Report Writing

The Advanced Higher investigation and report have been removed from the course this year. However, many of the S6 cohort will go on in forthcoming years to study a science or engineering degree that will involve laboratory work at some point. You will be asked to write a report of your work which may form part of an assessment or indeed your dissertation towards the end of the degree. To that end, the intention of this lesson is to outline the basic structure of a scientific report and the main points that should be included.

This lesson is completely informative and will not be assessed. The points covered in this lesson would normally have been taught and discussed during the investigation period. To that end, there is no requirement to copy the lesson. However, if you are interested in taking notes for your own personal interest then I would recommend that you only copy down **pages 1-3**. Pages 4-8 are example extracts taken from the introduction section of the investigations of two students.

The basic sections for a report should include the following sections.

- Title page
- Contents page
- Abstract
- Introduction
- Procedures
- Results
- Discussion (conclusion(s) and evaluation)
- List of references

Abstract

In your 'abstract' you must state the aim(s) and overall finding(s)/conclusion(s) of the investigation. The 'abstract' must be brief and should immediately follow the contents page and be separate from the 'introduction'. Although it appears early in the report, as the 'abstract' it summarises the investigation.

Introduction

This section contains the underlying chemistry in a concise account of the chemical theory underlying the experimental procedures used in your investigation. Diagrams, structural formulae, balanced chemical equations, must be included as appropriate. It is essentially "the chemical story" of your investigation.
Downloading directly from the internet or copying directly from books can be considered as plagiarism. There are software packages that can detect the extent to which a report has been plagiarised so it is always best to write in your own words. It is good to include information from other sources in your report, however this should be cited and referenced properly. There are many ways to use citations within a report and you should always adhere to the instructions and examples given. One of the most common methods is to number the information you are citing using a numbering system with a superscript, for example;

'The reduced form of indigo is soluble and colourless while the oxidised form is insoluble' [1]

This citation would then be listed in order in the **reference section** at the end of the report. There are many ways to reference and again you should always adhere to the instructions given. Citations taken from the internet will be referenced differently from citations taken from books and journals.

Procedures

This section must contain an account of the experimental procedures carried out in your investigation. The procedures must be clearly described and in sufficient detail to allow someone else to repeat the investigation without reference to any other source.

In giving quantitative data, you must quote these values to the correct number of decimal places appropriate to the equipment used. For example, if you use a balance reading to two decimal places, then masses must be quoted to two decimal places, e.g. 5·00 g and not 5 g.

The experimental procedures should describe accurately what was done in each experiment and should be written in the **past tense** using the **passive voice**, for example:
'25·0 cm^3 of 0·105 mol l^{-1} sodium hydroxide solution was pipetted into a conical flask.'
BUT NOT
'Pipette 25·0 cm^3 of 0·105 mol l^{-1} sodium hydroxide solution into a conical flask.'
or
'I pipetted 25·0 cm^3 of 0·105 mol l^{-1} sodium hydroxide solution into a conical flask.'

Results

The results must be relevant to the aim(s) of your investigation. In the results section, you must provide all raw data as well as processed or derived data. Raw data are the readings you actually record in the course of the investigation. For example, in titrations, the raw data are the initial and final burette readings not the titre volumes. Likewise if you are using a weighing boat when measuring out the mass of reactant, you should record all the masses.

Raw and processed data must be presented in a clear and concise manner with appropriate use of tables, graphs, diagrams and calculations.

Tables must have appropriate headings and units must be specified.

Graphs must be supported with tables of raw and/or processed data, i.e. a graph on its own is not sufficient — the data from which it has been derived must also be presented.
Where Excel or other software packages are used to present graphs, it is important that axes are adapted to suit the data in order that the results are presented in the most appropriate way.

Calculations must be clearly structured. You must also take care with significant figures in presenting and processing data. The number of significant figures in the final calculated result depends on the apparatus used and the accuracy of the measurements taken. This is usually the same as the lowest number of significant figures in any measurement used to determine the final result.

