NaOH solution has been added to neutralize the acid. Again you produce a salt solution. Describe the ions mainly present in the salt solution.
7. Some ion must influence the pH at the equivalence point as $\text{pH} > 7.0$. Give the equilibrium that is responsible for $\text{pH} > 7.0$ at the equivalence point.
8. Second acid/base equilibrium is always present in an aqueous solution. Explain why the influence of this equilibrium can be neglected.
9. The titration could be used to determine the amount of acetic acid.
10. Describe the differences between the graph of titration with the strong acid and titration graph with the weak acid. Explain these differences by

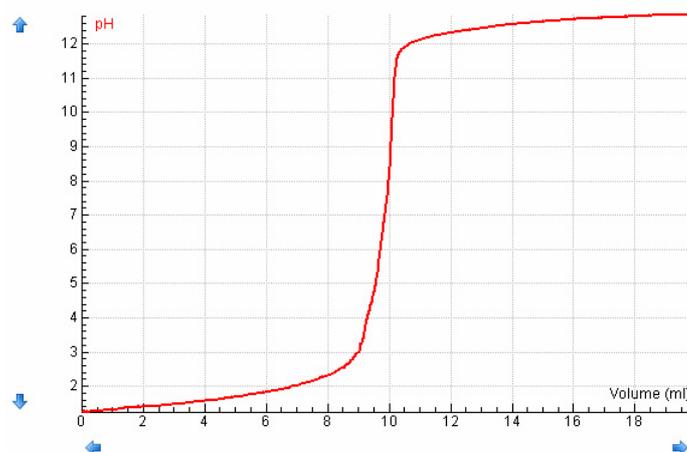
a chemical equilibrium.

11. In the second titration the [HAc] graph decreases almost linear during the titration. Explain why.

Analysing activities:

Students analyse the titration curves and the pH changes during adding the basic solution into the acidic solution. They find the correlation between the H_3O^+ ions concentration and pH.

To determine an equivalence points the steepest and the flattest parts of the graphs they can use the Derivative option.



Exemplary data: neutralization of a strong acid with a strong base.

Coach 6 Activity:

- 1A. Neutralization of strong and weak acids
- 1B. Neutralization of strong and weak acids with the step-motor burette

ACTIVITY 1. ACID-BASE TITRATION

Learning Objectives:

1. To determine a concentration of unknown acidic solution by using the titration method
2. To understand the titration method

Operational Skills:

- Connecting an interface and sensors/actuators
- Cleaning and preparation of a titration setup
- Starting and finishing real-time logging
- Defining formulae

Procedural Skills:

- Active observation during the experiment
- Analysing data using a graph
- Evaluating measurement quality
- Processing data

Materials:

- Interface (CoachLab II/II⁺)
- pH sensor
- 25-mL burette (method A) or CMA step-motor burette (art. nr 061) (method B)
- 0.1 mol/dm³ (M) sodium hydroxide NaOH (strong base)
- hydrochloric acid HCl of an unknown concentration
- several 100-mL beakers
- magnetic stirrer or stirring bar
- distilled water

APPLIED ICT TECHNOLOGY:
DATA LOGGING

STUDENT LEVEL:
AGE 17

RECOMMENDED SETTINGS:
STUDENT ACTIVITY IF
ENOUGH EQUIPMENT IS
AVAILABLE OTHERWISE
TEACHER DEMONSTRATION

Activity method:

1. If you use the CMA step-motor burette before you start the titration you need to enter a calibration factor in the control program. The calibration factor is the number of steps the motor has to turn to add 1 mL of titrant. The calibration factor can be determined in the Activity 0. Calibration of CMA step-motor burette
2. Prepare the experiment.
CAUTION: Avoid contact of all chemicals with eyes or skin
 - Rinse the proper parts of the experimental setup with the correct solution.
 - **Method A:**
Fill the burette with 0.1 mol/dm³ sodium hydroxide NaOH solution and clamp the burette above the reaction beaker.
 - **Method B:**
Fill the syringe with 0.1 mol/dm³ sodium hydroxide NaOH solution and place it in the burette.
 - Pipette the unknown acid into a beaker.
 - Place the beaker on a magnetic stirrer and add a stirring bar. If no magnetic stirrer is available you can stir with the stirring rod.
 - Connect the pH sensor to input 1 of the CoachLab II/II⁺ interface. If you use the step-motor burette connect it to four lower outputs of CoachLab II/II⁺. The connections are given on the bottom side of the burette.
 - Clamp the pH sensor and place its electrode in the beaker so that it is not in the way of the stirring bar. The solution must be well stirred during the titration. During the titration the salt bridge of the pH-sensor must be submerged in the solution.
3. Start the measurement by clicking the green Start button. First start stirring then start the addition NaOH solution.
Provide a dripping rate of about 1 drop per second when you use the burette (method A). Be sure to make measurements that will allow you to calculate the added volume for any time during the titration.