Observations, eg indicator colour changes, precipitates forming, gases forming, colours of solutions or precipitates, shapes and colours of crystals formed must be recorded.

Discussion (conclusion(s) and evaluation)

The conclusion(s) must be under a separate heading and must relate back to the aim(s) of the investigation. There must be a conclusion for each aim.
The 'evaluation' can written as one section but you may prefer to split it into two subsections.

Evaluation of the procedures you should address such points as accuracy of measurements:

- the main sources of error and how these were or could have been reduced.
- how close the results of control experiments were to the known values.
- precision of procedures, i.e. how close the results were in duplicate experiments.
- modifications made or could have been made to improve the procedures in your investigation.
- any procedures that were attempted but did not work.

In the **evaluation of the results** you may:

- discuss the differences between the calculated values from control experiments and known quantities used and estimate the uncertainties in your other experimental results based on these differences.
- discuss what effect the uncertainties you identified in the procedures and apparatus had on the final calculated results:
  - discuss how close your calculated results were to accepted values.
  - carry out uncertainty calculations to determine the error or percentage error in calculated results.

Pages 4-8 contain the introduction section of two separate investigations from students. You are not required to copy them. However, if you read them it will give you a general idea of how to set out an introduction and the type of information that can be included. Both introductions are well written. Although they are not perfect and have some minor mistakes, they are overall informative and "set the scene" for the investigation, i.e. that is the purpose of the introduction.

Example 1 – Determination of Iron in Iron tablets

Iron, Fe, is the fourth most abundant element in the Earth's crust and forms two common oxides, FeO and Fe_2O_3[1]. Iron has the atomic number 26 and is in group 8 of the periodic table, it is a transition metal which is an element whose atom has a partially filled d sub-shell. Transition metals are good catalysts and often form coloured compounds due to d-d transitions. Iron is used to manufacture steel, which is used in manufacturing and civil engineering, but it also has a biological role. It is an essential element for all forms of life as it is in haemoglobin which carries oxygen from the lungs to all the cells in the body via the blood. Each human contains an average of 4g of Iron and adults need 8.7-14.8mg of iron each day to prevent the development of anaemia[2].

Redox reactions are reactions where the oxidation states of atoms are changed. Redox reactions include reduction reactions, when an atom gains electrons, and oxidation reactions, when an atom loses electrons. The reduction reactions for iron are shown below:

$Fe^{2+}(aq) + 2e^- \leftrightarrow Fe(s)$
$Fe^{3+}(aq) + 3e^- \leftrightarrow Fe(s)$
$Fe^{3+}(aq) + e^- \leftrightarrow Fe^{2+}(aq)$ [3]

The oxidation equations are from right to left.

Titrations are a quantitative chemical analysis used to determine the concentration of a substance. Fe^{2+} ions in ferrous sulfate, which is present in Iron tablets, can be titrated using potassium permanganate in acidic conditions. The iron ions are oxidised and the permanganate is reduced, during this reaction there is a colour change from purple to colourless when the end point of the titration is reached. Potassium permanganate is self-indicating this due to the purple permanganate ions being converted to manganese ions which are colourless as the iron ions are oxidised. This reaction allows the mass of iron in iron tablets to be calculated by using the formulae n=m/gfm, n=cv and by using mole ratios. The equation for this reaction is:

$$2KMnO_4 + 8H_2SO_4 + 10FeSO_4 \text{-----> } 5Fe_2(SO_4)_3 + 2MnSO_4 + K_2SO_4 + H_2O$$

By combing the oxidation and reduction equations:

$Fe^{2+}(aq) \leftrightarrow Fe^{3+}(aq) + e^-$
$MnO^{4-}(aq) + 8H^+(aq) + 5e^- \leftrightarrow Mn^{2+}(aq) + 4H_2O(l)$ [3]

The REDOX equation can be obtained:

$$5Fe^{2+}(aq) + MnO^{4-}(aq) + 8H^+(aq) \leftrightarrow 5Fe^{3+}(aq) + Mn^{2+}(aq) + 4H_2O(l)$$

For this titration a control experiment can be set up where pure ferrous sulphate is used rather than using iron tablets as a source for the ferrous sulphate. This ensures that the potassium permanganate isn't reacting with any other ingredients in the tablets. The mass of iron calculated to be in the iron tablet can also be compared to what is quoted on the packaging of the tablets.