Questions/Assignments:

- Determine the volume of NaOH solution added at the equivalence point.
- Calculate the number of moles of NaOH used.
- Write down the neutralization reaction and determine of moles of acid used.

- Knowing the initial volume of the acid solution in a beaker calculate the acid concentration.

Analysing activities:

Exemplary calculations:

Concentration of NaOH (c_{NaOH}) = 0.1 mol/L

NaOH volume added before the largest pH increase = 10.10 mL

NaOH volume added after the largest pH increase = 10.15 mL

Volume of NaOH added at equivalence point (V_{NaOH}) = 10.125 mL

(This volume can also be found directly from the titration graph for example by using the *Derivative* option.)

Moles NaOH = $c_{\text{NaOH}} * V_{\text{NaOH}} = 0.1 * 0.01125 = 0.0010125$ mol

Moles HCL = 1 mol HCL/1 mol NaOH * 0.0010125 mol

Concentration of HCl (c_{HCl}) = Moles HCL/ $V_{\text{HCl}} = 0.0010125$ mol/0.01 L = 0.10125 mol/L

Coach 6 Activity:

2A. Acid-base titration

2B. Acid-base titration with the step-motor burette

ACTIVITY 3.

TITRATION CURVES OF STRONG AND WEAK ACID

Learning Objectives:

1. Explaining the changes in concentration of several chemical species in solution during titrations
2. Interpreting graphs
3. Evaluating several answers on questions related to Activity 1

APPLIED ICT TECHNOLOGY:
MODELLING

STUDENT LEVEL:
AGE 17

RECOMMENDED SETTINGS:
STUDENT ACTIVITY

Operational Skills:

- Manipulating model variables
- Using the Simulation option
- Changing model parameters

Procedural Skills:

- Analysing data using graphs
- Reading values/slopes
- Evaluating model quality

Activity method:

Ready-made graphical models which calculate the $[H_3O^+]$, $[OH^-]$ and pH changes during the titrations are available in the activities. Students use them as simulations.

Questions/Assignments

for titration of HCl (strong acid) with NaOH (strong base):

- Simulate curves using default starting values. Explain the nHCl and nNaOH curves.
- The nHCl vs time curve is linear before the equivalence point is reached. Explain why? The $[H_3O^+]$ vs volume is not linear before the equivalence point is reached. What is the reason for this?
- Scan the simulated pH curve. Put the cross at pH = 7.0. Describe the equilibrium that causes H_3O^+ ions to be present. Explain why it seems as if no H_3O^+ ions are present according to the $[H_3O^+]$ graph.

- Change the scales of the $[H_3O^+]$ diagram to show that even 0.01 mL before the equivalence point the equilibrium mentioned in question 3 is still not reached. What does this mean for the pH curve?
- Close to the equivalence point, the pH changes rapidly. Explain what is the consequence of this for the performance of a titration.
- Explain the sudden appearance of OH^- ions in the $[OH^-]$ graph.
- Sketch on paper what will appear with the $nHCl$ and $nNaOH$ curves and with the pH curve if you choose a more concentrated NaOH solution, for instance $[OH^-] = 0.2 \text{ mol/L}$. Evaluate your prediction by simulating graphs using a proper starting value.

Questions/Assignments for titration of HAc (weak acid) with NaOH (strong base):

- Simulate curves using default starting values. Discuss the shape of the $[H_3O^+]$ vs volume graph and of the $[OH^-]$ vs volume graph.
- Compare the pH curve with the graph in the case of a titration of a strong acid with a strong base.
- Determine the pH at the point of neutralization of the acetic acid solution.
- Determine the pH at the point where half of the amount of base has been added necessary for neutralization.
- Describe some peculiarities at the point mentioned in the previous question.
- The steepness of the pH curve has the unit pH/mL. It tells you how much the pH changes after adding a little base. Predict the point in the pH curve where the pH change while adding base is the lowest. Determine this point also by using the proper processing tools.
- When half of the amount of base has been added necessary for neutralization, holds $pH = pK_a$. Use the Henderson-Hasselbalch equation to explain this.
- Change the pK_a value into -3 and do a simulation. Compare the pH and $[H_3O^+]$ curves with the ones for the acetic acid titration discussed before.
- Also compare the curves obtained in question 8 with the ones found for the titration of a HCl solution with NaOH.

Analysing activities:

Scaling of diagrams to notice that the water equilibrium is only noticeable very close to the steep pH rising.

Zooming and scanning to find correspondences between several graphs.

Scanning and comparing several graphs shows the student the peculiarities of the buffer point. Using differentiation and zooming shows the slope minimum at the buffer point in the pH graph.

Coach 6 Activity:

3A. Titration curve of a strong acid

3B. Titration curve of a weak acid