The mass of iron in ferrous sulfate tablets can also be determined by using the oxidising agent potassium dichromate. For this reaction an indicator is needed as potassium dichromate is not self-indicating. The indicator N.phenylanthranilic acid can be used[4], this produces a colour change of colourless to purple when the reaction has completed. N.phenylanthranilic acid has the chemical formula $C_{13}H_{11}NO_2$, and can also be used in acid base titrations. The equation for the reaction is:

$$6\ FeSO_4 + K_2Cr_2O_7 + 7\ H_2SO_4 \rightarrow 3\ Fe_2(SO_4)_3 + K_2SO_4 + Cr_2(SO_4)_3 + 7\ H_2O$$

By combing the oxidation and reduction equations:

$$Fe^{2+}(aq) \leftrightarrow Fe^{3+}(aq) + e-$$
$$Cr_2O_2^{-7} + 14\ H^+ + 6e^- \rightarrow 2Cr^{3+} + 7H_2O\ ^3$$

The REDOX equation can be obtained:

$$Cr_2O_7^{2-} + 6\ Fe^{2+} + 14H^+ \rightarrow 2Cr^{3+} + 6\ Fe^{3+} + 7H_2O$$

The solutions used to titrate the iron solutions can be standardised. This is a process used to determine the exact concentration of a solution, this allows a more accurate value of the concentration of the solution that is being titrated to be calculated. The solution which is being used in the titration would be titrated against a primary standard. A primary standard is a substance which has a high purity, >99.9%, miscible in water, has a high gram formula mass to reduce errors when weighing and stable in air to prevent molecules being absorbed[5]. Therefore, in this case a more accurate value for the mass of iron in the tablet will be able to be determined. The potassium permanganate can be standardised by using ammonium iron(II) sulfate, the REDOX equation for the reaction is as follows:

$$MnO^{4-} + 8H^+ + 5Fe^{2+} \leftrightarrow Mn^{2+} + 5Fe^{3+} + 4H_2O$$

To prepare a 0.004mol l^{-1} of ammonium iron(II) sulfate, 0.3921g could be added to a 250cm^3 volumetric flask and filled to the graduation mark:

$$n = cv$$
$$= 4 \times 10^{-3} \times 0.25$$
$$= 1 \times 10^{-3}$$

$$m = n \times gfm$$
$$= 1 \times 10^{-3} \times 392.1$$
$$= 0.3921g$$

When preparing the primary standard solution it is good practice to weigh accurately approximately a certain mass of the solute, this allows the exact concentration of the solution to be determined. It is also good practice to add the washings into the conical flask to ensure no mass is lost and finally it is important to invert the conical flask multiple times to create a uniform solution.

Example 2 – Determination of Aspirin by back titration

Aspirin, also known as acetylsalicylic acid, is an aromatic compound which is prepared by the esterification of the phenolic hydroxyl group of salicylic acid. The production of aspirin can be reversed by a hydrolysis reaction. It has the chemical formula $C_9H_8O_4$. Due to the polarity of the molecule aspirin is soluble in water, ethanol, ethyl ether and chloroform. It has a molecular mass of 180g and a melting point of 135°C.[1]

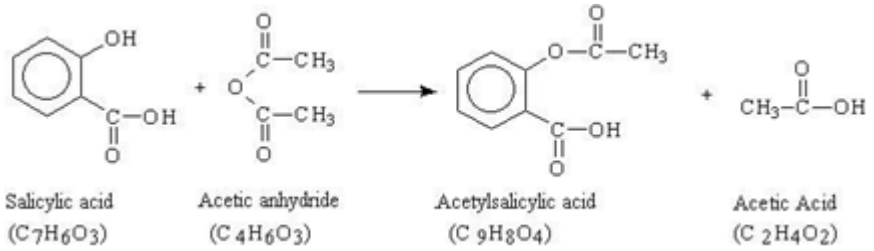
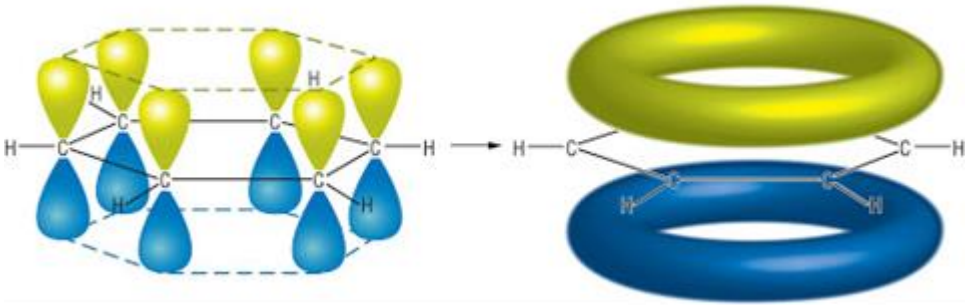


Figure 1: esterification of acetylsalicylic acid.[2]

The molecule of aspirin consists of a benzene ring attached to two functional groups: carboxylic acid and an ester group. The molecular shape of the compound is planar. In the benzene ring each carbon atom is sp^2 hybridised and the three filled sp^2 hybrid orbitals form sigma bonds with a hydrogen atom and the two neighbouring carbon atoms. This leaves an electron occupying a p orbital on each carbon atom. Each of these p orbitals overlap side on with the two p orbitals on either side and a pi molecular orbital forms.

Figure 2: Benzene.[3]



The delocalised electrons allow benzene to undergo substitution reactions rather than addition reactions which would disrupt the stability of the ring. Benzene is readily attacked by electrophiles, due to the high electron density of the delocalised ring system, through reactions such as alkylation, chlorination, nitration and sulfonation, which are all examples of electrophilic substitution.

Aspirin helps deactivate the enzyme which is produced when your body is in pain. This prevents pain messages being sent to your brain. Aspirin is also used in patients with coronary heart disease as it stops platelets from clumping together. This prevents blood clots from blocking the diseased arteries. A regular strength aspirin tablet contains 300-325mg.[4]

A back titration is used to determine the concentration of a substance by reacting it with a known amount of excess reagent. It is often used when substances are not readily soluble in water, one of the reactants are volatile or when a particular reaction is too slow. Two steps are followed in a back titration: the substance is reacted with excess reagent then a titration is conducted on the remaining quantity of the known solution. The chemical equations used to carry out a back titration calculation of aspirin are:

$C_9H_8O_4 + NaOH \longrightarrow C_9H_7O_4Na + H_2O$

$2NaOH + H_2SO_4 \longrightarrow Na_2SO_4 + 2H_2O$

When carrying out a back titration calculation the number of moles of acid is calculated. This is used, as well as the mole ratio, to determine the number of moles of excess alkali. The number of moles of alkali that reacted can then be calculated. Using the mole ratio, the number of moles of aspirin can be determined. The mass of aspirin can then be calculated.

Back Titration involves using a standard solution which is a solution of accurately known concentration. The process of standardisation allows an accurate concentration of the acid or alkali to be obtained. Although laboratory acids and alkalis are labelled with certain concentrations, they may become inaccurate overtime. A primary standard can be used to standardise laboratory acids. A primary standard should be readily available and have the following characteristics:

- High purity > 99.9%
- Stable in air and solution
- Reasonably high formula mass (to reduce errors when weighing)
- Readily soluble

To standardise an alkali the desired mass is dissolved in a small beaker with distilled water. The beaker is then rinsed several times with distilled water and the rinsings are transferred to a standard flask. Distilled water is added to the standard flask and made up to the graduation mark, ensuring the bottom of the meniscus touches the mark. The flask is stoppered and inverted several times to ensure the contents are completely mixed.

$H_2C_2O_4(s) + 2NaOH(aq) \longrightarrow Na_2C_2O_4(aq) + 2H_2O(l)$

The back titration of aspirin is an example of an acid base titration. An acid is any substance capable of donating a proton. A base is any substance capable of accepting a proton. When an acid donates a proton, the species left behind is called the conjugate base. For every acid there is a conjugate base that is formed when the acid loses a proton. When a base accepts a proton, the species that forms is called the conjugate acid. For every base there is a conjugate acid that is formed when the base gains a proton.[5]
Acids can be strong or weak. Strong acids completely dissociate when in solution. Weak acids partially dissociate when in solution. Bases can be strong or weak. Strong bases completely dissociate when in solution. Weak bases partially dissociate when in solution.
To determine the end point of titration the correct indicator must be used. This is determined by the pH of the salt produced which depends on the type of acid and alkali that was neutralised. Indicators (Hln) are usually weak acids in which the colour of the acid is different from its conjugate base. A weak acid with a certain colour can dissociate to form a conjugate base In with another colour.

$$HIn_{(aq)} + H_2O_{(l)} \rightleftharpoons H_3O^+_{(aq)} + In^-_{(aq)}$$

Adding an acid H_3O^+ will shift equilibrium to the left and give colour 1. Adding an alkali OH^- will shift equilibrium to the right and give colour 2.

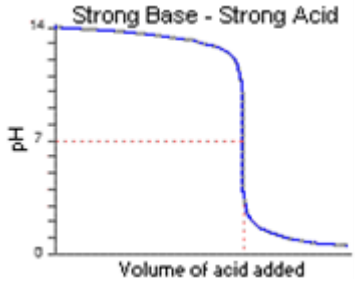
The acid indicator dissociation constant can be represented as:

$$K_{In} = \frac{[H_3O^+][In^-]}{[HIn]}$$

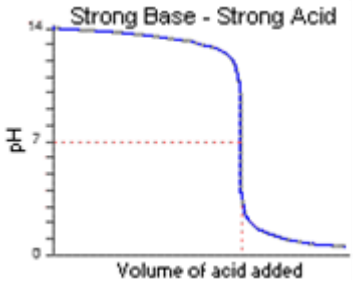
The theoretical point at which the indicator changes colour is when:

$$K_{In} = [H_3O^+]$$

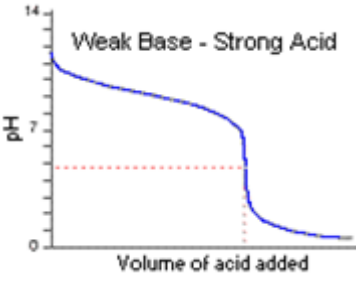
The colour between In^- and HIn is only distinguishable when they differ by a factor of 10. The pH range of an indicator chosen for a titration must coincide with the point at which the pH is changing very rapidly. Despite the term neutralisation, this does not always mean pH=7. The following diagrams are titration curves and can be drawn when a pH electrode is used.



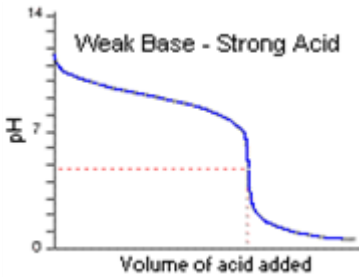
Salt Produced is neutral pH=7



Salt Produced is neutral pH=7



Salt Produced is acidic pH=5.5



Salt Produced is alkaline pH=9.5

In the case of the weak acid and weak base, the vertical point of the graph is almost non-existent and so no indicator is suitable for this reaction.